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A chemist's point of view: the noncylindrical symmetry of electron density means nothing but still means something

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Results of electron density analysis, integration and geometry data for all calculated systems

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B2H6

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\b2h6\b2h6.wfx

Sum File: D:\calc\ellipticity\b2h6\b2h6.sum

SumViz File: D:\calc\ellipticity\b2h6\b2h6.sumviz

Wfx Title: b2h6_mp2

Total memory allocated for AIMSum = 0.568 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	16.0000000074
Number of Alpha electrons (from MO Occs)	=	8.0000000037
Number of Beta electrons (from MO Occs)	=	8.0000000037
Number of electron pairs ($N*(N-1)/2$)	=	120.0000001148
Number of electron pairs (from Muller 2EDM)	=	119.9999948148
Number of electron pairs (from Muller 2EDM, no SOSI)	=	120.1691970426

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
B1	5.0	1.6705464100E+00	4.0174040500E-07	-2.0299600700E-07
B2	5.0	-1.6705471100E+00	3.9951427800E-07	2.0037355000E-07
H3	1.0	2.7524845100E+00	-1.9667145500E+00	2.1551642500E-06
H4	1.0	2.7524732900E+00	1.9667212800E+00	-1.0604733500E-06
H5	1.0	-2.7524819800E+00	-1.9667162700E+00	1.0822361000E-06
H6	1.0	-2.7524709600E+00	1.9667228600E+00	-2.1988634600E-06
H7	1.0	-1.4116116800E-06	-5.1961523300E-06	1.8419878800E+00
H8	1.0	6.3623635500E-08	-1.2132818600E-05	-1.8419878500E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
B1		1.9164618159E+00	-4.8280711155E-04	2.3886694204E+01	-2.3919881477E+01
B2		1.9164592297E+00	-4.8413797409E-04	2.3886694846E+01	-2.3919882120E+01
H3	-6.2839759670E-01	2.3069356408E-05	8.4216551866E-01	-8.4333559171E-01	3.0176330090E-01
H4	-6.2839521550E-01	2.5386162685E-05	8.4216618036E-01	-8.4333625433E-01	3.0176003037E-01
H5	-6.2839821980E-01	2.3353758530E-05	8.4216619526E-01	-8.4333626925E-01	3.0176479034E-01

H6 -6.2839634980E-01 2.4494078223E-05 8.4216615341E-01 -8.4333622734E-01 3.0176231922E-01

H7 -6.6024119220E-01 1.0406780961E-04 9.2077133287E-01 -9.2205061788E-01 4.2327430029E-01

H8 -6.6024122870E-01 1.0405515231E-04 9.2077135926E-01 -9.2205064430E-01 4.2327430091E-01

Total -1.1487571000E-03 -6.6251876787E-04 5.2983595790E+01 -5.3057209202E+01

Molecular charge q(Mol) from the wfx file: -7.4051063779E-09

Molecular energy E(Mol) from the wfx file: -5.3057048930E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0013893623E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0013893735E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR
B1	34	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00 13.00
B2	38	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00 13.00
H3	14	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H4	12	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00

H5	12	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H6	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H7	39	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H8	26	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00

Total 190

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 1.67053737102453E+00 4.01701230513439E-07 -2.02989829792090E-07

Type = (3,-3) NACP B1

Rho = 6.7092541661E+01 Rho at Nucleus = 6.7092538925E+01

GradRho = -2.4549806632E-12 -1.0310508550E-17 -4.3187033607E-18

HessRho_EigVals = -6.6981589109E+04 -6.6980676633E+04 -6.6979831685E+04

HessRho_EigVec1 = -1.5518255540E-06 9.2080166135E-07 1.0000000000E+00

HessRho_EigVec2 = 9.9999999999E-01 3.0412854076E-06 1.5518227535E-06

HessRho_EigVec3 = -3.0412839786E-06 9.9999999999E-01 -9.2080638089E-07

DelSqRho = -2.0094209743E+05

Bond Ellipticity = NA

V = -5.0238793645E+04

G = 1.6346441326E+00

K = 5.0237159001E+04

L = 5.0235524357E+04

Vnuc = 5.5316364161E+05

Ven = -3.7113154670E+07

Vrep = 3.7062915876E+07

DelSqV = 1.0705744529E+09

DelSqVen = 1.1115386176E+11

DelSqVrep = -1.1008328731E+11

DelSqG = 5.0155651658E+07

DelSqK = -1.1207301045E+09

Stress_EigVals = -1.6746522428E+04 -1.6746268631E+04 -1.6746002586E+04

Stress_EigVec1 = -2.9176484188E-06 1.0000000000E+00 -8.2201778210E-07

Stress_EigVec2 = 9.9999999999E-01 2.9176497727E-06 1.6470125637E-06

Stress_EigVec3 = -1.6470149621E-06 8.2201297670E-07 1.0000000000E+00

-DivStress = 3.1449705427E+03 1.3632232065E-02 -2.1548977547E-03

CP# 2 Coords = -1.67053807102673E+00 3.99477267070613E-07 2.00368490390096E-07

Type = (3,-3) NACP B2

Rho = 6.7092542733E+01 Rho at Nucleus = 6.7092539997E+01

GradRho = 5.6877835775E-12 -8.5245395812E-18 -6.0745331772E-18

HessRho_EigVals = -6.6981590420E+04 -6.6980677947E+04 -6.6979832998E+04

HessRho_EigVec1 = -1.4382771653E-06 9.3200450470E-07 1.0000000000E+00

HessRho_EigVec2 = 9.9999999999E-01 -3.1882088320E-06 1.4382801367E-06

HessRho_EigVec3 = 3.1882101725E-06 9.9999999999E-01 -9.3199991916E-07

DelSqRho = -2.0094210136E+05

Bond Ellipticity = NA

V = -5.0238794629E+04

G = 1.6346441011E+00

K = 5.0237159985E+04

L = 5.0235525341E+04

Vnuc = 5.5316377574E+05

Ven = -3.7113164262E+07

Vrep = 3.7062925468E+07

DelSqV = 1.0705744740E+09

DelSqVen = 1.1115389190E+11

DelSqVrep = -1.1008331743E+11

DelSqG = 5.0155652823E+07

DelSqK = -1.1207301268E+09

Stress_EigVals = -1.6746522757E+04 -1.6746268958E+04 -1.6746002914E+04

Stress_EigVec1 = 2.9678048675E-06 1.0000000000E+00 -8.3533545872E-07
Stress_EigVec2 = 9.999999999E-01 -2.9678035419E-06 1.5869429877E-06
Stress_EigVec3 = -1.5869405086E-06 8.3534016845E-07 1.0000000000E+00
-DivStress = -3.1449698488E+03 1.2874377886E-02 1.7606573557E-03

CP# 3 Coords = 2.74215019914726E+00 -1.94847675779717E+00 2.13370042862810E-06

Type = (3,-3) NACP H3

Rho = 4.1326003909E-01 Rho at Nucleus = 4.1149289918E-01

GradRho = -1.9519975913E-15 2.0484915847E-15 -4.7058305048E-20

HessRho_EigVals = -8.2780708899E+00 -8.2766227763E+00 -7.9146359553E+00

HessRho_EigVec1 = 8.6946969636E-01 4.9398628231E-01 9.6761794044E-08

HessRho_EigVec2 = -5.8392147659E-07 8.3188592400E-07 1.0000000000E+00

HessRho_EigVec3 = -4.9398628231E-01 8.6946969636E-01 -1.0117488011E-06

DelSqRho = -2.4469329622E+01

Bond Ellipticity = NA

V = -6.1266840480E+00

G = 4.6758213286E-03

K = 6.1220082267E+00

L = 6.1173324054E+00

Vnuc = 5.2096993139E+01

Ven = -2.1529605421E+01

Vrep = 1.5402921373E+01

DelSqV = 1.5988693823E+03

DelSqVen = 1.2747784974E+03

DelSqVrep = 3.2409088484E+02

DelSqG = 1.2166117225E+02

DelSqK = -1.7205305545E+03

Stress_EigVals = -2.0728748256E+00 -2.0718725274E+00 -1.9819366950E+00

Stress_EigVec1 = 8.6926882638E-01 4.9433966812E-01 9.6191439746E-07

Stress_EigVec2 = -1.3315286582E-06 3.9556193671E-07 1.0000000000E+00

Stress_EigVec3 = -4.9433966812E-01 8.6926882638E-01 -1.0020770955E-06

-DivStress = 5.2988853891E+00 -9.3462967570E+00 1.0986891946E-05

CP# 4 Coords = 2.74213908048928E+00 1.94848342088625E+00 -1.05396497630470E-06

Type = (3,-3) NACP H4

Rho = 4.1326012141E-01 Rho at Nucleus = 4.1149297979E-01

GradRho = -2.7955068815E-15 -1.8984380040E-15 -2.8574726786E-19

HessRho_EigVals = -8.2780725126E+00 -8.2766243974E+00 -7.9146373212E+00

HessRho_EigVec1 = 8.6947252407E-01 -4.9398130520E-01 -1.2057632233E-06

HessRho_EigVec2 = 1.2011826932E-06 -3.2666798013E-07 1.0000000000E+00

HessRho_EigVec3 = 4.9398130520E-01 8.6947252407E-01 -3.0933296134E-07

DelSqRho = -2.4469334231E+01

Bond Ellipticity = NA

V = -6.1266851990E+00

G = 4.6758205830E-03

K = 6.1220093784E+00

L = 6.1173335578E+00

Vnuc = 5.2096976417E+01

Ven = -2.1529602799E+01

Vrep = 1.5402917600E+01

DelSqV = 1.5988696635E+03

DelSqVen = 1.2747783284E+03

DelSqVrep = 3.2409133514E+02

DelSqG = 1.2166119368E+02

DelSqK = -1.7205308572E+03

Stress_EigVals = -2.0728752321E+00 -2.0718729301E+00 -1.9819370368E+00

Stress_EigVec1 = 8.6927165866E-01 -4.9433468769E-01 3.3686515803E-07

Stress_EigVec2 = -1.4395123358E-07 4.2831797104E-07 1.0000000000E+00

Stress_EigVec3 = 4.9433468769E-01 8.6927165866E-01 -3.0116458503E-07

-DivStress = 5.2988344240E+00 9.3463327613E+00 -3.3264288380E-06

CP# 5 Coords = -2.74214770534111E+00 -1.94847845393843E+00 1.07513341136102E-06

Type = (3,-3) NACP H5

Rho = 4.1325999811E-01 Rho at Nucleus = 4.1149285796E-01

GradRho = 6.6288120826E-16 2.8952534814E-15 6.9862847356E-20
HessRho_EigVals = -8.2780697876E+00 -8.2766216636E+00 -7.9146348023E+00
HessRho_EigVec1 = 8.6947071286E-01 -4.9398449316E-01 -1.1947591900E-06
HessRho_EigVec2 = 1.2007998802E-06 -3.0506800173E-07 1.0000000000E+00
HessRho_EigVec3 = 4.9398449316E-01 8.6947071286E-01 -3.2792882726E-07
DelSqRho = -2.4469326253E+01
Bond Ellipticity = NA
V = -6.1266832065E+00
G = 4.6758215876E-03
K = 6.1220073849E+00
L = 6.1173315634E+00
Vnuc = 5.2096987086E+01
Ven = -2.1529600785E+01
Vrep = 1.5402917578E+01
DelSqV = 1.5988691524E+03
DelSqVen = 1.2747781738E+03
DelSqVrep = 3.2409097859E+02
DelSqG = 1.2166115102E+02
DelSqK = -1.7205303034E+03
Stress_EigVals = -2.0728745479E+00 -2.0718722523E+00 -1.9819364064E+00
Stress_EigVec1 = 8.6926986898E-01 -4.9433783476E-01 2.5080675489E-07
Stress_EigVec2 = -6.0302518621E-08 4.0131986363E-07 1.0000000000E+00
Stress_EigVec3 = 4.9433783476E-01 8.6926986898E-01 -3.1904544879E-07
-DivStress = -5.2988660768E+00 -9.3463077301E+00 3.6216402905E-06

CP# 6 Coords = -2.74213678468293E+00 1.94848497961615E+00 -2.17730895952057E-06

Type = (3,-3) NACP H6

Rho = 4.1326010435E-01 Rho at Nucleus = 4.1149296260E-01

GradRho = 4.0462425077E-16 -3.0730626377E-15 -1.3138337144E-19

HessRho_EigVals = -8.2780718281E+00 -8.2766237042E+00 -7.9146366190E+00

HessRho_EigVec1 = 8.6947348601E-01 4.9397961206E-01 4.7962855463E-08

HessRho_EigVec2 = -5.4854109931E-07 8.6841455781E-07 1.0000000000E+00

HessRho_EigVec3 = -4.9397961206E-01 8.6947348601E-01 -1.0260315523E-06

DelSqRho = -2.4469332151E+01

Bond Ellipticity = NA

V = -6.1266846786E+00

G = 4.6758203725E-03

K = 6.1220088582E+00

L = 6.1173330378E+00

Vnuc = 5.2096973226E+01

Ven = -2.1529600591E+01

Vrep = 1.5402915913E+01

DelSqV = 1.5988695174E+03

DelSqVen = 1.2747781419E+03

DelSqVrep = 3.2409137546E+02

DelSqG = 1.2166117827E+02

DelSqK = -1.7205306957E+03

Stress_EigVals = -2.0728750586E+00 -2.0718727598E+00 -1.9819368601E+00

Stress_EigVec1 = 8.6927264621E-01 4.9433295110E-01 8.3000285023E-07

Stress_EigVec2 = -1.2244839449E-06 4.7418960894E-07 1.0000000000E+00

Stress_EigVec3 = -4.9433295110E-01 8.6927264621E-01 -1.0175028182E-06

-DivStress = -5.2988163767E+00 9.3463428865E+00 -1.1043229166E-05

CP# 7 Coords = -1.42156244192261E-06 -5.13024531091976E-06 1.82255904599282E+00

Type = (3,-3) NACP H7

Rho = 4.0547652787E-01 Rho at Nucleus = 4.0397009826E-01

GradRho = -1.7445358233E-17 9.0423414097E-19 -2.8449465006E-16

HessRho_EigVals = -8.1453861049E+00 -8.0517374835E+00 -7.8739516003E+00

HessRho_EigVec1 = -1.0573561554E-08 9.9999999999E-01 3.3817795842E-06

HessRho_EigVec2 = 1.0000000000E+00 1.0577108226E-08 -1.0487591225E-06

HessRho_EigVec3 = 1.0487591583E-06 -3.3817795731E-06 9.9999999999E-01

DelSqRho = -2.4071075189E+01

Bond Ellipticity = NA

V = -6.0350135039E+00

G = 8.6223533815E-03
K = 6.0263911505E+00
L = 6.0177687972E+00
Vnuc = 5.6828487025E+01
Ven = -2.3042617603E+01
Vrep = 1.7007604100E+01
DelSqV = 1.5774899817E+03
DelSqVen = 1.3679227840E+03
DelSqVrep = 2.0956719765E+02
DelSqG = 1.2013126021E+02
DelSqK = -1.6976212419E+03
Stress_EigVals = -2.0421736663E+00 -2.0185101698E+00 -1.9743296678E+00
Stress_EigVec1 = -2.1407394494E-08 9.9999999999E-01 3.2911711874E-06
Stress_EigVec2 = 1.0000000000E+00 2.1411121655E-08 -1.1324725490E-06
Stress_EigVec3 = 1.1324726195E-06 -3.2911711632E-06 9.9999999999E-01
-DivStress = 5.0377883351E-06 -3.3191907547E-05 9.7893533712E+00

CP# 8 Coords = 7.56971221966699E-08 -1.19808121064190E-05 -1.82255901448462E+00

Type = (3,-3) NACP H8

Rho = 4.0547654389E-01 Rho at Nucleus = 4.0397011396E-01

GradRho = -8.6602501412E-19 1.5000424100E-19 1.4779844015E-15

HessRho_EigVals = -8.1453864843E+00 -8.0517378564E+00 -7.8739519526E+00

HessRho_EigVec1 = -1.3655073665E-08 9.999999997E-01 -7.7187979778E-06

HessRho_EigVec2 = 1.0000000000E+00 1.3647854802E-08 -9.3523163392E-07

HessRho_EigVec3 = 9.3523152855E-07 7.7187979906E-06 9.999999997E-01

DelSqRho = -2.4071076293E+01

Bond Ellipticity = NA

V = -6.0350137801E+00

G = 8.6223533789E-03

K = 6.0263914267E+00

L = 6.0177690733E+00

Vnuc = 5.6828483075E+01

Ven = -2.3042616912E+01
Vrep = 1.7007603132E+01
DelSqV = 1.5774900514E+03
DelSqVen = 1.3679227517E+03
DelSqVrep = 2.0956729962E+02
DelSqG = 1.2013126648E+02
DelSqK = -1.6976213178E+03
Stress_EigVals = -2.0421737613E+00 -2.0185102633E+00 -1.9743297554E+00
Stress_EigVec1 = -2.8277860036E-08 9.9999999997E-01 -7.6833616472E-06
Stress_EigVec2 = 1.0000000000E+00 2.8270877937E-08 -9.0872982656E-07
Stress_EigVec3 = 9.0872960932E-07 7.6833616729E-06 9.9999999997E-01
-DivStress = -6.0805813529E-06 -7.6605543449E-05 -9.7893545588E+00

CP# 9 Coords = -6.85269113388475E-07 -2.35479769657017E-06 1.33307373179729E-08

Type = (3,+1) RCP B1 H7 B2 H8
Rho = 1.1446852411E-01
GradRho = 1.6110354899E-17 6.2517251906E-18 1.3460716726E-17
HessRho_EigVals = -1.6366177752E-01 1.7357459137E-02 9.6050050324E-02
HessRho_EigVec1 = -3.7640975039E-08 1.0000000000E+00 -1.6811414370E-06
HessRho_EigVec2 = 1.0000000000E+00 3.7645295379E-08 2.5698853647E-06
HessRho_EigVec3 = -2.5698854280E-06 1.6811413403E-06 1.0000000000E+00
DelSqRho = -5.0254268054E-02
Bond Ellipticity = NA
V = -1.1475022888E-01
G = 5.1093330931E-02
K = 6.3656897945E-02
L = 1.2563567014E-02
Vnuc = 8.2542596912E+00
Ven = -9.4485292445E-01
Vrep = 8.3010269558E-01
DelSqV = -1.9952650330E-01
DelSqVen = 4.1481177911E-01

DelSqVrep = -6.1433828242E-01

DelSqG = 8.2749386120E-02

DelSqK = 1.1677711718E-01

Stress_EigVals = -6.1076154259E-02 -5.1334647799E-02 -2.3394268171E-03

Stress_EigVec1 = -7.4943128834E-09 1.0000000000E+00 -2.5186219863E-06

Stress_EigVec2 = 4.0459890361E-07 2.5186219893E-06 1.0000000000E+00

Stress_EigVec3 = 1.0000000000E+00 7.4932938517E-09 -4.0459892248E-07

-DivStress = -1.2057419236E-07 1.6339714846E-07 -3.6339289741E-09

CP# 10 Coords = 2.12526780576302E+00 -8.65909906056977E-01 8.52650286286726E-07

Type = (3,-1) BCP B1 H3

Rho = 1.8011385020E-01

GradRho = 2.1684043450E-18 1.4484941024E-16 -1.7742693267E-18

HessRho_EigVals = -3.8736739867E-01 -3.5033560495E-01 4.9837515531E-01

HessRho_EigVec1 = -1.6823387085E-06 2.6327099952E-07 1.0000000000E+00

HessRho_EigVec2 = 8.7067231954E-01 4.9186350950E-01 1.3352723478E-06

HessRho_EigVec3 = -4.9186350950E-01 8.7067231954E-01 -1.0567037932E-06

DelSqRho = -2.3932784831E-01

Bond Ellipticity = 1.0570376859E-01

V = -3.2812265102E-01

G = 1.3414534447E-01

K = 1.9397730655E-01

L = 5.9831962077E-02

Vnuc = 8.5873801806E+00

Ven = -1.5467061074E+00

Vrep = 1.2185834564E+00

DelSqV = -3.7019143402E+00

DelSqVen = 2.0551992212E+00

DelSqVrep = -5.7571135614E+00

DelSqG = 5.9305178416E+00

DelSqK = -2.2286035014E+00

Stress_EigVals = -1.3856811141E-01 -1.2590573205E-01 -6.3648807562E-02

Stress_EigVec1 = 8.8936272079E-01 4.5720230847E-01 1.0015899665E-06

Stress_EigVec2 = -1.3451239533E-06 4.2587959143E-07 1.0000000000E+00

Stress_EigVec3 = -4.5720230847E-01 8.8936272079E-01 -9.9375520878E-07

-DivStress = -2.3048405745E-01 4.3478486081E-01 -5.3095203032E-07

BPL = 2.2241339761E+00 = 9.7813915836E-01 + 1.2459948178E+00

GBL_I = 2.2237169997E+00

GBL_II = 2.2446731953E+00

GBL_III = 2.2240408212E+00 = 9.7804929802E-01 + 1.2459915232E+00

GBL_IV = 2.2449987878E+00 = 9.7804509554E-01 + 1.2669536922E+00

CP# 11 Coords = 2.12526282252461E+00 8.65913191888061E-01 -6.41301214751113E-07

Type = (3,-1) BCP H4 B1

Rho = 1.8011391534E-01

GradRho = -1.3574211200E-16 -1.1275702594E-16 2.0829946380E-18

HessRho_EigVals = -3.8736768001E-01 -3.5033576495E-01 4.9837557833E-01

HessRho_EigVec1 = -1.1114874905E-06 1.0864768926E-06 1.0000000000E+00

HessRho_EigVec2 = 8.7067507796E-01 -4.9185862665E-01 1.5021374897E-06

HessRho_EigVec3 = 4.9185862665E-01 8.7067507796E-01 -3.9927364254E-07

DelSqRho = -2.3932786663E-01

Bond Ellipticity = 1.0570406670E-01

V = -3.2812284630E-01

G = 1.3414543982E-01

K = 1.9397740648E-01

L = 5.9831966658E-02

Vnuc = 8.5873821793E+00

Ven = -1.5467070268E+00

Vrep = 1.2185841805E+00

DelSqV = -3.7019169623E+00

DelSqVen = 2.0551998569E+00

DelSqVrep = -5.7571168193E+00

DelSqG = 5.9305231884E+00

DelSqK = -2.2286062261E+00

Stress_EigVals = -1.3856816717E-01 -1.2590577669E-01 -6.3648902439E-02
Stress_EigVec1 = 8.8936518781E-01 -4.5719750952E-01 1.2972950212E-06
Stress_EigVec2 = -1.0685971435E-06 7.5880098824E-07 1.0000000000E+00
Stress_EigVec3 = 4.5719750952E-01 8.8936518781E-01 -1.8629123075E-07
-DivStress = -2.3048175359E-01 -4.3478649649E-01 2.2042480388E-07
BPL = 2.2241337542E+00 = 1.2459947146E+00 + 9.7813903961E-01
GBL_I = 2.2237167760E+00
GBL_II = 2.2446729799E+00
GBL_III = 2.2240405989E+00 = 1.2459914199E+00 + 9.7804917895E-01
GBL_IV = 2.2449985736E+00 = 1.2669535972E+00 + 9.7804497645E-01

CP# 12 Coords = -2.12526741213998E+00 -8.65910505263003E-01 6.44880323263458E-07

Type = (3,-1) BCP B2 H5
Rho = 1.8011386566E-01
GradRho = 6.3100566439E-17 9.1072982489E-17 -5.3042129599E-20
HessRho_EigVals = -3.8736731357E-01 -3.5033573208E-01 4.9837505954E-01
HessRho_EigVec1 = -1.0835274077E-06 1.0828031260E-06 1.0000000000E+00
HessRho_EigVec2 = 8.7067305331E-01 -4.9186221062E-01 1.4759880557E-06
HessRho_EigVec3 = 4.9186221062E-01 8.7067305331E-01 -4.0982131786E-07
DelSqRho = -2.3932798612E-01
Bond Ellipticity = 1.0570312445E-01
V = -3.2812266701E-01
G = 1.3414533524E-01
K = 1.9397733177E-01
L = 5.9831996529E-02
Vnuc = 8.5873803821E+00
Ven = -1.5467062766E+00
Vrep = 1.2185836096E+00
DelSqV = -3.7019135114E+00
DelSqVen = 2.0552004529E+00
DelSqVrep = -5.7571139643E+00
DelSqG = 5.9305167388E+00

DelSqK = -2.2286032273E+00

Stress_EigVals = -1.3856809186E-01 -1.2590575691E-01 -6.3648818243E-02

Stress_EigVec1 = 8.8936382661E-01 -4.5720015740E-01 1.2795368830E-06

Stress_EigVec2 = -1.0380255307E-06 7.7942782646E-07 1.0000000000E+00

Stress_EigVec3 = 4.5720015740E-01 8.8936382661E-01 -2.1860947829E-07

-DivStress = 2.3048350187E-01 4.3478513227E-01 -2.2588804301E-07

BPL = 2.2241339089E+00 = 9.7813917760E-01 + 1.2459947313E+00

GBL_I = 2.2237169448E+00

GBL_II = 2.2446731435E+00

GBL_III = 2.2240407546E+00 = 9.7804931809E-01 + 1.2459914365E+00

GBL_IV = 2.2449987240E+00 = 9.7804511562E-01 + 1.2669536084E+00

CP# 13 Coords = -2.12526250307978E+00 8.65913684650633E-01 -8.74157282038063E-07

Type = (3,-1) BCP H6 B2

Rho = 1.8011391528E-01

GradRho = 5.3993268190E-17 -6.3317406873E-17 -7.6903643294E-19

HessRho_EigVals = -3.8736759867E-01 -3.5033587373E-01 4.9837579272E-01

HessRho_EigVec1 = -1.6484678041E-06 3.0259329097E-07 1.0000000000E+00

HessRho_EigVec2 = 8.7067576013E-01 4.9185741910E-01 1.2864482032E-06

HessRho_EigVec3 = -4.9185741910E-01 8.7067576013E-01 -1.0742717632E-06

DelSqRho = -2.3932767968E-01

Bond Ellipticity = 1.0570349116E-01

V = -3.2812289211E-01

G = 1.3414548609E-01

K = 1.9397740601E-01

L = 5.9831919920E-02

Vnuc = 8.5873826333E+00

Ven = -1.5467071081E+00

Vrep = 1.2185842160E+00

DelSqV = -3.7019176369E+00

DelSqVen = 2.0551983601E+00

DelSqVrep = -5.7571159970E+00

DelSqG = 5.9305244437E+00

DelSqK = -2.2286068069E+00

Stress_EigVals = -1.3856815597E-01 -1.2590580593E-01 -6.3648930211E-02

Stress_EigVec1 = 8.8936626675E-01 4.5719541071E-01 9.6006181094E-07

Stress_EigVec2 = -1.3115928655E-06 4.5150199342E-07 1.0000000000E+00

Stress_EigVec3 = -4.5719541070E-01 8.8936626675E-01 -1.0012048811E-06

-DivStress = 2.3048127610E-01 -4.3478679479E-01 5.3801883584E-07

BPL = 2.2241336655E+00 = 1.2459946625E+00 + 9.7813900300E-01

GBL_I = 2.2237167001E+00

GBL_II = 2.2446729057E+00

GBL_III = 2.2240405108E+00 = 1.2459913676E+00 + 9.7804914322E-01

GBL_IV = 2.2449984872E+00 = 1.2669535465E+00 + 9.7804494073E-01

CP# 14 Coords = 7.78748943720090E-01 -1.26887264059666E-06 4.89119687914463E-01

Type = (3,-1) BCP B1 H7

Rho = 1.2048179361E-01

GradRho = -4.8336334935E-14 3.8916895674E-18 4.3243186809E-14

HessRho_EigVals = -1.5352026509E-01 -8.7931719660E-02 3.8837122824E-01

HessRho_EigVec1 = -6.6395068542E-07 1.0000000000E+00 2.0568786023E-06

HessRho_EigVec2 = 6.1275615445E-01 -1.2186537777E-06 7.9027203872E-01

HessRho_EigVec3 = 7.9027203872E-01 1.7850666843E-06 -6.1275615444E-01

DelSqRho = 1.4691924348E-01

Bond Ellipticity = 7.4590313583E-01

V = -2.3249555436E-01

G = 1.3461268261E-01

K = 9.7882871744E-02

L = -3.6729810871E-02

Vnuc = 9.1633988841E+00

Ven = -1.1040227331E+00

Vrep = 8.7152717877E-01

DelSqV = -2.9319093816E+00

DelSqVen = -1.3462796318E+00

DelSqVrep = -1.5856297498E+00

DelSqG = 4.2202432135E+00

DelSqK = -1.2883338319E+00

Stress_EigVals = -1.0422459706E-01 -8.6432326183E-02 -4.1838631121E-02

Stress_EigVec1 = -2.0787360856E-06 1.0000000000E+00 5.4049626779E-07

Stress_EigVec2 = 5.4425404979E-01 6.7792715829E-07 8.3892045468E-01

Stress_EigVec3 = 8.3892045468E-01 2.0380615047E-06 -5.4425404979E-01

-DivStress = 2.6625741009E-01 4.9479763349E-07 -1.4513080327E-01

BPL = 2.5878343709E+00 = 1.0183891955E+00 + 1.5694451754E+00

GBL_I = 2.4723313034E+00

GBL_II = 2.4866946178E+00

GBL_III = 2.5613026841E+00 = 1.0171159554E+00 + 1.5441867287E+00

GBL_IV = 2.5781185831E+00 = 1.0171238806E+00 + 1.5609947025E+00

CP# 15 Coords = -7.78751905063715E-01 -1.33535941875764E-06 4.89122463070197E-01

Type = (3,-1) BCP H7 B2

Rho = 1.2048193575E-01

GradRho = 4.8350212722E-14 4.9056773408E-19 4.3270942385E-14

HessRho_EigVals = -1.5352061719E-01 -8.7932933640E-02 3.8837445890E-01

HessRho_EigVec1 = 6.0441886574E-07 1.0000000000E+00 2.1108594902E-06

HessRho_EigVec2 = -6.1275707219E-01 -1.2977897961E-06 7.9027132713E-01

HessRho_EigVec3 = 7.9027132713E-01 -1.7710989802E-06 6.1275707219E-01

DelSqRho = 1.4692090806E-01

Bond Ellipticity = 7.4588303652E-01

V = -2.3249622909E-01

G = 1.3461322806E-01

K = 9.7883001039E-02

L = -3.6730227016E-02

Vnuc = 9.1634010325E+00

Ven = -1.1040242945E+00

Vrep = 8.7152806539E-01

DelSqV = -2.9319284875E+00

DelSqVen = -1.3462952006E+00

DelSqVrep = -1.5856332869E+00

DelSqG = 4.2202709649E+00

DelSqK = -1.2883424774E+00

Stress_EigVals = -1.0422488901E-01 -8.6432559163E-02 -4.1838780923E-02

Stress_EigVec1 = 2.0565037813E-06 1.0000000000E+00 4.9163393096E-07

Stress_EigVec2 = -5.4425629617E-01 7.0682408669E-07 8.3891899733E-01

Stress_EigVec3 = 8.3891899732E-01 -1.9928149526E-06 5.4425629617E-01

-DivStress = -2.6625800975E-01 5.1191899868E-07 -1.4513215494E-01

BPL = 2.5878310079E+00 = 1.5694426852E+00 + 1.0183883227E+00

GBL_I = 2.4723295579E+00

GBL_II = 2.4866928926E+00

GBL_III = 2.5612995052E+00 = 1.5441843919E+00 + 1.0171151133E+00

GBL_IV = 2.5781154047E+00 = 1.5609923662E+00 + 1.0171230385E+00

CP# 16 Coords = 7.78750655923789E-01 -3.18461639192165E-06 -4.89121964921407E-01

Type = (3,-1) BCP B1 H8

Rho = 1.2048192946E-01

GradRho = -4.8308579359E-14 2.3736907207E-18 -4.3368086899E-14

HessRho_EigVals = -1.5352065683E-01 -8.7932817255E-02 3.8837358036E-01

HessRho_EigVec1 = 5.9861786466E-07 9.9999999998E-01 -6.9131566682E-06

HessRho_EigVec2 = -6.1275692992E-01 5.8300775024E-06 7.9027143742E-01

HessRho_EigVec3 = 7.9027143744E-01 3.7630140556E-06 6.1275692990E-01

DelSqRho = 1.4692010628E-01

Bond Ellipticity = 7.4588579803E-01

V = -2.3249604295E-01

G = 1.3461303476E-01

K = 9.7883008191E-02

L = -3.6730026569E-02

Vnuc = 9.1634002245E+00

Ven = -1.1040241395E+00

Vrep = 8.7152809651E-01

DelSqV = -2.9319231616E+00

DelSqVen = -1.3462877349E+00

DelSqVrep = -1.5856354268E+00

DelSqG = 4.2202631930E+00

DelSqK = -1.2883400314E+00

Stress_EigVals = -1.0422481332E-01 -8.6432492680E-02 -4.1838736949E-02

Stress_EigVec1 = -2.7499666476E-06 9.9999999999E-01 -3.3629291112E-06

Stress_EigVec2 = -5.4425580318E-01 1.3245408871E-06 8.3891931716E-01

Stress_EigVec3 = 8.3891931715E-01 4.1372938267E-06 5.4425580317E-01

-DivStress = 2.6625788556E-01 1.0766694744E-06 1.4513185210E-01

BPL = 2.5878317088E+00 = 1.0183885717E+00 + 1.5694431371E+00

GBL_I = 2.4723299692E+00

GBL_II = 2.4866933038E+00

GBL_III = 2.5613001976E+00 = 1.0171153539E+00 + 1.5441848437E+00

GBL_IV = 2.5781161004E+00 = 1.0171232792E+00 + 1.5609928213E+00

CP# 17 Coords = -7.78750280356795E-01 -3.24835026200669E-06 -4.89120296492234E-01

Type = (3,-1) BCP H8 B2

Rho = 1.2048180628E-01

GradRho = 4.8350212722E-14 -4.2985730933E-18 -4.3326453536E-14

HessRho_EigVals = -1.5352025087E-01 -8.7931893981E-02 3.8837224153E-01

HessRho_EigVec1 = -6.4269325893E-07 9.9999999998E-01 -6.9513356465E-06

HessRho_EigVec2 = 6.1275633190E-01 5.8872596007E-06 7.9027190111E-01

HessRho_EigVec3 = 7.9027190113E-01 -3.7515725090E-06 -6.1275633189E-01

DelSqRho = 1.4692009668E-01

Bond Ellipticity = 7.4589951294E-01

V = -2.3249576427E-01

G = 1.3461289422E-01

K = 9.7882870048E-02

L = -3.6730024169E-02

Vnuc = 9.1633997455E+00

Ven = -1.1040229530E+00

$V_{rep} = 8.7152718870E-01$
 $DelSqV = -2.9319153702E+00$
 $DelSqVen = -1.3462875765E+00$
 $DelSqVrep = -1.5856277937E+00$
 $DelSqG = 4.2202518292E+00$
 $DelSqK = -1.2883364591E+00$
 $Stress\_EigVals = -1.0422468496E-01 \ -8.6432406499E-02 \ -4.1838672808E-02$
 $Stress\_EigVec1 = 2.7100323641E-06 \ 9.9999999999E-01 \ -3.3334893095E-06$
 $Stress\_EigVec2 = 5.4425457674E-01 \ 1.3215837104E-06 \ 8.3892011282E-01$
 $Stress\_EigVec3 = 8.3892011282E-01 \ -4.0877674698E-06 \ -5.4425457673E-01$
 $-DivStress = -2.6625756102E-01 \ 1.0926742877E-06 \ 1.4513115025E-01$
 $BPL = 2.5878335293E+00 = 1.5694446104E+00 + 1.0183889190E+00$
 $GBL\_I = 2.4723308418E+00$
 $GBL\_II = 2.4866941584E+00$
 $GBL\_III = 2.5613018600E+00 = 1.5441861713E+00 + 1.0171156886E+00$
 $GBL\_IV = 2.5781177572E+00 = 1.5609941434E+00 + 1.0171236138E+00$

Number of NACPs = 8

Number of NNACPs = 0

Number of BCPs = 8

Number of RCPs = 1

Number of CCPs = 0

$NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H4	B1	H3	126.55556451	122.38097630	122.36778273	124.58815168	124.58908930
H6	B2	H5	126.55570015	122.38115646	122.36796334	124.58829102	124.58922864
H7	B1	H3	113.71426874	109.00284936	108.89312482	114.05700770	114.05666912
H7	B1	H4	113.71420203	109.00294826	108.89322650	114.05695909	114.05662051
H7	B2	H5	113.71417937	109.00280907	108.89308497	114.05691732	114.05657874
H7	B2	H6	113.71412469	109.00291301	108.89319168	114.05688213	114.05654356
B2	H7	B1	21.26626381	85.01606278	84.41140679	60.57130811	59.85202490
H8	B1	H3	113.71419263	109.00278907	108.89306411	114.05693422	114.05659564
H8	B1	H4	113.71424864	109.00305416	108.89333329	114.05700269	114.05666411
H8	B1	H7	53.14024726	94.98392566	95.58858165	57.48710110	57.48661139
H8	B2	H5	113.71413150	109.00270452	108.89297954	114.05687240	114.05653382
H8	B2	H6	113.71419766	109.00297205	108.89325113	114.05695245	114.05661387
H8	B2	H7	53.14034313	94.98394772	95.58860377	57.48718789	57.48669817
B2	H8	B1	21.26610002	85.01606384	84.41140780	60.57131416	59.85203080

Total time for electron density critical point search, analysis and connectivity = 11 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus
the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
B1	-2.3886694204E+01	2.3886694204E+01	-6.3534650288E+01	-5.2578865043E+01		
B2	-2.3886694846E+01	2.3886694846E+01	-6.3534665508E+01	-5.2578871882E+01		
H3	-8.4216551866E-01	8.4216551866E-01	-8.9773368030E+00	-1.6629713421E+00		
H4	-8.4216618036E-01	8.4216618036E-01	-8.9773301500E+00	-1.6629706632E+00		
H5	-8.4216619526E-01	8.4216619526E-01	-8.9773426310E+00	-1.6629717350E+00		
H6	-8.4216615341E-01	8.4216615341E-01	-8.9773362037E+00	-1.6629711038E+00		
H7	-9.2077133287E-01	9.2077133287E-01	-1.1036022556E+01	-1.7024561568E+00		
H8	-9.2077135926E-01	9.2077135926E-01	-1.1036022817E+01	-1.7024561948E+00		
Total	-5.2983595790E+01	5.2983595790E+01	-1.8505070696E+02	-1.1521453412E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
B1	-2.3886694099E+01	-2.3886694204E+01	1.0490203375E-07			
B2	-2.3886694631E+01	-2.3886694846E+01	2.1528925313E-07			
H3	-8.4216555758E-01	-8.4216551866E-01	-3.8917541150E-08			
H4	-8.4216620115E-01	-8.4216618036E-01	-2.0793608957E-08			
H5	-8.4216622778E-01	-8.4216619526E-01	-3.2522454918E-08			
H6	-8.4216616423E-01	-8.4216615341E-01	-1.0823244198E-08			
H7	-9.2077114945E-01	-9.2077133287E-01	1.8342487854E-07			
H8	-9.2077116886E-01	-9.2077135926E-01	1.9040005889E-07			
Total	-5.2983595199E+01	-5.2983595790E+01	5.9095937510E-07			

IQA Atomic Energy Components:

$E_{\text{IQA}}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{\text{ne}}(A, \text{Mol})/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{\text{en}}(A, \text{Mol})/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{\text{ee}}(A) = V_{\text{ee}}(A, \text{Mol}) = (1/2)[V_{\text{ee}}(A, \text{Mol}) + V_{\text{ee}}(\text{Mol}, A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{\text{nn}}(A, \text{Mol})/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{\text{eeC}}(A)$ = Coulomb Part of $V_{\text{ee}}(A)$

$V_{\text{eeX}}(A)$ = Exchange-Correlation Part of $V_{\text{ee}}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E_{\text{IQA}}(A)$	$T(A)$	$V_{\text{ne}}(A, \text{Mol})/2$	$V_{\text{en}}(A, \text{Mol})/2$	$V_{\text{ee}}(A)$	$V_{\text{nn}}(A, \text{Mol})/2$
$V_{\text{eeC}}(A)$	$V_{\text{eeX}}(A)$					

B1 9.0124239324E+00	2.3886694204E+01 -3.7573654449E+01 -3.1767325144E+01
B2 9.0124238797E+00	2.3886694846E+01 -3.7573654553E+01 -3.1767332754E+01
H3 2.1816715742E+00	8.4216551866E-01 -2.7517860119E+00 -4.4886684015E+00
H4 2.1816725981E+00	8.4216618036E-01 -2.7517871120E+00 -4.4886650750E+00
H5 2.1816718620E+00	8.4216619526E-01 -2.7517862395E+00 -4.4886713155E+00
H6 2.1816728771E+00	8.4216615341E-01 -2.7517873469E+00 -4.4886681018E+00
H7 2.6656508901E+00	9.2077133287E-01 -3.1835928916E+00 -5.5180112781E+00
H8 2.6656509122E+00	9.2077135926E-01 -3.1835929217E+00 -5.5180114087E+00

Total 3.2082838526E+01	5.2983595790E+01 -9.2521641526E+01 -9.2525353479E+01

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

B1	2.3886694204E+01 -5.2578865043E+01
B2	2.3886694846E+01 -5.2578871882E+01
H3	8.4216551866E-01 -1.6629713421E+00
H4	8.4216618036E-01 -1.6629706632E+00
H5	8.4216619526E-01 -1.6629717350E+00
H6	8.4216615341E-01 -1.6629711038E+00
H7	9.2077133287E-01 -1.7024561568E+00
H8	9.2077135926E-01 -1.7024561948E+00

Total	5.2983595790E+01 -1.1521453412E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$
	$VeeX(A,A')$					

B1	-1.1284221928E+01 -5.4778926225E+00	9.0124239324E+00
B2	-1.1284218612E+01 -5.4778968129E+00	9.0124238797E+00
H3	-1.9203003409E+00 -3.6571827305E+00	2.1816715742E+00
H4	-1.9203017804E+00 -3.6571797434E+00	2.1816725981E+00
H5	-1.9203003720E+00 -3.6571854480E+00	2.1816718620E+00
H6	-1.9203017950E+00 -3.6571825500E+00	2.1816728771E+00
H7	-2.3323648132E+00 -4.6667831997E+00	2.6656508901E+00
H8	-2.3323648243E+00 -4.6667833113E+00	2.6656509122E+00
Total	-3.4914374466E+01 -3.4918086418E+01	3.2082838526E+01

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$
B1	3.0835381840E+00	2.2253361285E+00	7.2168268909E+01	8.5820205543E-01	
	2.7831731091E+01				
B2	3.0835407701E+00	2.2253370342E+00	7.2168237753E+01	8.5820373594E-01	
	2.7831762247E+01				

H3	1.6283975966E+00 2.5908072748E+01	1.2065111627E+00	7.4091927252E+01	4.2188643395E-01
H4	1.6283952155E+00 2.5908088152E+01	1.2065091476E+00	7.4091911848E+01	4.2188606790E-01
H5	1.6283982200E+00 2.5908051399E+01	1.2065119722E+00	7.4091948601E+01	4.2188624781E-01
H6	1.6283963496E+00 2.5908072642E+01	1.2065102405E+00	7.4091927358E+01	4.2188610917E-01
H7	1.6602411922E+00 3.5032171542E+01	1.0786226497E+00	6.4967828458E+01	5.8161854246E-01
H8	1.6602412287E+00 3.5032171705E+01	1.0786226707E+00	6.4967828295E+01	5.8161855796E-01

Total	1.6001148757E+01 2.8542874140E+01	1.1433961006E+01	7.1457125860E+01	4.5671877506E+00

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$DI(A,A')/2$	$DI\_Bond(A,A')/2$	$DI\_NonBond(A,A')/2$

B1	3.0835381840E+00	2.2253361285E+00	8.5820205543E-01	8.1507904365E-01
4.3123011789E-02				
B2	3.0835407701E+00	2.2253370342E+00	8.5820373594E-01	8.1508155819E-01
4.3122177747E-02				
H3	1.6283975966E+00	1.2065111627E+00	4.2188643395E-01	2.5786749868E-01
1.6401893527E-01				
H4	1.6283952155E+00	1.2065091476E+00	4.2188606790E-01	2.5792536314E-01
1.6396070477E-01				
H5	1.6283982200E+00	1.2065119722E+00	4.2188624781E-01	2.5792621877E-01
1.6396002903E-01				
H6	1.6283963496E+00	1.2065102405E+00	4.2188610917E-01	2.5786853841E-01
1.6401757076E-01				
H7	1.6602411922E+00	1.0786226497E+00	5.8161854246E-01	2.9928641786E-01
2.8233212460E-01				
H8	1.6602412287E+00	1.0786226707E+00	5.8161855796E-01	2.9928656498E-01
2.8233199298E-01				

Total	1.6001148757E+01	1.1433961006E+01	4.5671877506E+00	3.2603212037E+00
1.3068665469E+00				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

B1	3.6414358017E+00	1.9485100522E+01	2.3126536324E+01
B2	3.6414433235E+00	1.9485112397E+01	2.3126555721E+01

H3	7.2258378499E-01	1.1490397087E+01	1.2212980872E+01
H4	7.2258091516E-01	1.1490382099E+01	1.2212963014E+01
H5	7.2258439531E-01	1.1490401152E+01	1.2212985547E+01
H6	7.2258221552E-01	1.1490389304E+01	1.2212971519E+01
H7	8.3888908326E-01	1.1612919500E+01	1.2451808584E+01
H8	8.3888913334E-01	1.1612919724E+01	1.2451808857E+01

Total	1.1850988653E+01	1.0815762178E+02	1.2000861044E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$

B1	B2	9.4812719210E+00	5.3887571061E-02	8.7379445050E-01	8.7379371764E-01
B1	H3	4.7633586691E+00	5.1573499735E-01	8.3627146250E+00	1.5835659498E+01 (Bonded)
B2	H3	5.0130721351E+00	1.6316488122E-02	2.6457389959E-01	5.0099828678E-01
B1	H4	4.7632934625E+00	5.1585072627E-01	8.3645911855E+00	1.5839236119E+01 (Bonded)
B2	H4	5.0130785355E+00	1.6289002903E-02	2.6412822332E-01	5.0015508361E-01
H3	H4	2.6014014481E+00	1.0054681447E-01	3.0872931364E+00	3.0872976507E+00
B1	H5	5.0130836691E+00	1.6288841723E-02	2.6412583129E-01	5.0014921177E-01
B2	H5	4.7633060825E+00	5.1585243755E-01	8.3646119186E+00	1.5839259440E+01 (Bonded)

H3	H5	2.6465228422E+00	1.0313811079E-02	3.1668589723E-01	3.1668577601E-01
H4	H5	2.6448984694E+00	1.3554802019E-02	4.1620123573E-01	4.1620046783E-01
B1	H6	5.0130640364E+00	1.6316572633E-02	2.6457549184E-01	5.0100126533E-01
B2	H6	4.7633579957E+00	5.1573707682E-01	8.3627413299E+00	1.5835735475E+01 (Bonded)
H3	H6	2.6448993020E+00	1.3554800108E-02	4.1620056847E-01	4.1620088718E-01
H4	H6	2.6465157991E+00	1.0314051197E-02	3.1669373314E-01	3.1669351258E-01
H5	H6	2.6014043020E+00	1.0054683025E-01	3.0872924392E+00	3.0872959852E+00
B1	H7	4.9697901985E+00	2.9925382431E-01	4.8524423317E+00	9.0123599424E+00 (Bonded)
B2	H7	4.9697618987E+00	2.9931901142E-01	4.8534952792E+00	9.0143231245E+00 (Bonded)
H3	H7	2.6566711756E+00	9.3723183030E-02	2.8777733161E+00	2.8225773301E+00
H4	H7	2.6566685160E+00	9.3720596013E-02	2.8776980895E+00	2.8224994192E+00
H5	H7	2.6566695722E+00	9.3728459688E-02	2.8779342344E+00	2.8227362424E+00
H6	H7	2.6566672111E+00	9.3726971521E-02	2.8778918456E+00	2.8226914246E+00
B1	H8	4.9697579535E+00	2.9931853936E-01	4.8534916953E+00	9.0143087098E+00 (Bonded)
B2	H8	4.9697942216E+00	2.9925459060E-01	4.8524506874E+00	9.0123828220E+00 (Bonded)
H3	H8	2.6566689191E+00	9.3727814883E-02	2.8779155373E+00	2.8227167614E+00
H4	H8	2.6566648570E+00	9.3728032749E-02	2.8779264350E+00	2.8227233227E+00
H5	H8	2.6566728826E+00	9.3721957815E-02	2.8777345942E+00	2.8225403693E+00
H6	H8	2.6566691882E+00	9.3723136215E-02	2.8777740823E+00	2.8225758581E+00
H7	H8	2.6612526096E+00	1.9029653438E-01	5.7309906317E+00	5.7309905058E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

B1	H3	5.2209598034E+01	4.0259796080E+01	3.2346881367E+01
B1	H4	5.2209602044E+01	4.0259798303E+01	3.2346882159E+01
B1	H7	3.6685568641E+01	2.8968506975E+01	2.3775530309E+01
B1	H8	3.6685590682E+01	2.8968486222E+01	2.3775480429E+01
B1	Total	1.7779035940E+02	1.3845658758E+02	1.1224477426E+02
B2	H5	5.2206638424E+01	4.0266718321E+01	3.2353928242E+01
B2	H6	5.2206643221E+01	4.0266721036E+01	3.2353929416E+01
B2	H7	3.6685631776E+01	2.8968517220E+01	2.3775523417E+01
B2	H8	3.6686276435E+01	2.8969203074E+01	2.3776236955E+01
B2	Total	1.7778518986E+02	1.3847115965E+02	1.1225961803E+02
H3	B1	5.2209598034E+01	4.0259796080E+01	3.2346881367E+01
H3	Total	5.2209598034E+01	4.0259796080E+01	3.2346881367E+01
H4	B1	5.2209602044E+01	4.0259798303E+01	3.2346882159E+01
H4	Total	5.2209602044E+01	4.0259798303E+01	3.2346882159E+01
H5	B2	5.2206638424E+01	4.0266718321E+01	3.2353928242E+01
H5	Total	5.2206638424E+01	4.0266718321E+01	3.2353928242E+01
H6	B2	5.2206643221E+01	4.0266721036E+01	3.2353929416E+01
H6	Total	5.2206643221E+01	4.0266721036E+01	3.2353929416E+01
H7	B1	3.6685571151E+01	2.8968509484E+01	2.3775532817E+01

H7	B2	3.6685631803E+01	2.8968517246E+01	2.3775523442E+01

H7	Total	7.3371202954E+01	5.7937026730E+01	4.7551056259E+01

H8	B1	3.6685590688E+01	2.8968486228E+01	2.3775480435E+01

H8	B2	3.6686265980E+01	2.8969192618E+01	2.3776226499E+01

H8	Total	7.3371856668E+01	5.7937678846E+01	4.7551706934E+01

Total	Total	7.1115109060E+02	5.5385548655E+02	4.4900877667E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N_{IAS}(A B)$	$G_{IAS}(A B)$	$K_{IAS}(A B)$	$L_{IAS}(A B)$	$\Delta \rho_{IAS}(A B)$ $V_{IAS}(A B)$

B1	H3	9.2761914076E-01	6.1039602719E-01	4.3097195464E-01	-1.7942407255E-01	7.1769629020E-01 -1.0413679818E+00

B1	H4	9.2761932812E-01	6.1039633312E-01	4.3097208704E-01	-1.7942424608E-01	7.1769698432E-01 -1.0413684202E+00

B1	H7	7.2598397529E-01	5.4935003585E-01	2.8838196674E-01	-2.6096806911E-01	1.0438722764E+00 -8.3773200259E-01

B1 H8 7.2597317899E-01 5.4934562202E-01 2.8837606528E-01 -2.6096955673E-01
1.0438782269E+00 -8.3772168730E-01

B1 Total 3.3071956232E+00 2.3194880182E+00 1.4387020737E+00 -8.8078594447E-01
3.5231437778E+00 -3.7581900919E+00

B2 H5 9.2761929063E-01 6.1039612799E-01 4.3097205626E-01 -1.7942407173E-01
7.1769628692E-01 -1.0413681842E+00

B2 H6 9.2761942435E-01 6.1039650828E-01 4.3097214340E-01 -1.7942436488E-01
7.1769745953E-01 -1.0413686517E+00

B2 H7 7.2597521072E-01 5.4934677624E-01 2.8837704739E-01 -2.6096972885E-01
1.0438789154E+00 -8.3772382364E-01

B2 H8 7.2606185196E-01 5.4938515832E-01 2.8842544889E-01 -2.6095970943E-01
1.0438388377E+00 -8.3781060720E-01

B2 Total 3.3072757777E+00 2.3195245708E+00 1.4387466959E+00 -8.8077787489E-01
3.5231114996E+00 -3.7582712667E+00

H3 B1 9.2761914076E-01 6.1039602719E-01 4.3097195464E-01 -1.7942407255E-01
7.1769629020E-01 -1.0413679818E+00

H3 Total 9.2761914076E-01 6.1039602719E-01 4.3097195464E-01 -1.7942407255E-01
7.1769629020E-01 -1.0413679818E+00

H4 B1 9.2761932812E-01 6.1039633312E-01 4.3097208704E-01 -1.7942424608E-01
7.1769698432E-01 -1.0413684202E+00

H4 Total 9.2761932812E-01 6.1039633312E-01 4.3097208704E-01 -1.7942424608E-01
7.1769698432E-01 -1.0413684202E+00

H5 B2 9.2761929063E-01 6.1039612799E-01 4.3097205626E-01 -1.7942407173E-01
7.1769628692E-01 -1.0413681842E+00

H5 Total 9.2761929063E-01 6.1039612799E-01 4.3097205626E-01 -1.7942407173E-01
7.1769628692E-01 -1.0413681842E+00

H6	B2	9.2761942435E-01	6.1039650828E-01	4.3097214340E-01	-1.7942436488E-01
		7.1769745953E-01	-1.0413686517E+00		

H6	Total	9.2761942435E-01	6.1039650828E-01	4.3097214340E-01	-1.7942436488E-01
		7.1769745953E-01	-1.0413686517E+00		

H7	B1	7.2598426327E-01	5.4935016492E-01	2.8838212909E-01	-2.6096803583E-01
		1.0438721433E+00	-8.3773229401E-01		

H7	B2	7.2597521376E-01	5.4934677761E-01	2.8837704902E-01	-2.6096972859E-01
		1.0438789144E+00	-8.3772382663E-01		

H7	Total	1.4519594770E+00	1.0986969425E+00	5.7675917811E-01	-5.2193776442E-01
		2.0877510577E+00	-1.6754561206E+00		

H8	B1	7.2597317966E-01	5.4934562232E-01	2.8837606564E-01	-2.6096955668E-01
		1.0438782267E+00	-8.3772168797E-01		

H8	B2	7.2606065082E-01	5.4938462126E-01	2.8842477166E-01	-2.6095984960E-01
		1.0438393984E+00	-8.3780939292E-01		

H8	Total	1.4520338305E+00	1.0987302436E+00	5.7680083730E-01	-5.2192940628E-01
		2.0877176251E+00	-1.6755310809E+00		

Total	Total	1.3228941892E+01	9.2780247717E+00	5.7548970264E+00	-3.5231277453E+00
		1.4092510981E+01	-1.5032921798E+01		

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

B1 5.7847894027E+00

B2 5.7847886741E+00

H3 7.4536051724E+01

H4 7.4775956099E+01

H5 7.4775924351E+01

H6 7.4536083241E+01

H7 3.6582049745E+01

H8 3.6582051975E+01

Total 3.8335769521E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1	5.7159661238E+00	6.7160713309E-02	2.4336895717E-02	-8.6268293799E-03	1.1749669584E-02
8.7728321899E-03	1.0370285683E-04				

B2	5.7159651319E+00	6.7160856804E-02	2.4336909775E-02	-8.6268016962E-03	1.1749696727E-02
8.7728152691E-03	1.0370263435E-04				

H3	6.1784558306E+01	-3.2506062963E-02	1.8091661610E-02	-8.6574029606E-03	-5.2611953301E-04
3.6310018957E-03	2.6243580011E-05				

H4	6.1805167405E+01	-3.0470376115E-02	1.9217890763E-02	-8.6628549870E-03	-4.9300693445E-04
3.6652181008E-03	2.6937978388E-05				

H5	6.1805143090E+01	-3.0463686338E-02	1.9217870969E-02	-8.6628171694E-03	-4.9289888859E-04
3.6652242289E-03	2.6937977849E-05				

H6	6.1784580486E+01	-3.2509153213E-02	1.8091616223E-02	-8.6573958264E-03	-5.2616936065E-04
3.6309950662E-03	2.6243629148E-05				

H7	3.2539908283E+01	7.3164407017E-01	3.0319589347E-02	6.8108535103E-04	2.2484515439E-02
5.4009386048E-03	4.3392498260E-05				

H8	3.2539907959E+01	7.3164397258E-01	3.0319583138E-02	6.8071433006E-04	2.2484512664E-02
5.4009357700E-03	4.3392445205E-05				

Total	3.2369119678E+02	1.4716603342E+00	3.0319589347E-02	-8.6628549870E-03	
4.5464947730E-03	1.1874006471E-04				

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
ESP-_Int_IDS(A)					

B1	7.7898598057E-02	1.3818782070E-03	4.6732823517E+00	7.2529655683E-02	1.0426837721E+00
-5.3689423739E-03					

B2	7.7898638004E-02	1.3818803414E-03	4.6732822240E+00	7.2529747404E-02
1.0426829079E+00 -5.3688905998E-03				
H3	2.3813588318E-01	1.6385500740E-03	1.7126320509E+01	1.0281491011E-01
4.4658237796E+01 -1.3532097307E-01				
H4	2.3968283284E-01	1.6799283705E-03	1.6803250955E+01	1.0460622836E-01
4.5001916450E+01 -1.3507660448E-01				
H5	2.3967991457E-01	1.6799210926E-03	1.6803266537E+01	1.0460811411E-01
4.5001876553E+01 -1.3507180045E-01				
H6	2.3813694746E-01	1.6385569377E-03	1.7126306475E+01	1.0281389712E-01
4.4658274011E+01 -1.3532305034E-01				
H7	7.3164407017E-01	1.7862650305E-02	3.2539908283E+01	7.3164407017E-01
0.0000000000E+00 NULL				
H8	7.3164397258E-01	1.7862644340E-02	3.2539907959E+01	7.3164397258E-01
0.0000000000E+00 NULL				

Total	2.5747208569E+00	4.5126009668E-02	1.4228552529E+02	2.0231905955E+00
1.8140567149E+02 -5.5153026131E-01				

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

B1	7.7225990582E-04	1.5520067102E-02	5.9253285523E-03	4.6983012516E-05
1.3452300063E-03				
B2	7.7192745835E-04	1.5520087152E-02	5.9253181457E-03	4.6982928289E-05
1.3452324845E-03				
H3	1.3136977554E-06	6.0033274544E-03	4.1137125404E-03	2.4254395543E-05
1.0326201244E-03				
H4	4.4759072081E-06	6.2253565483E-03	4.1611577222E-03	2.5377163904E-05
1.0776299223E-03				
H5	4.5280954353E-06	6.2254630004E-03	4.1611302449E-03	2.5376793640E-05
1.0776469714E-03				
H6	1.2138051669E-06	6.0032732260E-03	4.1137427135E-03	2.4254804311E-05
1.0326151280E-03				
H7	6.8108535103E-04	2.2484515439E-02	5.4009386048E-03	4.3392498260E-05
1.7862650305E-02				

H8	6.8071433006E-04	2.2484512664E-02	5.4009357700E-03	4.3392445205E-05
1.7862644340E-02				

Total	1.2138051669E-06	1.4219229900E-02	9.7466394031E-05	4.2636269282E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

B1	-1.1662558808E-04	-5.1491569329E-03	2.6023267546E-03	8.6341363747E-06
3.6648200730E-05				

B2	-1.1629084895E-04	-5.1491115458E-03	2.6023447750E-03	8.6343032323E-06
3.6647856978E-05				

H3	-5.0646817093E-05	-3.0301458308E-03	1.6505961654E-03	4.3863725243E-06
6.0592994963E-04				

H4	-3.2219200184E-05	-3.0015744913E-03	1.6453166237E-03	4.3743905455E-06
6.0229844822E-04				

H5	-3.2103301611E-05	-3.0014704008E-03	1.6453336020E-03	4.3744866950E-06
6.0227412127E-04				

H6	-5.0617660751E-05	-3.0301898883E-03	1.6505968513E-03	4.3863600934E-06
6.0594180975E-04				

H7	NULL	NULL	NULL	NULL	NULL

H8	NULL	NULL	NULL	NULL	NULL

Total	-3.2103301611E-05	-3.0403143231E-03	4.4811996606E-06	2.4897403866E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)

B1	5.4876610036E+00

B2	5.4876598249E+00

H3	5.2645740152E+01

H4 5.3123258049E+01
H5 5.3123238262E+01
H6 5.2645754490E+01
H7 2.9249106108E+01
H8 2.9249109700E+01

Total 2.8101152759E+02

Atomic Surface Area and Volume Data:

 $\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$

$\text{Vol(A)} = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$
 $\text{IsoSurface of the Electron Density Distribution (IsoDensity Surface)}$

$\text{N(Vol(A))} = \text{Average Number of Electrons in Vol(A)}$

$\text{N(Vol(A))}/\text{Vol(A)} = \text{Average Electron Density in Vol(A)}$

$\%N(\text{Vol(A)}) = 100 * \text{N(Vol(A))} / \text{N(A)}$

$= \text{Percentage of Atom A's Electron Population in Vol(A)}$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	1.8357514880E+02	2.7203809178E+01	3.0822671955E+00	1.1330277960E-01	
	9.9958781487E+01				
B2	1.8356997853E+02	2.7199643367E+01	3.0822679080E+00	1.1332015888E-01	
	9.9958720757E+01				
H3	1.2674564976E+02	1.1387000374E+02	1.6102961498E+00	1.4141530666E-02	
	9.8888388994E+01				
H4	1.2698555814E+02	1.1382029631E+02	1.6102743382E+00	1.4147514902E-02	
	9.8887194145E+01				
H5	1.2698256277E+02	1.1381039611E+02	1.6102732498E+00	1.4148736011E-02	
	9.8886944865E+01				

H6	1.2674272646E+02	1.1386110503E+02	1.6102916803E+00	1.4142596630E-02
9.8888190243E+01				
H7	1.0995325270E+02	7.3941431462E+01	1.6520573365E+00	2.2342782711E-02
9.9507068266E+01				
H8	1.0995390864E+02	7.3942840093E+01	1.6520579354E+00	2.2342365175E-02
9.9507102151E+01				

Total	1.0945087858E+03	6.5764952529E+02	1.5909785794E+01	2.4191891246E-02
9.9429022475E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	1.4417255370E+02	2.4440627001E+01	3.0804606380E+00	1.2603852748E-01	
9.9900194325E+01					
B2	1.4418712478E+02	2.4444059079E+01	3.0804661715E+00	1.2602105737E-01	
9.9900289990E+01					
H3	1.0204435439E+02	8.2720813846E+01	1.5902237663E+00	1.9223985988E-02	
9.7655742647E+01					
H4	1.0206496571E+02	8.2739749978E+01	1.5902387770E+00	1.9219767735E-02	
9.7656807258E+01					
H5	1.0207186141E+02	8.2741986751E+01	1.5902438674E+00	1.9219309685E-02	
9.7656939689E+01					
H6	1.0205130152E+02	8.2729708959E+01	1.5902320616E+00	1.9222019292E-02	
9.7656326839E+01					
H7	9.0476935013E+01	5.8903874475E+01	1.6423477915E+00	2.7881829610E-02	
9.8922240890E+01					
H8	9.0477586806E+01	5.8904687485E+01	1.6423486075E+00	2.7881458635E-02	
9.8922287865E+01					

Total	8.7754668333E+02	4.9762550757E+02	1.5806561681E+01	3.1763969974E-02	
9.8783918087E+01					

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	1.1773243526E+02	2.2404977632E+01	3.0775408042E+00	1.3735969099E-01
	9.9805503304E+01			
B2	1.1774727785E+02	2.2408081524E+01	3.0775491360E+00	1.3734103621E-01
	9.9805689798E+01			
H3	8.4992621519E+01	6.3024270977E+01	1.5620067555E+00	2.4784209817E-02
	9.5922934219E+01			
H4	8.5470140208E+01	6.3028905803E+01	1.5620088084E+00	2.4782419884E-02
	9.5923200555E+01			
H5	8.5477166504E+01	6.3024773880E+01	1.5620031229E+00	2.4783954416E-02
	9.5922674436E+01			
H6	8.4999683906E+01	6.3030577268E+01	1.5620188016E+00	2.4781921241E-02
	9.5923747421E+01			
H7	7.6800162367E+01	4.8320748556E+01	1.6273199115E+00	3.3677456582E-02
	9.8017078431E+01			
H8	7.6800816634E+01	4.8321215518E+01	1.6273208647E+00	3.3677150858E-02
	9.8017133689E+01			
Total	7.3002030426E+02	3.9356355116E+02	1.5657768205E+01	3.9784599358E-02
	9.7854025626E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
B1	H3	6.2825400206E-01		
B1	H4	6.2825162086E-01		
B1	H7	3.3004970298E-01		
B1	H8	3.2997828732E-01		
B1		1.9165336132E+00	1.9164618159E+00	
B2	H5	6.2825462516E-01		

B2	H6	6.2825275516E-01
B2	H7	3.2997609727E-01
B2	H8	3.3004754943E-01
B2		1.9165310270E+00 1.9164592297E+00
H3	B1	-6.2832579938E-01
H3		-6.2832579938E-01 -6.2839759670E-01
H4	B1	-6.2832341818E-01
H4		-6.2832341818E-01 -6.2839521550E-01
H5	B2	-6.2832642248E-01
H5		-6.2832642248E-01 -6.2839821980E-01
H6	B2	-6.2832455248E-01
H6		-6.2832455248E-01 -6.2839634980E-01
H7	B1	-3.3012150030E-01
H7	B2	-3.3004789459E-01
H7		-6.6016939488E-01 -6.6024119220E-01
H8	B1	-3.3005008464E-01
H8	B2	-3.3011934675E-01
H8		-6.6016943138E-01 -6.6024122870E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

B1	-9.2934821893E-02	1.7253864515E-02	-7.5680957378E-02
B2	9.2933470329E-02	-1.7250128005E-02	7.5683342324E-02
H3	1.3427880430E-01	-3.9409643707E-01	-2.5981763277E-01
H4	1.3427778541E-01	-3.9409102484E-01	-2.5981323943E-01

H5	-1.3427679808E-01	3.9409548555E-01	2.5981868747E-01
H6	-1.3427492335E-01	3.9409047301E-01	2.5981554966E-01
H7	3.9550011623E-06	5.7274885777E-05	6.1229886940E-05
H8	-4.4402276014E-06	-5.3855933305E-05	-5.8296160907E-05

Total	3.0314895609E-06	5.6521028939E-06	8.6835924546E-06

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

B1	-3.7417453959E-04	2.2371702547E-06	-3.7193736934E-04
B2	3.6642432334E-04	1.9002218491E-06	3.6832454519E-04
H3	-2.7024117465E-01	6.9166395787E-01	4.2142278322E-01
H4	2.7023802891E-01	-6.9166350068E-01	-4.2142547177E-01
H5	-2.7024383468E-01	6.9166534800E-01	4.2142151332E-01
H6	2.7024200684E-01	-6.9166543247E-01	-4.2142342563E-01
H7	2.3767881446E-05	2.5707260349E-06	2.6338607481E-05
H8	-3.0942904876E-05	5.8862897800E-06	-2.5056615096E-05

Total	-1.9898819680E-05	1.2967127239E-05	-6.9316924406E-06

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

B1	1.9912901040E-04	-3.4701273115E-05	1.6442773728E-04
B2	-1.8673187711E-04	3.4761847082E-05	-1.5197003003E-04
H3	2.7046308401E-06	-8.1840312746E-07	1.8862277126E-06
H4	2.3518134303E-06	2.6337566883E-07	2.6151890991E-06
H5	-1.3408177239E-06	-2.7480219055E-07	-1.6156199144E-06
H6	1.4963184446E-07	8.3234541644E-07	9.8197726090E-07
H7	4.2327429960E-01	-8.9312125979E-01	-4.6984696019E-01
H8	-4.2327429975E-01	8.9312125287E-01	4.6984695312E-01

Total	1.6262241681E-05	5.6169016993E-08	1.6318410698E-05

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

B1	9.2935788473E-02	1.7253899556E-02	7.5682049943E-02
B2	9.2934380306E-02	1.7250163135E-02	7.5684391147E-02
H3	3.0176330090E-01	7.9605969144E-01	4.9507813981E-01
H4	3.0176003037E-01	7.9605661485E-01	4.9507812278E-01
H5	3.0176479034E-01	7.9606042821E-01	4.9507761235E-01
H6	3.0176231922E-01	7.9605802011E-01	4.9507759343E-01
H7	4.2327430029E-01	8.9312126163E-01	4.6984696492E-01
H8	4.2327430091E-01	8.9312125451E-01	4.6984695740E-01

Total	2.5876890426E-05	1.4145522646E-05	1.9741926596E-05

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

B1	H3	-2.8568053671E-01	
B1	H4	-2.8567632320E-01	
B1	H7	2.9433748886E-01	
B1	H8	2.9427323557E-01	
B1		1.7253864515E-02	
B2	H5	2.8568013297E-01	
B2	H6	2.8567619852E-01	
B2	H7	-2.9427110129E-01	
B2	H8	-2.9433535821E-01	
B2		-1.7250128005E-02	

H3	B1	-3.9409643707E-01
H3		-3.9409643707E-01
H4	B1	-3.9409102484E-01
H4		-3.9409102484E-01
H5	B2	3.9409548555E-01
H5		3.9409548555E-01
H6	B2	3.9409047301E-01
H6		3.9409047301E-01
H7	B1	2.5708223566E-01
H7	B2	-2.5702496077E-01
H7		5.7274885777E-05
H8	B1	2.5702669890E-01
H8	B2	-2.5708055483E-01
H8		-5.3855933305E-05

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

B1	H3	5.4401161630E-01
B1	H4	-5.4401111394E-01
B1	H7	5.5138533949E-07
B1	H8	1.1834198736E-06
B1		2.2371702547E-06
B2	H5	5.4401253090E-01
B2	H6	-5.4401240712E-01
B2	H7	5.7246685171E-07
B2	H8	1.2039687521E-06
B2		1.9002218491E-06
H3	B1	6.9166395787E-01
H3		6.9166395787E-01
H4	B1	-6.9166350068E-01
H4		-6.9166350068E-01
H5	B2	6.9166534800E-01

H5		6.9166534800E-01
H6	B2	-6.9166543247E-01
H6		-6.9166543247E-01
H7	B1	1.2964794631E-06
H7	B2	1.2742465718E-06
H7		2.5707260349E-06
H8	B1	2.9533548961E-06
H8	B2	2.9329348839E-06
H8		5.8862897800E-06

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	H3	-6.6321400852E-07	
B1	H4	2.7536595720E-07	
B1	H7	-1.6143387471E-01	
B1	H8	1.6139956129E-01	
B1		-3.4701273115E-05	
B2	H5	-2.7926343622E-07	
B2	H6	6.7507695573E-07	
B2	H7	-1.6139865533E-01	
B2	H8	1.6143302136E-01	
B2		3.4761847082E-05	
H3	B1	-8.1840312746E-07	
H3		-8.1840312746E-07	
H4	B1	2.6337566883E-07	
H4		2.6337566883E-07	
H5	B2	-2.7480219055E-07	
H5		-2.7480219055E-07	
H6	B2	8.3234541644E-07	
H6		8.3234541644E-07	
H7	B1	-4.4661087727E-01	
H7	B2	-4.4651038252E-01	

H7		-8.9312125979E-01
H8	B1	4.4651349987E-01
H8	B2	4.4660775300E-01
H8		8.9312125287E-01

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

B1	H3	6.1446074547E-01	
B1	H4	6.1445834173E-01	
B1	H7	3.3570143469E-01	
B1	H8	3.3562859764E-01	
B1		1.7253899556E-02	
B2	H5	6.1446136751E-01	
B2	H6	6.1445942868E-01	
B2	H7	3.3562629068E-01	
B2	H8	3.3569915621E-01	
B2		1.7250163135E-02	
H3	B1	7.9605969144E-01	
H3		7.9605969144E-01	
H4	B1	7.9605661485E-01	
H4		7.9605661485E-01	
H5	B2	7.9606042821E-01	
H5		7.9606042821E-01	
H6	B2	7.9605802011E-01	
H6		7.9605802011E-01	
H7	B1	5.1531791313E-01	
H7	B2	5.1520224394E-01	
H7		8.9312126163E-01	
H8	B1	5.1520581278E-01	
H8	B2	5.1531436689E-01	
H8		8.9312125451E-01	

Atomic Traceless Quadrupole Moment Tensors:

$Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$
B1	1.4660238200E-01	1.7193184388E-03	-4.2165178728E-04	1.9209886215E-01	1.8241810792E-03	-3.3870124415E-01
B2	1.4660816451E-01	1.6924314074E-03	-4.7246848157E-04	1.9208328459E-01	1.8291341660E-03	-3.3869144909E-01
H3	7.9285969392E-02	-4.1538126323E-01	-1.5424984893E-05	4.4215343044E-01	-5.3487840726E-06	-5.2143939983E-01
H4	7.9266124531E-02	4.1537537428E-01	-2.1846506726E-05	4.4216028609E-01	6.0105788277E-06	-5.2142641062E-01
H5	7.9293716229E-02	4.1537871482E-01	1.3457703173E-06	4.4214663607E-01	-6.7268270155E-06	-5.2144035230E-01
H6	7.9280691076E-02	-4.1537431318E-01	-3.9351561430E-07	4.4215285667E-01	-4.7404629439E-06	-5.2143354774E-01
H7	5.0661168747E-01	7.9652360328E-07	-5.2609727260E-06	-1.4991490123E-01	5.4145155739E-05	-3.5669678624E-01
H8	5.0661192263E-01	7.7687540491E-07	-6.1552002832E-06	-1.4991522697E-01	4.6438307242E-05	-3.5669669566E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)

B1	1	-3.3870788985E-01	8.8100884640E-04	-3.4394519459E-03	9.9999369698E-01
B1	2	1.4653799625E-01	9.9928974223E-01	-3.7669497945E-02	-1.0099518968E-03
B1	3	1.9216989360E-01	3.7672734195E-02	9.9928433346E-01	3.4038218875E-03
B2	1	-3.3869822390E-01	9.8556921447E-04	-3.4492354685E-03	9.9999356569E-01
B2	2	1.4654586591E-01	9.9931110817E-01	-3.7095426257E-02	-1.1128482843E-03
B2	3	1.9215235799E-01	3.7099026049E-02	9.9930577509E-01	3.4102992083E-03
H3	1	-5.2143940061E-01	4.2049323410E-05	2.3677308927E-05	9.9999999884E-01
H3	2	-1.9255702761E-01	8.3674113090E-01	5.4759864640E-01	-4.8150060799E-05
H3	3	7.1399642822E-01	-5.4759864691E-01	8.3674113195E-01	3.2143743335E-06
H4	1	-5.2142641207E-01	5.7958789146E-05	-3.1222133518E-05	9.9999999783E-01
H4	2	-1.9256346892E-01	8.3674994360E-01	-5.4758517838E-01	-6.5593791243E-05
H4	3	7.1398988099E-01	5.4758517924E-01	8.3674994559E-01	-5.6122554326E-06
H5	1	-5.2144035239E-01	-1.0068288468E-05	1.1321219433E-05	9.9999999989E-01
H5	2	-1.9255130655E-01	8.3673772344E-01	-5.4760385496E-01	1.4624060178E-05
H5	3	7.1399165893E-01	5.4760385506E-01	8.3673772349E-01	-3.9594577970E-06
H6	1	-5.2143354778E-01	5.7795428310E-06	7.4109976487E-06	9.9999999996E-01
H6	2	-1.9255452697E-01	8.3674411448E-01	5.4759408946E-01	-8.8942169580E-06
H6	3	7.1398807475E-01	-5.4759408950E-01	8.3674411449E-01	-3.0362651709E-06
H7	1	-3.5669680045E-01	6.0942075588E-06	-2.6184670389E-04	9.9999996570E-01
H7	2	-1.4991488705E-01	-1.2111406277E-06	9.9999996572E-01	2.6184671128E-04
H7	3	5.0661168750E-01	9.9999999998E-01	1.2127363344E-06	-6.0938902166E-06
H8	1	-3.5669670613E-01	7.1299815510E-06	-2.2457674545E-04	9.9999997476E-01
H8	2	-1.4991521655E-01	-1.1812048949E-06	9.9999997478E-01	2.2457675388E-04
H8	3	5.0661192268E-01	9.9999999997E-01	1.1828060932E-06	-7.1297161001E-06

Atomic Radial Moments:

$$R-2(A) = \langle Rho/(r*r) \rangle(A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle(A)$$

$$R0(A) = \langle \text{Rho} \rangle(A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle(A)$$

$$R+2(A) = \langle \text{Rho} * r^2 \rangle(A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.2071063730E+01 2.2996344828E+00		1.0515773009E+01	3.0835381841E+00	1.9929734093E+00
B2	9.2071065526E+01 2.2996504968E+00		1.0515774376E+01	3.0835407703E+00	1.9929792884E+00
H3	3.1122336567E+00 3.7216818209E+00		1.6629713421E+00	1.6283975967E+00	2.1985572190E+00
H4	3.1122339186E+00 3.7216640772E+00		1.6629706632E+00	1.6283952155E+00	2.1985505701E+00
H5	3.1122337461E+00 3.7216818924E+00		1.6629717350E+00	1.6283982198E+00	2.1985579338E+00
H6	3.1122340125E+00 3.7216691422E+00		1.6629711038E+00	1.6283963498E+00	2.1985531373E+00
H7	3.1164077889E+00 3.2899284329E+00		1.7024561568E+00	1.6602411922E+00	2.1387048439E+00
H8	3.1164078813E+00 3.2899286783E+00		1.7024561948E+00	1.6602412287E+00	2.1387049199E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\text{Rho}/dx) + y^*(d\text{Rho}/dy) + z^*(d\text{Rho}/dz)$$

$$\text{GR-2}(A) = \langle \text{Dot}/(r^2) \rangle(A)$$

$$\text{GR-1}(A) = \langle \text{Dot}/r \rangle(A)$$

$$\text{GR0}(A) = \langle \text{Dot} \rangle(A)$$

$$\text{GR+1}(A) = \langle \text{Dot} * r \rangle(A)$$

$$\text{GR+2}(A) = \langle \text{Dot} * r^2 \rangle(A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)

B1 -9.0774394285E+01 -1.9388978543E+01 -7.0381870115E+00 -4.7349366632E+00 -
6.2240520929E+00

B2 -9.0774397137E+01 -1.9388982418E+01 -7.0381960744E+00 -4.7349629638E+00 -
6.2241409270E+00

H3 -2.6759155961E+00 -2.5706111106E+00 -3.5087408430E+00 -6.1276390162E+00 -
1.3053397556E+01

H4 -2.6759145727E+00 -2.5706075996E+00 -3.5087308722E+00 -6.1276098235E+00 -
1.3053297145E+01

H5 -2.6759156986E+00 -2.5706113527E+00 -3.5087405044E+00 -6.1276336813E+00 -
1.3053356425E+01

H6 -2.6759153412E+00 -2.5706094011E+00 -3.5087348409E+00 -6.1276195598E+00 -
1.3053334867E+01

H7 -2.4328763329E+00 -2.1628597596E+00 -2.6747350450E+00 -4.1572043188E+00 -
7.7697096257E+00

H8 -2.4328764152E+00 -2.1628598315E+00 -2.6747351719E+00 -4.1572046848E+00 -
7.7697109023E+00

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

B1	1.5417690921E+00	1.5417690921E+00	3.0835381841E+00	0.0000000000E+00
B2	1.5417703851E+00	1.5417703851E+00	3.0835407703E+00	0.0000000000E+00
H3	8.1419879836E-01	8.1419879836E-01	1.6283975967E+00	0.0000000000E+00
H4	8.1419760777E-01	8.1419760777E-01	1.6283952155E+00	0.0000000000E+00
H5	8.1419910992E-01	8.1419910992E-01	1.6283982198E+00	0.0000000000E+00
H6	8.1419817492E-01	8.1419817492E-01	1.6283963498E+00	0.0000000000E+00
H7	8.3012059611E-01	8.3012059611E-01	1.6602411922E+00	0.0000000000E+00
H8	8.3012061436E-01	8.3012061436E-01	1.6602412287E+00	0.0000000000E+00

Total 8.0005743786E+00 8.0005743786E+00 1.6001148757E+01 0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

BF3

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\bf3\bf3.wfx

Sum File: D:\calc\ellipticity\bf3\bf3.sum

SumViz File: D:\calc\ellipticity\bf3\bf3.sumviz

Wfx Title: bf3_as_plane_mp2

Total memory allocated for AIMSum = 0.459 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	31.9999999964
Number of Alpha electrons (from MO Occs)	=	15.9999999982
Number of Beta electrons (from MO Occs)	=	15.9999999982
Number of electron pairs ($N*(N-1)/2$)	=	495.9999998874
Number of electron pairs (from Muller 2EDM)	=	495.9993280212
Number of electron pairs (from Muller 2EDM, no SOSI)	=	496.2695879135

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z

B1	5.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
F2	9.0	0.0000000000E+00	2.4913044000E+00	0.0000000000E+00
F3	9.0	2.1575329000E+00	-1.2456522000E+00	0.0000000000E+00
F4	9.0	-2.1575329000E+00	-1.2456522000E+00	0.0000000000E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

B1		2.4144207924E+00	-4.0300064259E-04	2.3545169169E+01	-2.3561555812E+01
F2	-8.0492977030E-01	9.2605290897E-06	1.0007117934E+02	-1.0014082550E+02	4.6981347896E-01
F3	-8.0493068030E-01	8.9469809423E-06	1.0007117924E+02	-1.0014082541E+02	4.6981521048E-01
F4	-8.0493057340E-01	8.9159308053E-06	1.0007117918E+02	-1.0014082535E+02	4.6981500512E-01

Total -3.7023160000E-04 -3.7587720175E-04 3.2375870693E+02 -3.2398403207E+02

Molecular charge $q(Mol)$ from the wfx file: 3.5760244881E-09

Molecular energy $E(Mol)$ from the wfx file: -3.2398400584E+02

Molecular virial ratio $(-V(Mol))/T(Mol)$ from the wfx file: 2.0006959663E+00

Full molecular virial ratio $((-V(Mol)+W(Mol))/T(Mol))$ from the wfx file: 2.0006959664E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

B1	17	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
F2	16	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00
F3	19	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00
F4	14	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00

Total 66

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 9.03505269072073E-23 -1.45711814530638E-12 0.00000000000000E+00

 Type = (3,-3) NACP B1

 Rho = 6.7028922258E+01 Rho at Nucleus = 6.7028922258E+01

 GradRho = -2.1814695289E-17 2.6617163335E-17 0.0000000000E+00

HessRho_EigVals = -6.6913295791E+04 -6.6912038800E+04 -6.6912038800E+04

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

DelSqRho = -2.0073737339E+05

Bond Ellipticity = NA

V = -5.0187518718E+04

G = 1.5876849701E+00

K = 5.0185931033E+04

L = 5.0184343348E+04

Vnuc = 5.0000001084E+08

Ven = -3.3514461856E+10

Vrep = 3.3514411668E+10

DelSqV = 1.0694843676E+09

DelSqVen = 1.0054338125E+27

DelSqVrep = -1.0054338125E+27

DelSqG = 5.0100733040E+07

DelSqK = -1.1195851007E+09

Stress_EigVals = -1.6729334173E+04 -1.6729334173E+04 -1.6728850373E+04

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

-DivStress = -2.2846143672E-14 5.0640685350E-04 0.0000000000E+00

CP# 2 Coords = 1.94774314346660E-24 2.49129803755327E+00 0.00000000000000E+00

Type = (3,-3) NACP F2

Rho = 4.2590383807E+02 Rho at Nucleus = 4.2590380697E+02

GradRho = 4.6731117441E-19 1.0621015178E-10 0.0000000000E+00

HessRho_EigVals = -1.5363373697E+06 -1.5363136676E+06 -1.5363002465E+06

HessRho_EigVec1 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

DelSqRho = -4.6089512838E+06

Bond Ellipticity = NA

V = -1.1525688733E+06

G = 1.6552615009E+02

K = 1.1524033471E+06

L = 1.1522378210E+06

Vnuc = 1.4145563320E+06

Ven = -6.0246497095E+08

Vrep = 6.0131240208E+08

DelSqV = 9.7376560004E+10

DelSqVen = 6.5196212183E+12

DelSqVrep = -6.4222446583E+12

DelSqG = 4.1575486767E+09

DelSqK = -1.0153410868E+11

Stress_EigVals = -3.8419382306E+05 -3.8419050424E+05 -3.8418454595E+05

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

-DivStress = -5.6993223834E-14 2.0180255498E+05 0.0000000000E+00

CP# 3 Coords = 2.15752738995921E+00 -1.24564901877657E+00 0.00000000000000E+00

Type = (3,-3) NACP F3

Rho = 4.2590383508E+02 Rho at Nucleus = 4.2590380398E+02

GradRho = -9.1066709729E-11 -8.5853990583E-11 0.0000000000E+00

HessRho_EigVals = -1.5363373562E+06 -1.5363136541E+06 -1.5363002330E+06

HessRho_EigVec1 = 8.6602540719E-01 -4.9999999410E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 4.9999999410E-01 8.6602540719E-01 0.0000000000E+00

DelSqRho = -4.6089512433E+06

Bond Ellipticity = NA

V = -1.1525688631E+06

G = 1.6552614962E+02

K = 1.1524033370E+06
L = 1.1522378108E+06
Vnuc = 1.4145562688E+06
Ven = -6.0246493984E+08
Vrep = 6.0131237097E+08
DelSqV = 9.7376559139E+10
DelSqVen = 6.5196208947E+12
DelSqVrep = -6.4222443356E+12
DelSqG = 4.1575486328E+09
DelSqK = -1.0153410777E+11
Stress_EigVals = -3.8419381968E+05 -3.8419050086E+05 -3.8418454257E+05
Stress_EigVec1 = 4.9999999358E-01 8.6602540749E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602540749E-01 -4.9999999358E-01 0.0000000000E+00
-DivStress = 1.7476614690E+05 -1.0090127856E+05 0.0000000000E+00

CP# 4 Coords = -2.15752738995921E+00 -1.24564901877657E+00 0.00000000000000E+00

Type = (3,-3) NACP F4

Rho = 4.2590383508E+02 Rho at Nucleus = 4.2590380398E+02

GradRho = 9.1066709729E-11 -8.5850881959E-11 0.0000000000E+00

HessRho_EigVals = -1.5363373562E+06 -1.5363136541E+06 -1.5363002330E+06

HessRho_EigVec1 = 8.6602540720E-01 4.9999999409E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = -4.9999999409E-01 8.6602540720E-01 0.0000000000E+00

DelSqRho = -4.6089512433E+06

Bond Ellipticity = NA

V = -1.1525688631E+06

G = 1.6552614962E+02

K = 1.1524033370E+06

L = 1.1522378108E+06

Vnuc = 1.4145562688E+06

Ven = -6.0246493984E+08

Vrep = 6.0131237097E+08
DelSqV = 9.7376559139E+10
DelSqVen = 6.5196208968E+12
DelSqVrep = -6.4222443376E+12
DelSqG = 4.1575486328E+09
DelSqK = -1.0153410777E+11
Stress_EigVals = -3.8419381968E+05 -3.8419050086E+05 -3.8418454257E+05
Stress_EigVec1 = -4.9999999358E-01 8.6602540749E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602540749E-01 4.9999999358E-01 0.0000000000E+00
-DivStress = -1.7476614690E+05 -1.0090127856E+05 0.0000000000E+00

CP# 5 Coords = -2.63853527021271E-18 8.45090683635961E-01 0.00000000000000E+00

Type = (3,-1) BCP F2 B1
Rho = 1.9815918085E-01
GradRho = 1.1186627464E-19 -1.1102230246E-16 0.0000000000E+00
HessRho_EigVals = -5.8241919030E-01 -5.5169852601E-01 2.3673756431E+00
HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00
DelSqRho = 1.2332579268E+00
Bond Ellipticity = 5.5683788958E-02
V = -5.6770647094E-01
G = 4.3801047632E-01
K = 1.2969599462E-01
L = -3.0831448170E-01
Vnuc = 1.7374916645E+01
Ven = -3.4429992498E+00
Vrep = 2.8752927789E+00
DelSqV = -1.0922819058E+01
DelSqVen = -2.1427753680E+01
DelSqVrep = 1.0504934622E+01

DelSqG = 1.7533892209E+01

DelSqK = -6.6110731509E+00

Stress_EigVals = -2.4738482883E-01 -2.2958513617E-01 -9.0736505937E-02

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

-DivStress = 2.3644266395E-18 -7.8519264282E-01 0.0000000000E+00

BPL = 2.4912980376E+00 = 1.6462073539E+00 + 8.4509068364E-01

GBL_I = 2.4912980376E+00

GBL_II = 2.4913044000E+00

GBL_III = 2.4912980376E+00 = 1.6462073539E+00 + 8.4509068364E-01

GBL_IV = 2.4913044000E+00 = 1.6462137164E+00 + 8.4509068364E-01

CP# 6 Coords = 7.31869997765684E-01 -4.22545349373443E-01 0.00000000000000E+00

Type = (3,-1) BCP F3 B1

Rho = 1.9815918537E-01

GradRho = -7.3725747729E-18 0.0000000000E+00 0.0000000000E+00

HessRho_EigVals = -5.8241920560E-01 -5.5169854031E-01 2.3673756374E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 5.0000000340E-01 8.6602540182E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540182E-01 -5.0000000340E-01 0.0000000000E+00

DelSqRho = 1.2332578915E+00

Bond Ellipticity = 5.5683789330E-02

V = -5.6770646675E-01

G = 4.3801046982E-01

K = 1.2969599694E-01

L = -3.0831447288E-01

Vnuc = 1.7374916636E+01

Ven = -3.4429993265E+00

Vrep = 2.8752928598E+00

DelSqV = -1.0922819015E+01

DelSqVen = -2.1427753056E+01

DelSqVrep = 1.0504934041E+01

DelSqG = 1.7533892066E+01

DelSqK = -6.6110730507E+00

Stress_EigVals = -2.4738483005E-01 -2.2958513968E-01 -9.0736497027E-02

Stress_EigVec1 = 4.9999999192E-01 8.6602540845E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540845E-01 -4.9999999192E-01 0.0000000000E+00

-DivStress = -6.7999679933E-01 3.9259633459E-01 0.0000000000E+00

BPL = 2.4912980385E+00 = 1.6462073534E+00 + 8.4509068502E-01

GBL_I = 2.4912980385E+00

GBL_II = 2.4913044009E+00

GBL_III = 2.4912980385E+00 = 1.6462073534E+00 + 8.4509068502E-01

GBL_IV = 2.4913044009E+00 = 1.6462137159E+00 + 8.4509068502E-01

CP# 7 Coords = -7.31869997765684E-01 -4.22545349373443E-01 0.00000000000000E+00

Type = (3,-1) BCP B1 F4

Rho = 1.9815918537E-01

GradRho = -3.9031278209E-17 0.0000000000E+00 0.0000000000E+00

HessRho_EigVals = -5.8241920560E-01 -5.5169854031E-01 2.3673756374E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -5.0000000340E-01 8.6602540182E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540182E-01 5.0000000340E-01 0.0000000000E+00

DelSqRho = 1.2332578915E+00

Bond Ellipticity = 5.5683789330E-02

V = -5.6770646675E-01

G = 4.3801046982E-01

K = 1.2969599694E-01

L = -3.0831447288E-01

Vnuc = 1.7374916636E+01

Ven = -3.4429993265E+00

Vrep = 2.8752928598E+00

DelSqV = -1.0922819015E+01

$\text{DelSqVen} = -2.1427753056\text{E}+01$
 $\text{DelSqVrep} = 1.0504934041\text{E}+01$
 $\text{DelSqG} = 1.7533892066\text{E}+01$
 $\text{DelSqK} = -6.6110730507\text{E}+00$
 $\text{Stress\_EigVals} = -2.4738483005\text{E}-01 \ -2.2958513968\text{E}-01 \ -9.0736497027\text{E}-02$
 $\text{Stress\_EigVec1} = -4.9999999192\text{E}-01 \ 8.6602540845\text{E}-01 \ 0.0000000000\text{E}+00$
 $\text{Stress\_EigVec2} = 0.0000000000\text{E}+00 \ 0.0000000000\text{E}+00 \ 1.0000000000\text{E}+00$
 $\text{Stress\_EigVec3} = 8.6602540845\text{E}-01 \ 4.9999999192\text{E}-01 \ 0.0000000000\text{E}+00$
 $-\text{DivStress} = 6.7999679933\text{E}-01 \ 3.9259633459\text{E}-01 \ 0.0000000000\text{E}+00$
 $\text{BPL} = 2.4912980385\text{E}+00 = 8.4509068502\text{E}-01 + 1.6462073534\text{E}+00$
 $\text{GBL\_I} = 2.4912980385\text{E}+00$
 $\text{GBL\_II} = 2.4913044009\text{E}+00$
 $\text{GBL\_III} = 2.4912980385\text{E}+00 = 8.4509068502\text{E}-01 + 1.6462073534\text{E}+00$
 $\text{GBL\_IV} = 2.4913044009\text{E}+00 = 8.4509068502\text{E}-01 + 1.6462137159\text{E}+00$

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

 BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

F3	B1	F2	120.00000067	119.99999999	119.99999999	120.00000054	120.00000054
F4	B1	F2	120.00000067	119.99999999	119.99999999	120.00000054	120.00000054
F4	B1	F3	119.99999867	120.00000002	120.00000002	119.99999893	119.99999893

Total time for electron density critical point search, analysis and connectivity = 2 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus
the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
B1	-2.3545169169E+01	2.3545169169E+01	-7.8481473338E+01	-5.0700912820E+01		
F2	-1.0007117934E+02	1.0007117934E+02	-3.0497267640E+02	-2.4381883931E+02		
F3	-1.0007117924E+02	1.0007117924E+02	-3.0497268669E+02	-2.4381884177E+02		
F4	-1.0007117918E+02	1.0007117918E+02	-3.0497268552E+02	-2.4381884148E+02		

Total -3.2375870693E+02 3.2375870693E+02 -9.9339952195E+02 -7.8215743538E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$$V_{nn}(A) = \text{Contribution of Atom A to Nuclear Repulsion Energy of Molecule}$$

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$$V_{eeC}(A) = \text{Coulomb Part of } V_{ee}(A)$$

$$V_{eeX}(A) = \text{Exchange-Correlation Part of } V_{ee}(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
B1	-2.3545169155E+01	-2.3545169169E+01	1.3649638552E-08			
F2	-1.0007117933E+02	-1.0007117934E+02	8.8629736919E-09			
F3	-1.0007117923E+02	-1.0007117924E+02	8.8630873756E-09			
F4	-1.0007117917E+02	-1.0007117918E+02	8.8630643539E-09			

Total -3.2375870689E+02 -3.2375870693E+02 4.0238763974E-08

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$$T(A) = \text{Electronic Kinetic Energy of Atom A (Hamiltonian Form)}$$

$V_{ne}(A, \text{Mol})/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$V_{ne}(A, Mol)/2$	$V_{en}(A, Mol)/2$	$V_{ee}(A)$	$V_{nn}(A, Mol)/2$
$V_{eeC}(A)$	$V_{eeX}(A)$					
B1			2.3545169169E+01	-5.5216358905E+01	-3.9240736669E+01	
2.7094240264E+01						
F2			1.0007117934E+02	-1.4716037824E+02	-1.5248633820E+02	
2.7802853717E+01						
F3			1.0007117924E+02	-1.4716037787E+02	-1.5248634334E+02	
2.7802853711E+01						
F4			1.0007117918E+02	-1.4716037787E+02	-1.5248634276E+02	
2.7802853711E+01						
Total			3.2375870693E+02	-4.9669749288E+02	-4.9669976097E+02	
1.1050280140E+02						

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + V_{ne}(A, A) + V_{ee}(A, A)$$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{ne}(A, A) = (1/2)[V_{ne}(A, A) + V_{en}(A, A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A, A)$ = Two-electron Interaction Energy of Atom A With Itself

$V_{eeC}(A, A)$ = Coulomb Part of $V_{ee}(A, A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$
B1	2.3545169169E+01	-5.0700912820E+01				
F2	1.0007117934E+02	-2.4381883931E+02				
F3	1.0007117924E+02	-2.4381884177E+02				
F4	1.0007117918E+02	-2.4381884148E+02				
Total	3.2375870693E+02	-7.8215743538E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$	$VeeX(A,A')$

B1	-2.9865902495E+01 -1.3890280259E+01	2.7094240264E+01
F2	-2.5250958582E+01 -3.0576918543E+01	2.7802853717E+01
F3	-2.5250956984E+01 -3.0576922460E+01	2.7802853711E+01
F4	-2.5250957126E+01 -3.0576922018E+01	2.7802853711E+01

Total	-1.0561877519E+02 -1.0562104328E+02	1.1050280140E+02

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other

Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$

B1	2.5855792079E+00	2.0566066068E+00	7.9541427332E+01	5.2897260115E-01	2.0458572668E+01
F2	9.8049297705E+00	9.4566367105E+00	9.6447776087E+01	3.4829305999E-01	3.5522239133E+00
F3	9.8049306803E+00	9.4566376486E+00	9.6447776705E+01	3.4829303173E-01	3.5522232954E+00
F4	9.8049305731E+00	9.4566375272E+00	9.6447776521E+01	3.4829304597E-01	3.5522234795E+00

Total	3.2000370232E+01	3.0426518493E+01	9.5081770219E+01	1.5738517388E+00
	4.9182297812E+00			

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$DI(A,A')/2$	$DI\_Bond(A,A')/2$	$DI\_NonBond(A,A')/2$
B1	2.5855792079E+00	2.0566066068E+00	5.2897260115E-01	5.2906101780E-01	-
	8.8416656754E-05				
F2	9.8049297705E+00	9.4566367105E+00	3.4829305999E-01	1.7636618398E-01	
	1.7192687601E-01				
F3	9.8049306803E+00	9.4566376486E+00	3.4829303173E-01	1.7623557239E-01	
	1.7205745934E-01				
F4	9.8049305731E+00	9.4566375272E+00	3.4829304597E-01	1.7645926143E-01	
	1.7183378453E-01				
Total	3.2000370232E+01	3.0426518493E+01	1.5738517388E+00	1.0581220356E+00	
	5.1572970323E-01				

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A')$ = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$D2(A,A)$	$D2(A,A')$	$D2(A,Mol)$

B1	2.3143066168E+00	3.7762144733E+01	4.0076451349E+01
F2	4.3340005547E+01	1.0863619074E+02	1.5197619628E+02
F3	4.3340013999E+01	1.0863619639E+02	1.5197621039E+02
F4	4.3340013009E+01	1.0863619572E+02	1.5197620873E+02

Total	1.3233433917E+02	3.6367072758E+02	4.9600506675E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A)$ = Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A)$ = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	
B1	F2	2.5175056366E+01	3.5273236796E-01	6.8211479827E+00	1.7987500993E+00	(Bonded)
B1	F3	2.5175189330E+01	3.5247114477E-01	6.8160964417E+00	1.7974178312E+00	(Bonded)
F2	F3	9.6050416214E+01	1.7248102236E-01	8.7956276278E-01	8.7956268117E-01	
B1	F4	2.5174965363E+01	3.5291852287E-01	6.8247478512E+00	1.7996992443E+00	(Bonded)
F2	F4	9.6050414999E+01	1.7248135074E-01	8.7956443738E-01	8.7956436538E-01	
F3	F4	9.6050424008E+01	1.7248117459E-01	8.7956345747E-01	8.7956346709E-01	

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms
A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms
A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms
A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
B1	F2	4.5630952683E+01	3.7013151221E+01	3.0961500083E+01
B1	F3	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01
B1	F4	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01
B1	Total	1.3689285811E+02	1.1103945372E+02	9.2884500295E+01
F2	B1	4.5630952683E+01	3.7013151221E+01	3.0961500083E+01
F2	Total	4.5630952683E+01	3.7013151221E+01	3.0961500083E+01

F3	B1	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01

F3	Total	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01
F4	B1	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01

F4	Total	4.5630952714E+01	3.7013151248E+01	3.0961500106E+01

Total	Total	2.7378571622E+02	2.2207890743E+02	1.8576900059E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta^2 \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta^2 \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta^2 \rho\_IAS(A B)$ $V\_IAS(A B)$

B1	F2	9.2834152298E-01	1.1953838998E+00	3.9766163798E-01	-7.9772226187E-01	3.1908890475E+00 -1.5930455378E+00
B1	F3	9.2834153871E-01	1.1953838931E+00	3.9766164246E-01	-7.9772225068E-01	3.1908890027E+00 -1.5930455356E+00
B1	F4	9.2834153871E-01	1.1953838931E+00	3.9766164246E-01	-7.9772225068E-01	3.1908890027E+00 -1.5930455356E+00

B1 Total 2.7850246004E+00 3.5861516860E+00 1.1929849229E+00 -2.3931667632E+00
9.5726670529E+00 -4.7791366090E+00

F2 B1 9.2834152298E-01 1.1953838998E+00 3.9766163798E-01 -7.9772226187E-01
3.1908890475E+00 -1.5930455378E+00

F2 Total 9.2834152298E-01 1.1953838998E+00 3.9766163798E-01 -7.9772226187E-01
3.1908890475E+00 -1.5930455378E+00

F3 B1 9.2834153871E-01 1.1953838931E+00 3.9766164246E-01 -7.9772225068E-01
3.1908890027E+00 -1.5930455356E+00

F3 Total 9.2834153871E-01 1.1953838931E+00 3.9766164246E-01 -7.9772225068E-01
3.1908890027E+00 -1.5930455356E+00

F4 B1 9.2834153871E-01 1.1953838931E+00 3.9766164246E-01 -7.9772225068E-01
3.1908890027E+00 -1.5930455356E+00

F4 Total 9.2834153871E-01 1.1953838931E+00 3.9766164246E-01 -7.9772225068E-01
3.1908890027E+00 -1.5930455356E+00

Total Total 5.5700492008E+00 7.1723033720E+00 2.3859698458E+00 -4.7863335265E+00
1.9145334106E+01 -9.5582732180E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

B1	2.3994115233E+00						

F2	1.0053143505E+02						

F3	1.0076238857E+02						

F4	1.0066066320E+02						

Total	3.0435389834E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

B1	2.4756175168E+00	1.9159956023E-01	8.9016714274E-02	2.5799044756E-02	7.7394653629E-02
	1.0480726427E-02	1.9780546560E-04			

F2	8.7897805794E+01	4.8431269533E-01	8.5416387207E-02	-1.3728536551E-02	5.5099520512E-03
	1.6628346796E-02	4.7552498325E-04			

F3	8.7915168742E+01	4.7784273074E-01	8.4616466782E-02	-1.3731523180E-02	5.4352705862E-03
	1.6529652514E-02	4.7037122373E-04			

F4	8.7556784818E+01	4.6289982725E-01	8.4663934930E-02	-1.3731874142E-02	5.2868527347E-03
	1.6404131092E-02	4.6082383864E-04			

Total	2.6584537687E+02	1.6166548136E+00	8.9016714274E-02	-1.3731874142E-02	
	6.0811846066E-03	5.1420471108E-04			

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
	ESP-_Int_IDS(A)				

B1	1.9159956023E-01	1.5318472275E-02	2.4756175168E+00	1.9159956023E-01	
	0.0000000000E+00	NULL			

F2	1.3644885125E+00	4.4466142357E-02	3.9614783658E+01	9.2440060392E-01	
	4.8283022136E+01	-4.4008790859E-01			

F3	1.3581320984E+00	4.3949970045E-02	3.9515870708E+01	9.1798741458E-01	
	4.8399298033E+01	-4.4014468384E-01			

F4	1.3429887490E+00	4.2795536896E-02	3.9420332934E+01	9.0294428814E-01	
	4.8136451884E+01	-4.4004446088E-01			

Total	4.2572089201E+00	1.4653012157E-01	1.2102660482E+02	2.9369318669E+00	
	1.4481877205E+02	-1.3202770533E+00			

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
	ESP+*ESP+_Int_IDS(A)			

B1	2.5799044756E-02	7.7394653629E-02	1.0480726427E-02	1.9780546560E-04
	1.5318472275E-02			
F2	1.5145036411E-05	2.3334738160E-02	1.7446777163E-02	4.5714945760E-04
	3.9680522909E-02			
F3	9.3345835504E-05	2.3230853784E-02	1.7307512092E-02	4.5143146600E-04
	3.9164338848E-02			
F4	1.1161204009E-05	2.2905546984E-02	1.7089771464E-02	4.3955554229E-04
	3.8009858636E-02			

Total	1.1161204009E-05	2.4266828532E-02	5.0322134325E-04	1.3217319267E-01

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

B1	NULL	NULL	NULL	NULL	NULL
F2	-9.4877884005E-06	-9.1147548169E-03	3.4389428668E-03	1.6037232728E-05	4.7856194475E-03
F3	-2.2982373734E-05	-9.0940303211E-03	3.4540798356E-03	1.6176724214E-05	4.7856311969E-03
F4	-2.8348446515E-05	-9.1416056577E-03	3.4178941035E-03	1.5850053290E-05	4.7856782608E-03

Total	-9.4877884005E-06	-9.1167535437E-03	1.6022014052E-05	1.4356928905E-02	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

B1	2.6495717763E+00				
F2	7.8459306075E+01				
F3	7.8292827386E+01				

F4 7.8320126515E+01

Total 2.3772183175E+02

Atomic Surface Area and Volume Data:

$$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$$

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

N(Vol(A)) = Average Number of Electrons in Vol(A)

N(Vol(A))/Vol(A) = Average Electron Density in Vol(A)

%N(Vol(A)) = 100 * N(Vol(A)) / N(A)
= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1 9.9981146027E+01	1.3929226963E+02	1.2944093572E+01	2.5850917232E+00	1.9971207013E-01	
F2 9.9823446262E+01	1.4616238773E+02	1.4745609544E+02	9.7876188003E+00	6.6376495128E-02	
F3 9.9823620159E+01	1.4639334128E+02	1.4749969097E+02	9.7876367592E+00	6.6356998411E-02	
F4 9.9823341233E+01	1.4629161591E+02	1.4742965815E+02	9.7876093039E+00	6.6388333438E-02	
Total 9.9836209253E+01	5.7813961456E+02	4.5532953813E+02	3.1947956587E+01	7.0164471907E-02	

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	1.1351507124E+02	1.2021761185E+01	2.5844868150E+00	2.1498404229E-01
	9.9957750565E+01			
F2	1.2491095702E+02	1.1714462302E+02	9.7680236520E+00	8.3384310782E-02
	9.9623596301E+01			
F3	1.2492831999E+02	1.1719822975E+02	9.7680773597E+00	8.3346628875E-02
	9.9624134817E+01			
F4	1.2456993607E+02	1.1721347215E+02	9.7680939161E+00	8.3335931754E-02
	9.9624304762E+01			

Total	4.8792428431E+02	3.6357808611E+02	3.1888681743E+01	8.7707931147E-02
	9.9650977510E+01			

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	9.5534072072E+01	1.1291463227E+01	2.5834284907E+00	2.2879483719E-01
	9.9916818758E+01			
F2	1.0942080616E+02	9.6768155535E+01	9.7389468547E+00	1.0064206351E-01
	9.9327043465E+01			
F3	1.0925432749E+02	9.6793313499E+01	9.7389998863E+00	1.0061645308E-01
	9.9327575113E+01			
F4	1.0928162662E+02	9.6825002817E+01	9.7390615655E+00	1.0058415990E-01
	9.9328205260E+01			

Total	4.2349083234E+02	3.0167793508E+02	3.1800436797E+01	1.0541187505E-01
	9.9375215245E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

```

-----
B1    F2    8.0482398984E-01
B1    F3    8.0482489984E-01
B1    F4    8.0482479294E-01
B1                                2.4144736826E+00 2.4144207924E+00
F2    B1    -8.0487688007E-01
F2                                -8.0487688007E-01 -8.0492977030E-01
F3    B1    -8.0487779007E-01
F3                                -8.0487779007E-01 -8.0493068030E-01
F4    B1    -8.0487768317E-01
F4                                -8.0487768317E-01 -8.0493057340E-01

```

Atomic Dipole Moments:

```

-----
Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A
Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A
Mu(A) = Mu_Intra(A) + Mu_Bond(A)
      = Total Dipole Moment Contribution of Atom A

```

```

Atom A  Mu_Intra_X(A)  Mu_Bond_X(A)  Mu_X(A)
-----
B1      9.0313086782E-04 -7.8236903400E-08 9.0305263092E-04
F2      3.8396135165E-07 -2.1236960362E-18 3.8396135165E-07
F3      4.0687184193E-01 -1.1474844061E+00 -7.4061256421E-01
F4     -4.0687149607E-01 1.1474842537E+00 7.4061275766E-01
-----
Total   9.0386068917E-04 -2.3064026888E-07 9.0363004890E-04

```

```

Atom A  Mu_Intra_Y(A)  Mu_Bond_Y(A)  Mu_Y(A)
-----
B1     -1.1630174481E-04 7.3602407302E-07 -1.1556572074E-04
F2      4.6981347895E-01 -1.3249993600E+00 -8.5518588101E-01

```

F3 -2.3490771858E-01 6.6250042292E-01 4.2759270434E-01

F4 -2.3490790689E-01 6.6250033493E-01 4.2759242804E-01

Total -1.1844826481E-04 2.1339259862E-06 -1.1631433882E-04

Atom A Mu_Intra_Z(A) Mu_Bond_Z(A) Mu_Z(A)

B1 -3.1722404903E-04 0.0000000000E+00 -3.1722404903E-04

F2 3.0990196150E-06 0.0000000000E+00 3.0990196150E-06

F3 -4.2138208598E-07 0.0000000000E+00 -4.2138208598E-07

F4 1.4582086865E-06 0.0000000000E+00 1.4582086865E-06

Total -3.1308820281E-04 0.0000000000E+00 -3.1308820281E-04

Atom A |Mu_Intra(A)| |Mu_Bond(A)| |Mu(A)|

B1 9.6426270152E-04 7.4017055408E-07 9.6410092174E-04

F2 4.6981347896E-01 1.3249993600E+00 8.5518588101E-01

F3 4.6981521048E-01 1.3250008576E+00 8.5518564714E-01

F4 4.6981500512E-01 1.3250006816E+00 8.5518567653E-01

Total 9.6385598489E-04 2.1463538964E-06 9.6337973481E-04

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A Atom B Mu_Bond_X(A|B) Mu_Bond_X(A)

B1 F2 2.1235564835E-18

B1	F3	-5.8902719765E-01
B1	F4	5.8902711941E-01
B1		-7.8236903400E-08
F2	B1	-2.1236960362E-18
F2		-2.1236960362E-18
F3	B1	-1.1474844061E+00
F3		-1.1474844061E+00
F4	B1	1.1474842537E+00
F4		1.1474842537E+00

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

B1	F2	-6.8014925578E-01
B1	F3	3.4007501849E-01
B1	F4	3.4007497332E-01
B1		7.3602407302E-07
F2	B1	-1.3249993600E+00
F2		-1.3249993600E+00
F3	B1	6.6250042292E-01
F3		6.6250042292E-01
F4	B1	6.6250033493E-01
F4		6.6250033493E-01

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	F2	0.0000000000E+00
B1	F3	0.0000000000E+00
B1	F4	0.0000000000E+00
B1		0.0000000000E+00
F2	B1	0.0000000000E+00
F2		0.0000000000E+00
F3	B1	0.0000000000E+00

```

F3          0.0000000000E+00
F4   B1     0.0000000000E+00
F4          0.0000000000E+00

```

```

Atom A  Atom B  |Mu_Bond(A|B)|  |Mu_Bond(A)|
-----

```

```

B1   F2   6.8014925578E-01
B1   F3   6.8015002593E-01
B1   F4   6.8014993559E-01
B1          7.4017055408E-07
F2   B1   1.3249993600E+00
F2          1.3249993600E+00
F3   B1   1.3250008576E+00
F3          1.3250008576E+00
F4   B1   1.3250006816E+00
F4          1.3250006816E+00

```

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$

$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$

$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$

$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

```

Atom A  Q_XX(A)  Q_XY(A)  Q_XZ(A)  Q_YY(A)  Q_YZ(A)  Q_ZZ(A)
-----

```

```

B1      2.3030360886E-01  2.9921949248E-03 -4.2294518298E-04  2.3124799608E-01  2.2537390092E-
03 -4.6155160495E-01

```

F2 2.0322959979E-01 -2.2012474433E-06 -1.7602847938E-05 1.9751881034E-01 -1.8620439274E-05 -4.0074841014E-01

F3 1.9894460943E-01 2.4765553012E-03 -7.3482677661E-06 2.0180227128E-01 -1.7718123467E-05 -4.0074688071E-01

F4 1.9894632282E-01 -2.4771774914E-03 1.5515065774E-05 2.0180085652E-01 -1.0016125242E-05 -4.0074717934E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
B1	1	-4.6155920708E-01	6.2539082588E-04	-3.2557368122E-03	9.9999450452E-01
B1	2	2.2775120233E-01	7.6062049705E-01	-6.4919161656E-01	-2.5892963545E-03
B1	3	2.3380800475E-01	6.4919647900E-01	7.6061793640E-01	2.0703816711E-03
F2	1	-4.0074841123E-01	2.9144962419E-05	3.1124057512E-05	9.999999909E-01
F2	2	1.9751881008E-01	3.8535812352E-04	9.9999992526E-01	-3.1135286462E-05
F2	3	2.0322960115E-01	9.9999992532E-01	-3.8535903061E-04	-2.9132966333E-05
F3	1	-4.0074688132E-01	1.2132183926E-05	2.9355410019E-05	9.999999950E-01
F3	2	1.9751426497E-01	8.6594899973E-01	-5.0013231234E-01	4.1757365592E-06
F3	3	2.0323261635E-01	5.0013231221E-01	8.6594899924E-01	-3.1487985143E-05
F4	1	-4.0074717990E-01	-2.5803432061E-05	1.6516866626E-05	9.999999953E-01
F4	2	1.9751465660E-01	8.6580324019E-01	5.0038460115E-01	1.4075909375E-05
F4	3	2.0323252331E-01	-5.0038460069E-01	8.6580324015E-01	-2.7211996703E-05

Atomic Radial Moments:

$R-2(A) = \langle \rho / (r^2) \rangle(A)$

$R-1(A) = \langle \rho / r \rangle(A)$

$$R0(A) = \langle Rho \rangle(A) = N(A)$$

$$R+1(A) = \langle Rho * r \rangle(A)$$

$$R+2(A) = \langle Rho * r^2 \rangle(A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.1694433660E+01	1.0140182564E+01	2.5855792076E+00	1.2460979643E+00	1.0207286711E+00
F2	3.3044483115E+02	2.7090982146E+01	9.8049297703E+00	9.0807110966E+00	1.2603446729E+01
F3	3.3044482957E+02	2.7090982419E+01	9.8049306803E+00	9.0807133843E+00	1.2603452186E+01
F4	3.3044482956E+02	2.7090982387E+01	9.8049305734E+00	9.0807130747E+00	1.2603451349E+01

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(dRho/dx) + y^*(dRho/dy) + z^*(dRho/dz)$$

$$GR-2(A) = \langle \text{Dot} / (r^3) \rangle(A)$$

$$GR-1(A) = \langle \text{Dot} / r^2 \rangle(A)$$

$$GR0(A) = \langle \text{Dot} \rangle(A)$$

$$GR+1(A) = \langle \text{Dot} * r \rangle(A)$$

$$GR+2(A) = \langle \text{Dot} * r^2 \rangle(A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
B1	-9.0394536694E+01	-1.8902952017E+01	-6.2193516177E+00	-3.1414780909E+00	-2.6725172889E+00
F2	-3.3008199282E+02	-5.3412798921E+01	-2.7735968407E+01	-3.2536421936E+01	-5.4153393019E+01
F3	-3.3008199150E+02	-5.3412799720E+01	-2.7735970743E+01	-3.2536427415E+01	-5.4153404246E+01
F4	-3.3008199138E+02	-5.3412799416E+01	-2.7735969984E+01	-3.2536425536E+01	-5.4153399645E+01

Atomic Electronic Spin Populations:

$$N_{\alpha}(A) = \text{Average number of Alpha electrons in Atom A}$$
$$N_{\beta}(A) = \text{Average number of Beta electrons in Atom A}$$
$$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$$
$$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

B1	1.2927896038E+00	1.2927896038E+00	2.5855792076E+00	0.0000000000E+00
F2	4.9024648852E+00	4.9024648852E+00	9.8049297703E+00	0.0000000000E+00
F3	4.9024653401E+00	4.9024653401E+00	9.8049306803E+00	0.0000000000E+00
F4	4.9024652867E+00	4.9024652867E+00	9.8049305734E+00	0.0000000000E+00

Total	1.6000185116E+01	1.6000185116E+01	3.2000370232E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional

of the corresponding DFT model and atomic contributions $VeeX(A)$ to $VeeX$ are explicitly calculated and unambiguous. However, since $VeeX$ is at least partly just a one-electron functional for DFT models, the partitioning of $VeeX(A)$ into interatomic ($VeeX(A,B)$ and $VeeX(A,A')$) and intraatomic ($VeeX(A,A)$) contributions is ambiguous. Currently, interatomic contributions $VeeX(A,B)$ and $VeeX(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$. For wavefunctions of non-supported DFT models, $VeeX$ is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E\_IQA(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

BH3

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\bh3\neu\bh3plane.wfx

Sum File: D:\calc\ellipticity\bh3\neu\bh3plane.sum

SumViz File: D:\calc\ellipticity\bh3\neu\bh3plane.sumviz

Wfx Title: bh3_plane_mp2

Total memory allocated for AIMSum = 0.328 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	8.0000000044
Number of Alpha electrons (from MO Occs)	=	4.0000000022
Number of Beta electrons (from MO Occs)	=	4.0000000022
Number of electron pairs ($N*(N-1)/2$)	=	28.0000000330
Number of electron pairs (from Muller 2EDM)	=	27.9999997702
Number of electron pairs (from Muller 2EDM, no SOSI)	=	28.0715931155

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
B1	5.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
H2	1.0	0.0000000000E+00	2.2498469000E+00	0.0000000000E+00
H3	1.0	1.9484245700E+00	-1.1249234500E+00	0.0000000000E+00
H4	1.0	-1.9484245700E+00	-1.1249234500E+00	0.0000000000E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

B1 1.9856166069E+00 5.2398712511E-05 2.3882665884E+01 -2.3911670827E+01 1.0297249867E-04

H2 -6.6184595150E-01 6.7823983479E-06 8.6003533956E-01 -8.6107983248E-01 3.4817475575E-01

H3 -6.6184523750E-01 8.0708065804E-06 8.6003564561E-01 -8.6108013890E-01 3.4817336706E-01

H4 -6.6184543430E-01 8.3485032214E-06 8.6003615424E-01 -8.6108064815E-01 3.4817352238E-01

Total 7.9983600000E-05 7.5600420661E-05 2.6462773023E+01 -2.6494911447E+01

Molecular charge q(Mol) from the wfx file: -4.3943122587E-09

Molecular energy E(Mol) from the wfx file: -2.6494886934E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0012144767E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0012144776E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	
B1	15	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

H3	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 36

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -1.11802520551933E-22 2.70578448080495E-14 0.00000000000000E+00

Type = (3,-3) NACP B1

Rho = 6.7255818610E+01 Rho at Nucleus = 6.7255818610E+01

GradRho = 2.0337888807E-17 7.6032768803E-18 0.0000000000E+00

HessRho_EigVals = -6.7148737761E+04 -6.7145933500E+04 -6.7145933500E+04

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

DelSqRho = -2.0144060476E+05

Bond Ellipticity = NA

V = -5.0363202120E+04

G = 1.5254650137E+00

K = 5.0361676655E+04

L = 5.0360151190E+04

Vnuc = 5.0000000133E+08

Ven = -3.3627909395E+10

Vrep = 3.3627859032E+10

DelSqV = 1.0732188901E+09

DelSqVen = 1.0088372791E+27

DelSqVrep = -1.0088372791E+27

DelSqG = 5.0282313860E+07

DelSqK = -1.1235012040E+09

Stress_EigVals = -1.6788005574E+04 -1.6788005574E+04 -1.6787190973E+04

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

-DivStress = 3.7614647429E-14 -8.5911908657E-06 0.0000000000E+00

CP# 2 Coords = -1.70089136208909E-20 2.22875651895114E+00 0.00000000000000E+00

Type = (3,-3) NACP H2

Rho = 4.1675451712E-01 Rho at Nucleus = 4.1495478155E-01

GradRho = -1.7179057017E-19 -4.6430300341E-11 0.0000000000E+00

HessRho_EigVals = -8.3305113039E+00 -8.3294877939E+00 -7.9614291476E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

DelSqRho = -2.4621428245E+01

Bond Ellipticity = NA

V = -6.1642634090E+00

G = 4.4531738331E-03

K = 6.1598102352E+00

L = 6.1553570614E+00

Vnuc = 5.0174033783E+01

Ven = -2.0910255221E+01

Vrep = 1.4745991812E+01

DelSqV = 1.6078506491E+03

DelSqVen = 1.2353563728E+03

DelSqVrep = 3.7249427638E+02

DelSqG = 1.2214366654E+02

DelSqK = -1.7299943157E+03

Stress_EigVals = -2.0863549750E+00 -2.0842516464E+00 -1.9936567877E+00

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

-DivStress = 8.7204657327E-18 1.0870266956E+01 0.0000000000E+00

CP# 3 Coords = 1.93015976480119E+00 -1.11437826002413E+00 0.00000000000000E+00

Type = (3,-3) NACP H3

Rho = 4.1675453236E-01 Rho at Nucleus = 4.1495479680E-01

GradRho = -2.7724667697E-15 1.4859623562E-15 0.0000000000E+00

HessRho_EigVals = -8.3305118084E+00 -8.3294883010E+00 -7.9614296497E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 4.9999999365E-01 8.6602540745E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540745E-01 -4.9999999365E-01 0.0000000000E+00

DelSqRho = -2.4621429759E+01

Bond Ellipticity = NA

V = -6.1642637866E+00

G = 4.4531733927E-03

K = 6.1598106132E+00

L = 6.1553574398E+00

Vnuc = 5.0174035498E+01

Ven = -2.0910256701E+01

Vrep = 1.4745992914E+01

DelSqV = 1.6078507531E+03

DelSqVen = 1.2353564908E+03

DelSqVrep = 3.7249426238E+02

DelSqG = 1.2214367693E+02

DelSqK = -1.7299944301E+03

Stress_EigVals = -2.0863551011E+00 -2.0842517725E+00 -1.9936569129E+00

Stress_EigVec1 = 4.9999999661E-01 8.6602540574E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540574E-01 -4.9999999661E-01 0.0000000000E+00

-DivStress = 9.4139276355E+00 -5.4351335454E+00 0.0000000000E+00

CP# 4 Coords = -1.93015976480119E+00 -1.11437826002413E+00 0.00000000000000E+00

Type = (3,-3) NACP H4

Rho = 4.1675453236E-01 Rho at Nucleus = 4.1495479680E-01

GradRho = 2.7785383017E-15 1.4824929090E-15 0.0000000000E+00

HessRho_EigVals = -8.3305118084E+00 -8.3294883010E+00 -7.9614296497E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -4.9999999365E-01 8.6602540745E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540745E-01 4.9999999365E-01 0.0000000000E+00

DelSqRho = -2.4621429759E+01

Bond Ellipticity = NA

V = -6.1642637866E+00

G = 4.4531733927E-03

K = 6.1598106132E+00

L = 6.1553574398E+00

Vnuc = 5.0174035498E+01

Ven = -2.0910256701E+01

Vrep = 1.4745992914E+01

DelSqV = 1.6078507531E+03

DelSqVen = 1.2353564908E+03

DelSqVrep = 3.7249426238E+02

DelSqG = 1.2214367693E+02

DelSqK = -1.7299944301E+03

Stress_EigVals = -2.0863551011E+00 -2.0842517725E+00 -1.9936569129E+00

Stress_EigVec1 = -4.9999999661E-01 8.6602540574E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540574E-01 4.9999999661E-01 0.0000000000E+00

-DivStress = -9.4139276355E+00 -5.4351335454E+00 0.0000000000E+00

CP# 5 Coords = -2.39885562184847E-20 9.73771734822802E-01 0.00000000000000E+00

Type = (3,-1) BCP H2 B1

Rho = 1.8070317313E-01

GradRho = -1.1758239781E-18 3.1859389732E-17 0.0000000000E+00

HessRho_EigVals = -4.4738509017E-01 -3.2757906921E-01 5.2203643741E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

DelSqRho = -2.5292772197E-01

Bond Ellipticity = 3.6573161173E-01

V = -3.2675773554E-01

G = 1.3176290253E-01

K = 1.9499483302E-01

L = 6.3231930492E-02

Vnuc = 6.6167193085E+00

Ven = -1.1956621747E+00

Vrep = 8.6890443919E-01

DelSqV = -3.7972515739E+00

DelSqVen = 1.6735517416E+00

DelSqVrep = -5.4708033155E+00

DelSqG = 6.1431214123E+00

DelSqK = -2.3458698384E+00

Stress_EigVals = -1.4785587069E-01 -1.1305528119E-01 -6.5846583666E-02

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

-DivStress = 6.0348745000E-19 -5.0102446953E-01 0.0000000000E+00

BPL = 2.2287565193E+00 = 1.2549847845E+00 + 9.7377173482E-01

GBL_I = 2.2287565193E+00

GBL_II = 2.2498469000E+00

GBL_III = 2.2287565193E+00 = 1.2549847845E+00 + 9.7377173482E-01

GBL_IV = 2.2498469000E+00 = 1.2760751652E+00 + 9.7377173482E-01

CP# 6 Coords = 8.43311054879503E-01 -4.86885860801952E-01 0.00000000000000E+00

Type = (3,-1) BCP H3 B1

Rho = 1.8070317161E-01

GradRho = 3.1649892273E-17 1.0819165270E-16 0.0000000000E+00

HessRho_EigVals = -4.4738509109E-01 -3.2757907072E-01 5.2203647889E-01
HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec2 = 5.0000000695E-01 8.6602539977E-01 0.0000000000E+00
HessRho_EigVec3 = 8.6602539977E-01 -5.0000000695E-01 0.0000000000E+00
DelSqRho = -2.5292768292E-01
Bond Ellipticity = 3.6573160827E-01
V = -3.2675774118E-01
G = 1.3176291022E-01
K = 1.9499483095E-01
L = 6.3231920731E-02
Vnuc = 6.6167193453E+00
Ven = -1.1956621714E+00
Vrep = 8.6890443020E-01
DelSqV = -3.7972517845E+00
DelSqVen = 1.6735514926E+00
DelSqVrep = -5.4708032771E+00
DelSqG = 6.1431217617E+00
DelSqK = -2.3458699772E+00
Stress_EigVals = -1.4785587269E-01 -1.1305528143E-01 -6.5846587062E-02
Stress_EigVec1 = 5.0000001670E-01 8.6602539414E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602539414E-01 -5.0000001670E-01 0.0000000000E+00
-DivStress = -4.3389992652E-01 2.5051223913E-01 0.0000000000E+00
BPL = 2.2287565201E+00 = 1.2549847929E+00 + 9.7377172722E-01
GBL_I = 2.2287565201E+00
GBL_II = 2.2498469000E+00
GBL_III = 2.2287565201E+00 = 1.2549847929E+00 + 9.7377172722E-01
GBL_IV = 2.2498469000E+00 = 1.2760751728E+00 + 9.7377172722E-01

CP# 7 Coords = -8.43311054879503E-01 -4.86885860801952E-01 0.00000000000000E+00

Type = (3,-1) BCP B1 H4

Rho = 1.8070317161E-01

GradRho = 9.9834712892E-18 4.2272160773E-17 0.0000000000E+00
HessRho_EigVals = -4.4738509109E-01 -3.2757907072E-01 5.2203647889E-01
HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec2 = -5.0000000695E-01 8.6602539977E-01 0.0000000000E+00
HessRho_EigVec3 = 8.6602539977E-01 5.0000000695E-01 0.0000000000E+00
DelSqRho = -2.5292768292E-01
Bond Ellipticity = 3.6573160827E-01
V = -3.2675774118E-01
G = 1.3176291022E-01
K = 1.9499483095E-01
L = 6.3231920731E-02
Vnuc = 6.6167193453E+00
Ven = -1.1956621714E+00
Vrep = 8.6890443020E-01
DelSqV = -3.7972517845E+00
DelSqVen = 1.6735514926E+00
DelSqVrep = -5.4708032771E+00
DelSqG = 6.1431217617E+00
DelSqK = -2.3458699772E+00
Stress_EigVals = -1.4785587269E-01 -1.1305528143E-01 -6.5846587062E-02
Stress_EigVec1 = -5.0000001670E-01 8.6602539414E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602539414E-01 5.0000001670E-01 0.0000000000E+00
-DivStress = 4.3389992652E-01 2.5051223913E-01 0.0000000000E+00
BPL = 2.2287565201E+00 = 9.7377172722E-01 + 1.2549847929E+00
GBL_I = 2.2287565201E+00
GBL_II = 2.2498469000E+00
GBL_III = 2.2287565201E+00 = 9.7377172722E-01 + 1.2549847929E+00
GBL_IV = 2.2498469000E+00 = 9.7377172722E-01 + 1.2760751728E+00

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H3	B1	H2	119.99999960	120.00000001	120.00000000	119.99999981	119.99999981
H4	B1	H2	119.99999960	120.00000001	120.00000000	119.99999981	119.99999981
H4	B1	H3	120.00000080	119.99999999	120.00000000	120.00000038	120.00000038

Total time for electron density critical point search, analysis and connectivity = 0 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$E_e(A) = E(A) - W(A) = -T(A)$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$Vee(A) = Vee(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $Vnn(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
B1	-2.3882665884E+01	2.3882665884E+01	-5.6266058610E+01	-5.2320348701E+01		
H2	-8.6003533956E-01	8.6003533956E-01	-6.3986446376E+00	-1.6832937090E+00		
H3	-8.6003564561E-01	8.6003564561E-01	-6.3986428040E+00	-1.6832935528E+00		
H4	-8.6003615424E-01	8.6003615424E-01	-6.3986452705E+00	-1.6832938248E+00		
Total	-2.6462773023E+01	2.6462773023E+01	-7.5461991322E+01	-5.7370229788E+01		

More Virial-Based Atomic Energy Components:

$$E(A) = Ee(A) + W(A)$$

= $T(A) + Ven(A) + Vee(A) + Vnn(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$Ee(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$Vnn(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $Vnn(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

B1	-2.3882665874E+01	-2.3882665884E+01	1.0370041627E-08			
H2	-8.6003533503E-01	-8.6003533956E-01	4.5297907027E-09			
H3	-8.6003564108E-01	-8.6003564561E-01	4.5297940614E-09			
H4	-8.6003614971E-01	-8.6003615424E-01	4.5297937622E-09			

Total	-2.6462772999E+01	-2.6462773023E+01	2.3959420153E-08			

IQA Atomic Energy Components:

$E_{\text{IQA}}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{\text{ne}}(A, \text{Mol})/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{\text{en}}(A, \text{Mol})/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{\text{ee}}(A) = V_{\text{ee}}(A, \text{Mol}) = (1/2)[V_{\text{ee}}(A, \text{Mol}) + V_{\text{ee}}(\text{Mol}, A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{\text{nn}}(A, \text{Mol})/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{\text{eeC}}(A)$ = Coulomb Part of $V_{\text{ee}}(A)$

$V_{\text{eeX}}(A)$ = Exchange-Correlation Part of $V_{\text{ee}}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E_{\text{IQA}}(A)$	$T(A)$	$V_{\text{ne}}(A, \text{Mol})/2$	$V_{\text{en}}(A, \text{Mol})/2$	$V_{\text{ee}}(A)$	$V_{\text{nn}}(A, \text{Mol})/2$

B1			2.3882665884E+01	-3.1911062957E+01	-2.8133029305E+01	
	3.3335601636E+00					
H2			8.6003533956E-01	-1.9400066127E+00	-3.1993223188E+00	
	1.3678043022E+00					

H3	8.6003564561E-01	-1.9400066172E+00	-3.1993214020E+00
1.3678043022E+00			
H4	8.6003615424E-01	-1.9400066172E+00	-3.1993226353E+00
1.3678043022E+00			

Total	2.6462773023E+01	-3.7731082804E+01	-3.7730995661E+01
7.4369730702E+00			

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)
B1	2.3882665884E+01	-5.2320348701E+01				
H2	8.6003533956E-01	-1.6832937090E+00				
H3	8.6003564561E-01	-1.6832935528E+00				
H4	8.6003615424E-01	-1.6832938248E+00				

Total	2.6462773023E+01	-5.7370229788E+01				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= V_{ne}(A,A')/2 + V_{en}(A,A')/2 + V_{ee}(A,A') + V_{nn}(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$V_{ne}(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[V_{ne}(A,Mol) - V_{ne}(A,A)]$$

$V_{en}(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[V_{en}(A,Mol) - V_{en}(A,A)]$$

$V_{ee}(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= V_{ee}(A,Mol) - V_{ee}(A,A)$$

$V_{nn}(A) = V_{nn}(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A,A')$ = Coulomb Part of $V_{ee}(A,A')$

$V_{eeX}(A,A')$ = Exchange-Correlation Part of $V_{ee}(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$V_{ne}(A,A')/2$	$V_{en}(A,A')/2$	$V_{ee}(A,A')$	$V_{nn}(A)$	$V_{eeC}(A,A')$ $V_{eeX}(A,A')$
B1	-5.7508886067E+00	-1.9728549545E+00		3.3335601636E+00		
H2	-1.0983597583E+00	-2.3576754643E+00		1.3678043022E+00		
H3	-1.0983598408E+00	-2.3576746256E+00		1.3678043022E+00		
H4	-1.0983597048E+00	-2.3576757228E+00		1.3678043022E+00		
Total	-9.0459679106E+00	-9.0458807672E+00		7.4369730702E+00		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$$\%Loc(A) = 100 * LI(A) / N(A)$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A)$$

$$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
B1	3.0143833932E+00	2.2299064562E+00	7.3975542105E+01	7.8447693696E-01	2.6024457895E+01
H2	1.6618459516E+00	1.2799275356E+00	7.7018422458E+01	3.8191841599E-01	2.2981577542E+01
H3	1.6618452376E+00	1.2799268457E+00	7.7018414037E+01	3.8191839185E-01	2.2981585963E+01
H4	1.6618454341E+00	1.2799272990E+00	7.7018432205E+01	3.8191813508E-01	2.2981567795E+01
Total	7.9999200165E+00	6.0696881366E+00	7.5871860270E+01	1.9302318799E+00	2.4128139730E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that
are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

DI_Bond(A,A')/2 = Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A that
are Shared With Atoms to Which Atom A is Bonded

DI_NonBond(A,A')/2 = Non-Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
B1	3.0143833932E+00		2.2299064562E+00	7.8447693696E-01	7.8446416313E-01
	1.2773824440E-05				
H2	1.6618459516E+00		1.2799275356E+00	3.8191841599E-01	2.6148095396E-01
	1.2043746203E-01				
H3	1.6618452376E+00		1.2799268457E+00	3.8191839185E-01	2.6149901201E-01
	1.2041937984E-01				
H4	1.6618454341E+00		1.2799272990E+00	3.8191813508E-01	2.6148419716E-01
	1.2043393793E-01				
Total	7.9999200165E+00		6.0696881366E+00	1.9302318799E+00	1.5689283263E+00
	3.6130355362E-01				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
B1	3.4283003925E+00	7.1220414824E+00	1.0550341875E+01
H2	7.4090221560E-01	5.0755585329E+00	5.8164607485E+00

H3 7.4090137399E-01 5.0755568757E+00 5.8164582497E+00

H4 7.4090147394E-01 5.0755574636E+00 5.8164589375E+00

Total 5.6510054560E+00 2.2348714355E+01 2.7999719811E+01

Diatomic Electron Pair Contributions and Delocalization Data:

 $2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized
(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$

B1	H2	4.7479598846E+00	5.2296190792E-01	8.6744424930E+00	1.5734367780E+01 (Bonded)
B1	H3	4.7479396743E+00	5.2299802403E-01	8.6750415559E+00	1.5735461167E+01 (Bonded)
H2	H3	2.7015266381E+00	1.2040828436E-01	3.6227270115E+00	3.6227285680E+00
B1	H4	4.7479550815E+00	5.2296839431E-01	8.6745500837E+00	1.5734567836E+01 (Bonded)
H2	H4	2.7015270824E+00	1.2040804887E-01	3.6227199263E+00	3.6227210544E+00
H3	H4	2.7015260350E+00	1.2040777061E-01	3.6227131109E+00	3.6227126825E+00

Areas of Interatomic Surfaces:

 $Area\_IAS(A|B),0.0004 =$ Area of the Part of Interatomic Surface Between Atoms
A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
B1	H2	4.8431999970E+01	3.7122603821E+01	2.9763325195E+01
B1	H3	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
B1	H4	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
B1	Total	1.4529600011E+02	1.1136781161E+02	8.9289975691E+01
H2	B1	4.8431999970E+01	3.7122603821E+01	2.9763325195E+01
H2	Total	4.8431999970E+01	3.7122603821E+01	2.9763325195E+01
H3	B1	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
H3	Total	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
H4	B1	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
H4	Total	4.8432000071E+01	3.7122603894E+01	2.9763325248E+01
Total	Total	2.9059200022E+02	2.2273562322E+02	1.7857995138E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$DelSqRho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $DelSqRho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$DelSqRho\_IAS(A B)$	$V\_IAS(A B)$

B1	H2	8.5643388692E-01	5.7748534277E-01	4.3376483315E-01	-1.4372050962E-01	5.7488203847E-01	-1.0112501759E+00

B1	H3	8.5643388592E-01	5.7748535680E-01	4.3376483753E-01	-1.4372051926E-01	5.7488207706E-01	-1.0112501943E+00

B1	H4	8.5643388584E-01	5.7748535661E-01	4.3376483762E-01	-1.4372051899E-01	5.7488207597E-01	-1.0112501942E+00

B1	Total	2.5693016587E+00	1.7324560562E+00	1.3012945083E+00	-4.3116154787E-01	1.7246461915E+00	-3.0337505644E+00

H2	B1	8.5643388692E-01	5.7748534277E-01	4.3376483315E-01	-1.4372050962E-01	5.7488203847E-01	-1.0112501759E+00

H2	Total	8.5643388692E-01	5.7748534277E-01	4.3376483315E-01	-1.4372050962E-01	5.7488203847E-01	-1.0112501759E+00

H3	B1	8.5643388592E-01	5.7748535680E-01	4.3376483753E-01	-1.4372051926E-01	5.7488207706E-01	-1.0112501943E+00

H3	Total	8.5643388592E-01	5.7748535680E-01	4.3376483753E-01	-1.4372051926E-01	5.7488207706E-01	-1.0112501943E+00

H4	B1	8.5643388584E-01	5.7748535661E-01	4.3376483762E-01	-1.4372051899E-01	5.7488207596E-01	-1.0112501942E+00

H4 Total 8.5643388584E-01 5.7748535661E-01 4.3376483762E-01 -1.4372051899E-01
5.7488207596E-01 -1.0112501942E+00

Total Total 5.1386033174E+00 3.4649121124E+00 2.6025890166E+00 -8.6232309574E-01
3.4492923830E+00 -6.0675011288E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP_-Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1 9.9956828144E+00

H2 8.7206192765E+01

H3 8.7178156646E+01

H4 8.6748644819E+01

Total 2.7112867704E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1 1.0008052708E+01 2.6906048562E-01 7.0075363253E-02 -8.4685772887E-03 2.6884399340E-02 2.3781911510E-02 7.1088432920E-04

H2 7.0484043148E+01 2.9015208910E-01 6.5813140596E-02 -8.4696763453E-03 4.1165642057E-03 9.7098473755E-03 1.8714392528E-04

H3 7.0336626524E+01 2.8917505530E-01 6.5367032796E-02 -8.4676784829E-03 4.1113011754E-03 9.6924616073E-03 1.8378954693E-04

H4 7.0429511404E+01 2.8681156445E-01 6.4275164645E-02 -8.4446150992E-03 4.0723208032E-03 9.6134132738E-03 1.8188963182E-04

Total 2.2125823378E+02 1.1351991945E+00 7.0075363253E-02 -8.4696763453E-03 5.1306528804E-03 2.3051473730E-04

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)	ESP-_Int_IDS(A)

B1	2.9442754794E-01	1.4348097378E-02	7.7583175864E+00	2.8174401678E-01	2.2497351216E+00	-1.2683531156E-02

H2	5.8966209171E-01	1.4385090209E-02	2.8150660114E+01	4.3990709040E-01	4.2333383034E+01	-1.4975500130E-01

H3	5.8692329325E-01	1.4116022466E-02	2.8034538872E+01	4.3804917428E-01	4.2302087652E+01	-1.4887411897E-01

H4	5.8362188438E-01	1.3978386599E-02	2.8625523656E+01	4.3521672442E-01	4.1803987749E+01	-1.4840515997E-01

Total	2.0546348173E+00	5.6827596652E-02	9.2569040228E+01	1.5949170059E+00	1.2868919356E+02	-4.5971781140E-01

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)

B1	3.6884622831E-05	3.6315091982E-02	2.0253266636E-02	5.1957892608E-04

H2	1.4888874004E-05	1.5626883655E-02	1.2373598340E-02	2.3974889813E-04

H3	1.8023177381E-05	1.5625339025E-02	1.2262630842E-02	2.3242929282E-04

H4	2.4217182442E-06	1.5203799576E-02	1.2138898538E-02	2.3095985426E-04

Total	2.4217182442E-06	1.7229486251E-02	2.9162551218E-04	5.4475094393E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

B1	-1.7969306756E-04	-5.6377886597E-03	2.1330825477E-03	6.2105558221E-06
8.5479173674E-05				
H2	-1.7901915676E-05	-3.5375155627E-03	2.0122266155E-03	5.4770698693E-06
7.6162354438E-04				
H3	-2.6416556008E-05	-3.5193090279E-03	2.0100708058E-03	5.4695535288E-06
7.5530756373E-04				
H4	-3.8682462483E-05	-3.5500240039E-03	1.9894525915E-03	5.3404019347E-06
7.5009197723E-04				

Total	-1.7901915676E-05	-3.5723109197E-03	5.5190904670E-06	2.3525022590E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1	9.3115194969E+00

H2	5.8858847263E+01

H3	5.9439925131E+01

H4	5.8825528767E+01

Total	1.8643582066E+02

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A | \text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A) = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$

$\text{Isosurface of the Electron Density Distribution (IsoDensity Surface)}$

$N(\text{Vol}(A)) = \text{Average Number of Electrons in Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A) = \text{Average Electron Density in Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

$= \text{Percentage of Atom A's Electron Population in Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1 9.9925601945E+01	1.5529168292E+02		3.3062464619E+01	3.0121407505E+00	9.1104543631E-02
H2 9.8722909637E+01	1.3563819273E+02		1.2312343511E+02	1.6406226770E+00	1.3325023587E-02
H3 9.8718064876E+01	1.3561015672E+02		1.2292315147E+02	1.6405414597E+00	1.3346073869E-02
H4 9.8721139285E+01	1.3518064489E+02		1.2304403507E+02	1.6405927459E+00	1.3333378940E-02
Total 9.9174711956E+01	5.6172067727E+02		4.0215308627E+02	7.9338976331E+00	1.9728550903E-02

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1 9.9824708844E+01	1.2137586432E+02		2.8406189245E+01	3.0090994456E+00	1.0593112014E-01
H2 9.7357165635E+01	1.0760664697E+02		8.7780622927E+01	1.6179261156E+00	1.8431472250E-02
H3 9.7353509255E+01	1.0745923042E+02		8.7719359674E+01	1.6178646571E+00	1.8443644175E-02
H4 9.7355801593E+01	1.0755211530E+02		8.7756495336E+01	1.6179029438E+00	1.8436275715E-02
Total 9.8285897182E+01	4.4399385700E+02		2.9166266718E+02	7.8627931621E+00	2.6958517654E-02

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	9.8601495188E+01	2.5032758295E+01	3.0042583811E+00	1.2001307829E-01
	9.9664110013E+01			
H2	8.8622172458E+01	6.6144145784E+01	1.5870215554E+00	2.3993378954E-02
	9.5497513110E+01			
H3	8.9203250379E+01	6.6149508852E+01	1.5870281660E+00	2.3991533626E-02
	9.5497951926E+01			
H4	8.8588854015E+01	6.6148600404E+01	1.5870266962E+00	2.3991840894E-02
	9.5497852174E+01			

Total	3.6501577204E+02	2.2347501333E+02	7.7653347987E+00	3.4748112027E-02
	9.7067655460E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

B1	H2	6.6186880396E-01		
B1	H3	6.6186808996E-01		
B1	H4	6.6186828676E-01		
B1		1.9856051807E+00	1.9856166069E+00	
H2	B1	-6.6185737773E-01		
H2		-6.6185737773E-01	-6.6184595150E-01	
H3	B1	-6.6185666373E-01		
H3		-6.6185666373E-01	-6.6184523750E-01	
H4	B1	-6.6185686053E-01		
H4		-6.6185686053E-01	-6.6184543430E-01	

Atomic Dipole Moments:

$\mu_{\text{Intra}}(A)$ = Intraatomic Dipole Moment Contribution of Atom A

$\text{Mu\_Bond(A)} = \text{Bonding Dipole Moment Contribution of Atom A}$

$\text{Mu(A)} = \text{Mu\_Intra(A)} + \text{Mu\_Bond(A)}$

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

B1	-1.0046864716E-04	1.6596361485E-07	-1.0030268355E-04
H2	-7.3560340920E-07	-1.5877002914E-20	-7.3560340920E-07
H3	3.0152718542E-01	-7.3142674416E-01	-4.2989955874E-01
H4	-3.0152684605E-01	7.3142696165E-01	4.2990011560E-01

Total	-1.0086488057E-04	3.8344995335E-07	-1.0048143062E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

B1	2.1828387358E-05	-6.0820304837E-07	2.1220184310E-05
H2	3.4817475574E-01	-8.4457976261E-01	-4.9640500687E-01
H3	-1.7408632911E-01	4.2228943012E-01	2.4820310101E-01
H4	-1.7408722754E-01	4.2228955569E-01	2.4820232815E-01

Total	2.3027477358E-05	-1.3850059028E-06	2.1642471455E-05

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

B1	5.7365429503E-06	0.0000000000E+00	5.7365429503E-06
H2	6.5351777292E-07	0.0000000000E+00	6.5351777292E-07
H3	-5.4728333238E-07	0.0000000000E+00	-5.4728333238E-07
H4	1.2304554110E-06	0.0000000000E+00	1.2304554110E-06

Total	7.0732328018E-06	0.0000000000E+00	7.0732328018E-06

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

```

-----
B1   1.0297249867E-04  6.3044021882E-07  1.0268316548E-04
H2   3.4817475575E-01  8.4457976261E-01  4.9640500687E-01
H3   3.4817336706E-01  8.4457885651E-01  4.9640548945E-01
H4   3.4817352238E-01  8.4457910764E-01  4.9640558527E-01
-----

```

```

Total  1.0370158855E-04  1.4371065435E-06  1.0302885563E-04

```

Bond Contributions to Atomic Dipole Moments:

```

-----
Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

```

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Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

```

```

= Total Bonding Dipole Moment Contribution of Atom A

```

```

Atom A  Atom B  Mu_Bond_X(A|B)  Mu_Bond_X(A)
-----

```

```

B1   H2   1.5877277013E-20
B1   H3  -5.5816067713E-01
B1   H4   5.5816084310E-01
B1                                1.6596361485E-07
H2   B1  -1.5877002914E-20
H2                                -1.5877002914E-20
H3   B1  -7.3142674416E-01
H3                                -7.3142674416E-01
H4   B1   7.3142696165E-01
H4                                7.3142696165E-01

```

```

Atom A  Atom B  Mu_Bond_Y(A|B)  Mu_Bond_Y(A)
-----

```

```

B1   H2  -6.4450913345E-01
B1   H3   3.2225421472E-01
B1   H4   3.2225431054E-01

```

B1		-6.0820304837E-07
H2	B1	-8.4457976261E-01
H2		-8.4457976261E-01
H3	B1	4.2228943012E-01
H3		4.2228943012E-01
H4	B1	4.2228955569E-01
H4		4.2228955569E-01

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	H2	0.0000000000E+00	
B1	H3	0.0000000000E+00	
B1	H4	0.0000000000E+00	
B1		0.0000000000E+00	
H2	B1	0.0000000000E+00	
H2		0.0000000000E+00	
H3	B1	0.0000000000E+00	
H3		0.0000000000E+00	
H4	B1	0.0000000000E+00	
H4		0.0000000000E+00	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

B1	H2	6.4450913345E-01	
B1	H3	6.4450843315E-01	
B1	H4	6.4450862479E-01	
B1		6.3044021882E-07	
H2	B1	8.4457976261E-01	
H2		8.4457976261E-01	
H3	B1	8.4457885651E-01	
H3		8.4457885651E-01	
H4	B1	8.4457910764E-01	

H4

8.4457910764E-01

Atomic Traceless Quadrupole Moment Tensors:

$$Q(A) = \text{Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge}$$

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$

B1	5.7184060293E-02	-1.4929730691E-04	1.3037594608E-04	5.7977430395E-02	5.1595346250E-05	-1.1516149069E-01
H2	-9.2780476176E-02	3.8804193882E-06	-1.5795907202E-05	7.0023485516E-01	-2.0206402255E-06	-6.0745437899E-01
H3	5.0198226887E-01	-3.4338749540E-01	-7.1636474722E-06	1.0547052027E-01	-1.6133909834E-05	-6.0745278915E-01
H4	5.0197772202E-01	3.4338665112E-01	1.4344059983E-05	1.0546416503E-01	-1.0721666533E-05	-6.0744188705E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$$Q_{\text{EigVal}_n}(A) = \text{nth Eigenvalue of } Q(A)$$

$$Q_{\text{EigVal}_n\_X}(A) = \text{X Component of the nth Eigenvector of } Q(A)$$

$$Q_{\text{EigVal}_n\_Y}(A) = \text{Y Component of the nth Eigenvector of } Q(A)$$

$$Q_{\text{EigVal}_n\_Z}(A) = \text{Z Component of the nth Eigenvector of } Q(A)$$

Atom A	n	$Q_{\text{EigVal}_n}(A)$	$Q_{\text{EigVec}_n\_X}(A)$	$Q_{\text{EigVec}_n\_Y}(A)$	$Q_{\text{EigVec}_n\_Z}(A)$

B1	1	-1.1516160476E-01	-7.5673786645E-04	-2.9865193632E-04	9.999966908E-01
B1	2	5.7157005197E-02	9.8385117856E-01	1.7898665225E-01	7.9797241611E-04
B1	3	5.8004599561E-02	-1.7898683134E-01	9.8385145684E-01	1.5838308218E-04
H2	1	-6.0745437947E-01	3.0691086331E-05	1.5451080247E-06	9.999999953E-01
H2	2	-9.2780475710E-02	9.999999952E-01	-4.8933245688E-06	-3.0691078770E-05
H2	3	7.0023485518E-01	4.8932771454E-06	9.999999999E-01	-1.5452582055E-06
H3	1	-6.0745278975E-01	1.5820036789E-05	3.0250536532E-05	9.999999942E-01
H3	2	-9.2783836333E-02	4.9999904325E-01	8.6602595549E-01	-3.4107753083E-05
H3	3	7.0023662608E-01	8.6602595602E-01	-4.9999904350E-01	1.4246768478E-06
H4	1	-6.0744188762E-01	-2.0665222454E-05	2.4993234374E-05	9.999999947E-01
H4	2	-9.2789008390E-02	-4.9999772682E-01	8.6602671561E-01	-3.1977372946E-05
H4	3	7.0023089601E-01	8.6602671596E-01	4.9999772722E-01	5.4000743564E-06

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.2190894096E+01	1.0464069740E+01	3.0143833931E+00	1.9108245033E+00	2.2063473965E+00
H2	3.1409499059E+00	1.6832937090E+00	1.6618459515E+00	2.2776237954E+00	3.9401024820E+00
H3	3.1409499654E+00	1.6832935528E+00	1.6618452375E+00	2.2776215044E+00	3.9400956029E+00
H4	3.1409502012E+00	1.6832938248E+00	1.6618454343E+00	2.2776209289E+00	3.9400896894E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
B1	-9.0998064248E+01	-1.9449640775E+01	-7.0990778506E+00	-4.8712405656E+00	-6.6289671455E+00
H2	-2.7550857987E+00	-2.7062570073E+00	-3.7957958913E+00	-6.8272276551E+00	-1.4970001078E+01
H3	-2.7550853376E+00	-2.7062554025E+00	-3.7957912375E+00	-6.8272139590E+00	-1.4969950200E+01
H4	-2.7550853341E+00	-2.7062551648E+00	-3.7957898387E+00	-6.8272063452E+00	-1.4969905091E+01

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
B1	1.5071916966E+00	1.5071916966E+00	3.0143833931E+00	0.0000000000E+00
H2	8.3092297574E-01	8.3092297574E-01	1.6618459515E+00	0.0000000000E+00
H3	8.3092261877E-01	8.3092261877E-01	1.6618452375E+00	0.0000000000E+00
H4	8.3092271713E-01	8.3092271713E-01	1.6618454343E+00	0.0000000000E+00

Total 3.9999600082E+00 3.9999600082E+00 7.9999200164E+00 0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

BH3NH3

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\bh3nh3\bh3nh3.wfx

Sum File: D:\calc\ellipticity\bh3nh3\bh3nh3.sum

SumViz File: D:\calc\ellipticity\bh3nh3\bh3nh3.sumviz

Wfx Title: bh3nh3_mp2

Total memory allocated for AIMSum = 0.549 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	18.0000000120
Number of Alpha electrons (from MO Occs)	=	9.0000000060
Number of Beta electrons (from MO Occs)	=	9.0000000060
Number of electron pairs ($N*(N-1)/2$)	=	153.0000002108
Number of electron pairs (from Muller 2EDM)	=	152.9999482236
Number of electron pairs (from Muller 2EDM, no SOSI)	=	153.1984726326

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
B1	5.0	0.0000000000E+00	0.0000000000E+00	-1.7578205300E+00
H2	1.0	0.0000000000E+00	-2.2095054400E+00	-2.3377815000E+00
H3	1.0	1.9134878400E+00	1.1047527200E+00	-2.3377815000E+00
H4	1.0	-1.9134878400E+00	1.1047527200E+00	-2.3377815000E+00
N5	7.0	0.0000000000E+00	0.0000000000E+00	1.3720698400E+00
H6	1.0	0.0000000000E+00	1.7921056000E+00	2.0659860900E+00
H7	1.0	-1.5520089800E+00	-8.9605280000E-01	2.0659860900E+00
H8	1.0	1.5520089800E+00	-8.9605280000E-01	2.0659860900E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
B1	1.9249496754E+00	-4.1180657778E-04	2.3852685255E+01	-2.3874874059E+01	6.9576218771E-02
H2	-6.7477463140E-01	5.1219608506E-05	8.4708630120E-01	-8.4787429767E-01	2.1849926066E-01
H3	-6.7478175670E-01	4.5168883303E-05	8.4708559639E-01	-8.4787359221E-01	2.1850673710E-01
H4	-6.7477858210E-01	4.8348199279E-05	8.4708646477E-01	-8.4787446139E-01	2.1850398238E-01
N5	-1.1138082501E+00	1.0199809089E-05	5.5112088086E+01	-5.5163355744E+01	1.9762390711E-01

H6 4.0432191635E-01 3.3843092090E-05 4.5939993828E-01 -4.5982729206E-01 1.7301765497E-01

H7 4.0432021278E-01 3.2742096762E-05 4.5940027180E-01 -4.5982762588E-01 1.7301736591E-01

H8 4.0432161354E-01 3.3050693886E-05 4.5939951312E-01 -4.5982686651E-01 1.7301792304E-01

Total -2.2980223000E-04 -1.5723419486E-04 8.2884231427E+01 -8.2961333939E+01

Molecular charge q(Mol) from the wfx file: -1.2047593831E-08

Molecular energy E(Mol) from the wfx file: -8.2961339914E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0009302434E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0009302444E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR
B1	31	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00 13.00
H2	13	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H3	14	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H4	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00

N5	35	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H6	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H7	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 129

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -1.14051007231369E-24 5.66389372600270E-14 -1.75781203399839E+00

Type = (3,-3) NACP B1

Rho = 6.7013615016E+01 Rho at Nucleus = 6.7013612601E+01

GradRho = 3.5083501627E-18 3.6856309359E-17 2.8697044741E-12

HessRho_EigVals = -6.6901219954E+04 -6.6899952377E+04 -6.6899952377E+04

HessRho_EigVec1 = 0.0000000000E+00 7.7334623759E-09 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 -7.7334623759E-09

DelSqRho = -2.0070112471E+05

Bond Ellipticity = NA

V = -5.0178599024E+04

G = 1.6589235285E+00

K = 5.0176940101E+04

L = 5.0175281177E+04

Vnuc = 5.8851638971E+05

Ven = -3.9438610771E+07

Vrep = 3.9388432172E+07

DelSqV = 1.0692956609E+09

DelSqVen = 1.1811590118E+11

DelSqVrep = -1.1704660552E+11

DelSqG = 5.0094366723E+07

DelSqK = -1.1193900277E+09

Stress_EigVals = -1.6726326416E+04 -1.6726326416E+04 -1.6725946193E+04

Stress_EigVec1 = 0.0000000000E+00 1.0000000000E+00 -5.7591513929E-09

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 5.7591513929E-09 1.0000000000E+00

-DivStress = 3.6325020209E-15 -1.9858962672E-05 -2.9531411454E+03

CP# 2 Coords = -3.82192147027182E-20 -2.19181426325052E+00 -2.33209277745974E+00

Type = (3,-3) NACP H2

Rho = 4.1419480114E-01 Rho at Nucleus = 4.1279690861E-01

GradRho = -6.4419232082E-20 1.0182826804E-15 4.6837533851E-16

HessRho_EigVals = -8.3002497880E+00 -8.2976153318E+00 -7.9942954416E+00

HessRho_EigVec1 = 0.0000000000E+00 -2.9034396577E-01 9.5692234875E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 9.5692234875E-01 2.9034396577E-01

DelSqRho = -2.4592160561E+01

Bond Ellipticity = NA

V = -6.1583988758E+00

G = 5.1793677470E-03

K = 6.1532195081E+00

L = 6.1480401403E+00

Vnuc = 5.8751234377E+01

Ven = -2.4334455840E+01

Vrep = 1.8176056964E+01

DelSqV = 1.6117489621E+03

DelSqVen = 1.4448197890E+03

DelSqVrep = 1.6692917316E+02

DelSqG = 1.2263479314E+02

DelSqK = -1.7343837553E+03

Stress_EigVals = -2.0784786913E+00 -2.0779159791E+00 -2.0020042054E+00

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 -2.9204284570E-01 9.5640523643E-01
Stress_EigVec3 = 0.0000000000E+00 9.5640523643E-01 2.9204284570E-01
-DivStress = 2.0035946119E-17 -9.1135556101E+00 -2.9269523246E+00

CP# 3 Coords = 1.89816683222649E+00 1.09590713217711E+00 -2.33209277806696E+00

Type = (3,-3) NACP H3

Rho = 4.1419480647E-01 Rho at Nucleus = 4.1279691407E-01

GradRho = -4.6837533851E-17 -2.0816681712E-17 1.6991616447E-15

HessRho_EigVals = -8.3002498786E+00 -8.2976154228E+00 -7.9942955465E+00

HessRho_EigVec1 = 2.5144533796E-01 1.4517181280E-01 9.5692235149E-01

HessRho_EigVec2 = -4.9999994995E-01 8.6602543268E-01 1.8225358471E-07

HessRho_EigVec3 = 8.2871906703E-01 4.7846117368E-01 -2.9034395674E-01

DelSqRho = -2.4592160848E+01

Bond Ellipticity = NA

V = -6.1583989473E+00

G = 5.1793676825E-03

K = 6.1532195796E+00

L = 6.1480402120E+00

Vnuc = 5.8751237381E+01

Ven = -2.4334457397E+01

Vrep = 1.8176058449E+01

DelSqV = 1.6117489822E+03

DelSqVen = 1.4448198797E+03

DelSqVrep = 1.6692910250E+02

DelSqG = 1.2263479442E+02

DelSqK = -1.7343837766E+03

Stress_EigVals = -2.0784787140E+00 -2.0779160018E+00 -2.0020042315E+00

Stress_EigVec1 = -5.0000006354E-01 8.6602536710E-01 -2.3877211943E-07

Stress_EigVec2 = 2.5291639136E-01 1.4602163507E-01 9.5640523894E-01

Stress_EigVec3 = 8.2827123302E-01 4.7820261985E-01 -2.9204283749E-01

-DivStress = 7.8925704021E+00 4.5567775774E+00 -2.9269520510E+00

CP# 4 Coords = -1.89816683222649E+00 1.09590713217711E+00 -2.33209277806696E+00

Type = (3,-3) NACP H4

Rho = 4.1419480647E-01 Rho at Nucleus = 4.1279691407E-01

GradRho = 4.8572257327E-17 -1.7347234760E-17 1.7026310917E-15

HessRho_EigVals = -8.3002498786E+00 -8.2976154228E+00 -7.9942955465E+00

HessRho_EigVec1 = -2.5144533796E-01 1.4517181280E-01 9.5692235149E-01

HessRho_EigVec2 = 4.9999994995E-01 8.6602543268E-01 1.8225342919E-07

HessRho_EigVec3 = 8.2871906703E-01 -4.7846117368E-01 2.9034395674E-01

DelSqRho = -2.4592160848E+01

Bond Ellipticity = NA

V = -6.1583989473E+00

G = 5.1793676825E-03

K = 6.1532195796E+00

L = 6.1480402120E+00

Vnuc = 5.8751237381E+01

Ven = -2.4334457397E+01

Vrep = 1.8176058449E+01

DelSqV = 1.6117489822E+03

DelSqVen = 1.4448198797E+03

DelSqVrep = 1.6692910250E+02

DelSqG = 1.2263479442E+02

DelSqK = -1.7343837766E+03

Stress_EigVals = -2.0784787140E+00 -2.0779160018E+00 -2.0020042315E+00

Stress_EigVec1 = 5.0000006354E-01 8.6602536710E-01 -2.3877185071E-07

Stress_EigVec2 = -2.5291639136E-01 1.4602163507E-01 9.5640523894E-01

Stress_EigVec3 = 8.2827123302E-01 -4.7820261985E-01 2.9204283749E-01

-DivStress = -7.8925704021E+00 4.5567775774E+00 -2.9269520510E+00

CP# 5 Coords = -3.51974343407875E-23 6.02487587169278E-13 1.37207589097775E+00

Type = (3,-3) NACP N5

Rho = 1.9384291788E+02 Rho at Nucleus = 1.9384291050E+02

GradRho = 6.2912301054E-17 -1.8968752282E-16 -1.6487700094E-11
HessRho_EigVals = -4.0309386561E+05 -4.0309386561E+05 -4.0308807986E+05
HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 -1.4759915407E-08
HessRho_EigVec3 = 0.0000000000E+00 1.4759915407E-08 1.0000000000E+00
DelSqRho = -1.2092758111E+06
Bond Ellipticity = NA
V = -3.0236944166E+05
G = 2.5244443625E+01
K = 3.0234419721E+05
L = 3.0231895277E+05
Vnuc = 1.1568416883E+06
Ven = -2.2424556838E+08
Vrep = 2.2394319894E+08
DelSqV = 1.4120525269E+10
DelSqVen = 1.3989406659E+12
DelSqVrep = -1.3848201406E+12
DelSqG = 6.2877678321E+08
DelSqK = -1.4749302052E+10
Stress_EigVals = -1.0079065378E+05 -1.0078939394E+05 -1.0078939394E+05
Stress_EigVec1 = 0.0000000000E+00 4.1639790670E-08 1.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 -4.1639790670E-08
Stress_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
-DivStress = 1.5047258694E-13 -2.7327901242E-03 -2.7803170018E+04

CP# 6 Coords = 1.60567667390962E-20 1.75564482151782E+00 2.05319297918269E+00

Type = (3,-3) NACP H6

Rho = 4.2103515557E-01 Rho at Nucleus = 4.1531159958E-01

GradRho = 8.8687515844E-20 -6.2116978228E-14 -2.4130003551E-14

HessRho_EigVals = -8.3662834904E+00 -8.3584484012E+00 -7.2270989466E+00

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 -3.4450253167E-01 9.3878538851E-01

HessRho_EigVec3 = 0.0000000000E+00 9.3878538851E-01 3.4450253167E-01

DelSqRho = -2.3951830838E+01

Bond Ellipticity = NA

V = -6.0235981590E+00

G = 1.7820224725E-02

K = 6.0057779343E+00

L = 5.9879577096E+00

Vnuc = 3.2022418705E+01

Ven = -1.3482564041E+01

Vrep = 7.4589658822E+00

DelSqV = 1.5160353061E+03

DelSqVen = 7.6699555586E+02

DelSqVrep = 7.4903975022E+02

DelSqG = 1.1520683841E+02

DelSqK = -1.6312421445E+03

Stress_EigVals = -2.1041746423E+00 -2.1024006389E+00 -1.8170228778E+00

Stress_EigVec1 = 0.0000000000E+00 -3.3936144647E-01 9.4065605226E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 9.4065605226E-01 3.3936144647E-01

-DivStress = -9.6768548860E-18 1.8302660088E+01 6.4231010173E+00

CP# 7 Coords = -1.52043301858148E+00 -8.77822410458869E-01 2.05319297948449E+00

Type = (3,-3) NACP H7

Rho = 4.2103515011E-01 Rho at Nucleus = 4.1531159388E-01

GradRho = 2.5404209014E-09 1.4667125084E-09 -1.0396044095E-09

HessRho_EigVals = -8.3662832931E+00 -8.3584482046E+00 -7.2270987468E+00

HessRho_EigVec1 = -5.0000000840E-01 8.6602539893E-01 -3.6907593698E-08

HessRho_EigVec2 = 2.9834791847E-01 1.7225129491E-01 9.3878539132E-01

HessRho_EigVec3 = 8.1301199939E-01 4.6939269253E-01 -3.4450252401E-01

DelSqRho = -2.3951830245E+01

Bond Ellipticity = NA

V = -6.0235980111E+00

G = 1.7820224990E-02
K = 6.0057777861E+00
L = 5.9879575611E+00
Vnuc = 3.2022418118E+01
Ven = -1.3482563619E+01
Vrep = 7.4589656079E+00
DelSqV = 1.5160352634E+03
DelSqVen = 7.6699552693E+02
DelSqVrep = 7.4903973650E+02
DelSqG = 1.1520683441E+02
DelSqK = -1.6312420978E+03
Stress_EigVals = -2.1041745927E+00 -2.1024005898E+00 -1.8170228287E+00
Stress_EigVec1 = 2.9389557683E-01 1.6968081086E-01 9.4065605422E-01
Stress_EigVec2 = -5.0000002591E-01 8.6602538882E-01 -1.0011244142E-07
Stress_EigVec3 = 8.1463204209E-01 4.7032802206E-01 -3.3936144103E-01
-DivStress = -1.5850568687E+01 -9.1513299558E+00 6.4231007152E+00

CP# 8 Coords = 1.52043301858148E+00 -8.77822410458869E-01 2.05319297948449E+00

Type = (3,-3) NACP H8

Rho = 4.2103515011E-01 Rho at Nucleus = 4.1531159388E-01

GradRho = -2.5404208737E-09 1.4667124945E-09 -1.0396044242E-09

HessRho_EigVals = -8.3662832931E+00 -8.3584482046E+00 -7.2270987468E+00

HessRho_EigVec1 = 5.0000000840E-01 8.6602539893E-01 -3.6907524440E-08

HessRho_EigVec2 = -2.9834791847E-01 1.7225129491E-01 9.3878539132E-01

HessRho_EigVec3 = 8.1301199939E-01 -4.6939269253E-01 3.4450252401E-01

DelSqRho = -2.3951830245E+01

Bond Ellipticity = NA

V = -6.0235980111E+00

G = 1.7820224990E-02

K = 6.0057777861E+00

L = 5.9879575611E+00

Vnuc = 3.2022418118E+01

Ven = -1.3482563619E+01
Vrep = 7.4589656079E+00
DelSqV = 1.5160352634E+03
DelSqVen = 7.6699552693E+02
DelSqVrep = 7.4903973650E+02
DelSqG = 1.1520683441E+02
DelSqK = -1.6312420978E+03
Stress_EigVals = -2.1041745927E+00 -2.1024005898E+00 -1.8170228287E+00
Stress_EigVec1 = -2.9389557683E-01 1.6968081086E-01 9.4065605422E-01
Stress_EigVec2 = 5.0000002591E-01 8.6602538882E-01 -1.0011228711E-07
Stress_EigVec3 = 8.1463204209E-01 -4.7032802206E-01 3.3936144103E-01
-DivStress = 1.5850568687E+01 -9.1513299558E+00 6.4231007152E+00

CP# 9 Coords = -2.34540511770533E-18 -1.46974193554782E-09 -7.85716059423827E-01

Type = (3,-1) BCP N5 B1
Rho = 9.8620388791E-02
GradRho = 3.3719232268E-19 3.8851479033E-14 -2.9515279110E-13
HessRho_EigVals = -1.0319500641E-01 -1.0319500268E-01 6.8336079302E-01
HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 1.0144879609E-09
HessRho_EigVec3 = 0.0000000000E+00 -1.0144879609E-09 1.0000000000E+00
DelSqRho = 4.7697078393E-01
Bond Ellipticity = 3.6179943042E-08
V = -2.2929978280E-01
G = 1.7427123939E-01
K = 5.5028543409E-02
L = -1.1924269598E-01
Vnuc = 1.0389314387E+01
Ven = -1.0245982241E+00
Vrep = 7.9529844134E-01
DelSqV = -4.2834390692E+00
DelSqVen = -4.9553994278E+00

DelSqVrep = 6.7196035857E-01

DelSqG = 6.0758650055E+00

DelSqK = -1.7924259363E+00

Stress_EigVals = -9.7833436796E-02 -9.7833435763E-02 -3.3632910242E-02

Stress_EigVec1 = 0.0000000000E+00 1.0000000000E+00 3.4941025604E-09

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 -3.4941025604E-09 1.0000000000E+00

-DivStress = -3.3842415144E-22 3.9463330153E-10 -3.0148411311E-01

BPL = 3.1298879250E+00 = 2.1577919504E+00 + 9.7209597457E-01

GBL_I = 3.1298879250E+00

GBL_II = 3.1298903700E+00

GBL_III = 3.1298879250E+00 = 2.1577919504E+00 + 9.7209597457E-01

GBL_IV = 3.1298903700E+00 = 2.1577858994E+00 + 9.7210447058E-01

CP# 10 Coords = -6.66578472006688E-18 -9.52761945178238E-01 -1.98216579010225E+00

Type = (3,-1) BCP B1 H2

Rho = 1.6377738753E-01

GradRho = 1.8528373277E-18 3.4694469520E-17 6.9388939039E-18

HessRho_EigVals = -3.3954497690E-01 -2.8826528710E-01 5.2356469603E-01

HessRho_EigVec1 = 0.0000000000E+00 -2.5311824624E-01 9.6743534844E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 9.6743534844E-01 2.5311824624E-01

DelSqRho = -1.0424556797E-01

Bond Ellipticity = 1.7789061705E-01

V = -3.0669006984E-01

G = 1.4031433892E-01

K = 1.6637573091E-01

L = 2.6061391993E-02

Vnuc = 9.2532402415E+00

Ven = -1.5154715130E+00

Vrep = 1.2087814431E+00

DelSqV = -3.7824889210E+00

DelSqVen = 9.6460928456E-01

DelSqVrep = -4.7470982056E+00

DelSqG = 5.8528968501E+00

DelSqK = -2.0704079291E+00

Stress_EigVals = -1.3259026374E-01 -1.1868475087E-01 -5.5415055228E-02

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 -2.2242467342E-01 9.7494987802E-01

Stress_EigVec3 = 0.0000000000E+00 9.7494987802E-01 2.2242467342E-01

-DivStress = 4.1833855315E-18 4.3812343783E-01 1.0594318038E-01

BPL = 2.2664454430E+00 = 9.7887845517E-01 + 1.2875669878E+00

GBL_I = 2.2657996683E+00

GBL_II = 2.2843530848E+00

GBL_III = 2.2663374972E+00 = 9.7882068432E-01 + 1.2875168129E+00

GBL_IV = 2.2849070743E+00 = 9.7881873700E-01 + 1.3060883373E+00

CP# 11 Coords = 8.25116042917672E-01 4.76380976567859E-01 -1.98216579349076E+00

Type = (3,-1) BCP H3 B1

Rho = 1.6377738591E-01

GradRho = 1.2143064332E-16 6.2450045135E-17 2.2551405188E-17

HessRho_EigVals = -3.3954497257E-01 -2.8826528011E-01 5.2356470651E-01

HessRho_EigVec1 = 2.1920684408E-01 1.2655910354E-01 9.6743534813E-01

HessRho_EigVec2 = -4.9999999141E-01 8.6602540874E-01 2.1483376410E-08

HessRho_EigVec3 = 8.3782359008E-01 4.8371767047E-01 -2.5311824743E-01

DelSqRho = -1.0424554618E-01

Bond Ellipticity = 1.7789063058E-01

V = -3.0669006946E-01

G = 1.4031434146E-01

K = 1.6637572800E-01

L = 2.6061386544E-02

Vnuc = 9.2532402492E+00

Ven = -1.5154714992E+00

Vrep = 1.2087814297E+00

DelSqV = -3.7824889690E+00

DelSqVen = 9.6460908367E-01

DelSqVrep = -4.7470980527E+00

DelSqG = 5.8528969220E+00

DelSqK = -2.0704079529E+00

Stress_EigVals = -1.3259026418E-01 -1.1868475000E-01 -5.5415055284E-02

Stress_EigVec1 = -4.9999999452E-01 8.6602540695E-01 -1.4242635739E-08

Stress_EigVec2 = 1.9262541553E-01 1.1121234992E-01 9.7494987693E-01

Stress_EigVec3 = 8.4433136550E-01 4.8747493037E-01 -2.2242467822E-01

-DivStress = -3.7942602769E-01 -2.1906172193E-01 1.0594318263E-01

BPL = 2.2664454431E+00 = 1.2875669898E+00 + 9.7887845335E-01

GBL_I = 2.2657996686E+00

GBL_II = 2.2843530841E+00

GBL_III = 2.2663374973E+00 = 1.2875168148E+00 + 9.7882068251E-01

GBL_IV = 2.2849070735E+00 = 1.3060883383E+00 + 9.7881873519E-01

CP# 12 Coords = -8.25116042917672E-01 4.76380976567859E-01 -1.98216579349076E+00

Type = (3,-1) BCP B1 H4

Rho = 1.6377738591E-01

GradRho = -1.0755285551E-16 4.1633363423E-17 1.6479873022E-17

HessRho_EigVals = -3.3954497257E-01 -2.8826528011E-01 5.2356470651E-01

HessRho_EigVec1 = -2.1920684408E-01 1.2655910354E-01 9.6743534813E-01

HessRho_EigVec2 = 4.9999999141E-01 8.6602540874E-01 2.1483377700E-08

HessRho_EigVec3 = 8.3782359008E-01 -4.8371767047E-01 2.5311824743E-01

DelSqRho = -1.0424554618E-01

Bond Ellipticity = 1.7789063058E-01

V = -3.0669006946E-01

G = 1.4031434146E-01

K = 1.6637572800E-01

L = 2.6061386544E-02

Vnuc = 9.2532402492E+00

Ven = -1.5154714992E+00

Vrep = 1.2087814297E+00
DelSqV = -3.7824889690E+00
DelSqVen = 9.6460908367E-01
DelSqVrep = -4.7470980527E+00
DelSqG = 5.8528969220E+00
DelSqK = -2.0704079529E+00
Stress_EigVals = -1.3259026418E-01 -1.1868475000E-01 -5.5415055284E-02
Stress_EigVec1 = 4.9999999452E-01 8.6602540695E-01 -1.4242636573E-08
Stress_EigVec2 = -1.9262541553E-01 1.1121234992E-01 9.7494987693E-01
Stress_EigVec3 = 8.4433136550E-01 -4.8747493037E-01 2.2242467822E-01
-DivStress = 3.7942602769E-01 -2.1906172193E-01 1.0594318263E-01
BPL = 2.2664454431E+00 = 9.7887845335E-01 + 1.2875669898E+00
GBL_I = 2.2657996686E+00
GBL_II = 2.2843530841E+00
GBL_III = 2.2663374973E+00 = 9.7882068251E-01 + 1.2875168148E+00
GBL_IV = 2.2849070735E+00 = 9.7881873519E-01 + 1.3060883383E+00

CP# 13 Coords = -1.66840426635400E-18 1.32717445641142E+00 1.89231873508784E+00

Type = (3,-1) BCP H6 N5
Rho = 3.3520444406E-01
GradRho = 2.7781518447E-18 -1.5959455979E-16 7.6327832943E-17
HessRho_EigVals = -1.2574602835E+00 -1.2358913467E+00 8.2415500537E-01
HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec2 = 0.0000000000E+00 -3.5994076732E-01 9.3297515723E-01
HessRho_EigVec3 = 0.0000000000E+00 9.3297515723E-01 3.5994076732E-01
DelSqRho = -1.6691966248E+00
Bond Ellipticity = 1.7452130243E-02
V = -5.3416013397E-01
G = 5.8430488883E-02
K = 4.7572964509E-01
L = 4.1729915620E-01
Vnuc = 9.5605694456E+00

Ven = -3.2047453659E+00
Vrep = 2.6705852320E+00
DelSqV = -1.4351045977E+00
DelSqVen = 1.5958470250E+01
DelSqVrep = -1.7393574848E+01
DelSqG = 3.1918157092E+00
DelSqK = -1.7567111116E+00
Stress_EigVals = -3.5754062333E-01 -3.5247560882E-01 1.7585609818E-01
Stress_EigVec1 = 0.0000000000E+00 -3.5412474120E-01 9.3519819700E-01
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 9.3519819700E-01 3.5412474120E-01
-DivStress = 4.3588946159E-18 1.1891284009E+00 4.5225658542E-01
BPL = 1.8831996391E+00 = 4.5768345276E-01 + 1.4255161864E+00
GBL_I = 1.8831381328E+00
GBL_II = 1.9217601941E+00
GBL_III = 1.8831740977E+00 = 4.5767606032E-01 + 1.4254980374E+00
GBL_IV = 1.9218079310E+00 = 4.9630768525E-01 + 1.4255002457E+00

CP# 14 Coords = -1.14936680265323E+00 -6.63587232397108E-01 1.89231874103902E+00

Type = (3,-1) BCP N5 H7
Rho = 3.3520444387E-01
GradRho = 4.8572257327E-17 -6.2450045135E-17 -1.6046192153E-16
HessRho_EigVals = -1.2574602840E+00 -1.2358913493E+00 8.2415497096E-01
HessRho_EigVec1 = -4.9999998965E-01 8.6602540976E-01 2.4447569276E-08
HessRho_EigVec2 = 3.1171785933E-01 1.7997035869E-01 9.3297515839E-01
HessRho_EigVec3 = 8.0798018944E-01 4.6648757716E-01 -3.5994076433E-01
DelSqRho = -1.6691966624E+00
Bond Ellipticity = 1.7452128527E-02
V = -5.3416014534E-01
G = 5.8430489871E-02
K = 4.7572965547E-01
L = 4.1729916560E-01

Vnuc = 9.5605694327E+00
Ven = -3.2047453598E+00
Vrep = 2.6705852145E+00
DelSqV = -1.4351036667E+00
DelSqVen = 1.5958470588E+01
DelSqVrep = -1.7393574254E+01
DelSqG = 3.1918156057E+00
DelSqK = -1.7567119390E+00
Stress_EigVals = -3.5754062206E-01 -3.5247560843E-01 1.7585608516E-01
Stress_EigVec1 = 3.0668096325E-01 1.7706247312E-01 9.3519819685E-01
Stress_EigVec2 = -5.0000003496E-01 8.6602538360E-01 -1.1105015408E-07
Stress_EigVec3 = 8.0990539683E-01 4.6759909707E-01 -3.5412474159E-01
-DivStress = -1.0298154163E+00 -5.9456420497E-01 4.5225658492E-01
BPL = 1.8831996412E+00 = 1.4255161970E+00 + 4.5768344417E-01
GBL_I = 1.8831381349E+00
GBL_II = 1.9217601974E+00
GBL_III = 1.8831740998E+00 = 1.4254980481E+00 + 4.5767605173E-01
GBL_IV = 1.9218079344E+00 = 1.4255002564E+00 + 4.9630767795E-01

CP# 15 Coords = 1.14936680265323E+00 -6.63587232397108E-01 1.89231874103902E+00

Type = (3,-1) BCP H8 N5
Rho = 3.3520444387E-01
GradRho = 1.3183898417E-16 -2.6367796835E-16 2.5153490402E-17
HessRho_EigVals = -1.2574602840E+00 -1.2358913493E+00 8.2415497096E-01
HessRho_EigVec1 = 4.9999998965E-01 8.6602540976E-01 2.4447572844E-08
HessRho_EigVec2 = -3.1171785933E-01 1.7997035869E-01 9.3297515839E-01
HessRho_EigVec3 = 8.0798018944E-01 -4.6648757716E-01 3.5994076433E-01
DelSqRho = -1.6691966624E+00
Bond Ellipticity = 1.7452128527E-02
V = -5.3416014534E-01
G = 5.8430489871E-02
K = 4.7572965547E-01

$L = 4.1729916560E-01$
 $V_{nuc} = 9.5605694327E+00$
 $V_{en} = -3.2047453598E+00$
 $V_{rep} = 2.6705852145E+00$
 $DelSqV = -1.4351036667E+00$
 $DelSqVen = 1.5958470588E+01$
 $DelSqVrep = -1.7393574254E+01$
 $DelSqG = 3.1918156057E+00$
 $DelSqK = -1.7567119390E+00$
 $Stress\_EigVals = -3.5754062206E-01 \ -3.5247560843E-01 \ 1.7585608516E-01$
 $Stress\_EigVec1 = -3.0668096325E-01 \ 1.7706247312E-01 \ 9.3519819685E-01$
 $Stress\_EigVec2 = 5.0000003496E-01 \ 8.6602538360E-01 \ -1.1105016738E-07$
 $Stress\_EigVec3 = 8.0990539683E-01 \ -4.6759909707E-01 \ 3.5412474159E-01$
 $-DivStress = 1.0298154163E+00 \ -5.9456420497E-01 \ 4.5225658492E-01$
 $BPL = 1.8831996412E+00 = 4.5768344417E-01 + 1.4255161970E+00$
 $GBL\_I = 1.8831381349E+00$
 $GBL\_II = 1.9217601974E+00$
 $GBL\_III = 1.8831740998E+00 = 4.5767605173E-01 + 1.4254980481E+00$
 $GBL\_IV = 1.9218079344E+00 = 4.9630767795E-01 + 1.4255002564E+00$

Number of NACPs = 8

Number of NNACPs = 0

Number of BCPs = 7

Number of RCPs = 0

Number of CCPs = 0

$NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H2	B1	N5	102.41023196	104.68212097	104.70747402	103.25046132	103.24997724
H3	B1	N5	102.41023237	104.68212098	104.70747402	103.25046168	103.24997760
H3	B1	H2	115.51330701	113.80593117	113.78553440	114.91008018	114.91043741
H4	B1	N5	102.41023237	104.68212098	104.70747402	103.25046168	103.24997760
H4	B1	H2	115.51330701	113.80593117	113.78553440	114.91008018	114.91043741
H4	B1	H3	115.51330536	113.80593113	113.78553437	114.91007909	114.91043633
H6	N5	B1	111.69306615	111.20417955	111.16676367	111.40482237	111.40504880
H7	N5	B1	111.69306654	111.20417953	111.16676363	111.40482240	111.40504883
H7	N5	H6	107.16087801	107.68404215	107.72374589	107.47031343	107.47007145
H8	N5	B1	111.69306654	111.20417953	111.16676363	111.40482240	111.40504883
H8	N5	H6	107.16087801	107.68404215	107.72374589	107.47031343	107.47007145
H8	N5	H7	107.16087768	107.68404230	107.72374606	107.47031342	107.47007145

Total time for electron density critical point search, analysis and connectivity = 6 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$Ee(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular Ee unless molecular electronic virial theorem is satisfied.

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Ven(A) = Ven(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$VenO(A) = Ven(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$Vee(A) = Vee(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
B1	-2.3852685255E+01	2.3852685255E+01	-6.5441613104E+01	-5.2511819264E+01		
H2	-8.4708630120E-01	8.4708630120E-01	-1.0073225822E+01	-1.6867308303E+00		
H3	-8.4708559639E-01	8.4708559639E-01	-1.0073264821E+01	-1.6867335131E+00		
H4	-8.4708646477E-01	8.4708646477E-01	-1.0073250068E+01	-1.6867325675E+00		
N5	-5.5112088086E+01	5.5112088086E+01	-1.6533911724E+02	-1.3437380828E+02		
H6	-4.5939993828E-01	4.5939993828E-01	-4.1108760800E+00	-9.0540339668E-01		
H7	-4.5940027180E-01	4.5940027180E-01	-4.1108874391E+00	-9.0540491301E-01		
H8	-4.5939951312E-01	4.5939951312E-01	-4.1108766409E+00	-9.0540326839E-01		
Total	-8.2884231427E+01	8.2884231427E+01	-2.7333311122E+02	-1.9466203603E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$E_e(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

VeeX(A) = Exchange-Correlation Part of Vee(A)

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
B1	-2.3852685234E+01	-2.3852685255E+01	2.0882020017E-08			
H2	-8.4708629250E-01	-8.4708630120E-01	8.6960270283E-09			
H3	-8.4708558769E-01	-8.4708559639E-01	8.6960472968E-09			
H4	-8.4708645607E-01	-8.4708646477E-01	8.6960508071E-09			
N5	-5.5112088058E+01	-5.5112088086E+01	2.8277001506E-08			
H6	-4.5939993564E-01	-4.5939993828E-01	2.6365813705E-09			
H7	-4.5940026916E-01	-4.5940027180E-01	2.6365777861E-09			
H8	-4.5939951048E-01	-4.5939951312E-01	2.6365794061E-09			
Total	-8.2884231343E+01	-8.2884231427E+01	8.3156885218E-08			

IQA Atomic Energy Components:

E_IQA(A) = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

Vne(A,Mol)/2 = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

Ven(A,Mol)/2 = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

Vnn(A,Mol)/2 = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

VeeC(A) = Coulomb Part of Vee(A)

VeeX(A) = Exchange-Correlation Part of Vee(A)

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	E_IQA(A) VeeX(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2

B1 1.0650473367E+01			2.3852685255E+01	-3.9429643476E+01	-3.2720806552E+01	
H2 2.4564647330E+00			8.4708630120E-01	-3.0642331670E+00	-5.0366129111E+00	
H3 2.4564647335E+00			8.4708559639E-01	-3.0642331728E+00	-5.0366324105E+00	
H4 2.4564647335E+00			8.4708646477E-01	-3.0642331728E+00	-5.0366250339E+00	
N5 1.3486686369E+01			5.5112088086E+01	-7.7509554928E+01	-8.2669558618E+01	
H6 3.0256110654E+00			4.5939993828E-01	-3.5113331348E+00	-2.0554380400E+00	
H7 3.0256110616E+00			4.5940027180E-01	-3.5113331315E+00	-2.0554437196E+00	
H8 3.0256110616E+00			4.5939951312E-01	-3.5113331315E+00	-2.0554383205E+00	

Total 4.0583387125E+01			8.2884231427E+01	-1.3666589731E+02	-1.3666655561E+02	

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)
B1	2.3852685255E+01	-5.2511819264E+01				
H2	8.4708630120E-01	-1.6867308303E+00				
H3	8.4708559639E-01	-1.6867335131E+00				
H4	8.4708646477E-01	-1.6867325675E+00				
N5	5.5112088086E+01	-1.3437380828E+02				
H6	4.5939993828E-01	-9.0540339668E-01				
H7	4.5940027180E-01	-9.0540491301E-01				
H8	4.5939951312E-01	-9.0540326839E-01				
Total	8.2884231427E+01	-1.9466203603E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A VeeX(A,A')	E_IQA_Inter(A)	Vne(A,A')/2	Ven(A,A')/2	Vee(A,A')	Vnn(A)	VeeC(A,A')

B1	-1.3173733844E+01	-6.4648969202E+00		1.0650473367E+01		
H2	-2.2208677518E+00	-4.1932474960E+00		2.4564647330E+00		
H3	-2.2208664162E+00	-4.1932656539E+00		2.4564647335E+00		
H4	-2.2208668890E+00	-4.1932587502E+00		2.4564647335E+00		
N5	-1.0322650789E+01	-1.5482654479E+01		1.3486686369E+01		
H6	-3.0586314365E+00	-1.6027363417E+00		3.0256110654E+00		
H7	-3.0586306750E+00	-1.6027412630E+00		3.0256110616E+00		
H8	-3.0586314973E+00	-1.6027366863E+00		3.0256110616E+00		

Total	-3.9334879299E+01	-3.9335537590E+01		4.0583387125E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')

B1	3.0750503246E+00	2.2166790610E+00	7.2085944195E+01	8.5837126364E-01	
2.7914055805E+01					

H2	1.6747746311E+00 2.5696069145E+01	1.2444233839E+00	7.4303930855E+01	4.3035124724E-01
H3	1.6747817567E+00 2.5696050650E+01	1.2444289882E+00	7.4303949350E+01	4.3035276848E-01
H4	1.6747785821E+00 2.5696042936E+01	1.2444267586E+00	7.4303957064E+01	4.3035182354E-01
N5	8.1138082500E+00 1.7551500909E+01	6.6897131212E+00	8.2448499091E+01	1.4240951288E+00
H6	5.9567808361E-01 6.4908893758E+01	2.0903002918E-01	3.5091106242E+01	3.8664805443E-01
H7	5.9567978715E-01 6.4908824671E+01	2.0903103851E-01	3.5091175329E+01	3.8664874864E-01
H8	5.9567838666E-01 6.4908886667E+01	2.0903017776E-01	3.5091113333E+01	3.8664820889E-01

Total	1.8000229802E+01 2.6296704518E+01	1.3266762558E+01	7.3703295482E+01	4.7334672436E+00

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2

B1	3.0750503246E+00		2.2166790610E+00	8.5837126364E-01	8.5109522700E-01
	7.2760366451E-03				
H2	1.6747746311E+00		1.2444233839E+00	4.3035124724E-01	2.3536361127E-01
	1.9498763597E-01				
H3	1.6747817567E+00		1.2444289882E+00	4.3035276848E-01	2.3531692994E-01
	1.9503583854E-01				
H4	1.6747785821E+00		1.2444267586E+00	4.3035182354E-01	2.3527369142E-01
	1.9507813212E-01				
N5	8.1138082500E+00		6.6897131212E+00	1.4240951288E+00	1.2352295802E+00
	1.8886554857E-01				
H6	5.9567808361E-01	2.0903002918E-01	3.8664805443E-01	3.6334818767E-01	2.3299866756E-02
H7	5.9567978715E-01	2.0903103851E-01	3.8664874864E-01	3.6337183798E-01	2.3276910663E-02
H8	5.9567838666E-01	2.0903017776E-01	3.8664820889E-01	3.6336856020E-01	2.3279648698E-02

Total	1.8000229802E+01		1.3266762558E+01	4.7334672436E+00	3.8823676257E+00
	8.5109961796E-01				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

B1	3.6196277190E+00	2.2518299000E+01	2.6137926719E+01
H2	7.8022334057E-01	1.3455355358E+01	1.4235578699E+01
H3	7.8023247215E-01	1.3455406794E+01	1.4235639266E+01
H4	7.8022827023E-01	1.3455384012E+01	1.4235612282E+01
N5	2.9572085598E+01	3.9395269079E+01	6.8967354677E+01
H6	7.2901175055E-02	4.9903564057E+00	5.0632575807E+00
H7	7.2901685155E-02	4.9903703756E+00	5.0632720608E+00
H8	7.2901281284E-02	4.9903588753E+00	5.0632601565E+00

Total	3.5751101541E+01	1.1725079990E+02	1.5300190144E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$
B1	H2	4.9146526618E+00	4.7072722255E-01	7.6539759167E+00	1.4053449754E+01 (Bonded)
B1	H3	4.9147212546E+00	4.7063385988E-01	7.6524578495E+00	1.4050602653E+01 (Bonded)
H2	H3	2.7428371195E+00	1.2408975844E-01	3.7046703519E+00	3.7046545900E+00
B1	H4	4.9147547311E+00	4.7054738284E-01	7.6510517417E+00	1.4048047541E+01 (Bonded)
H2	H4	2.7428322708E+00	1.2408882248E-01	3.7046424090E+00	3.7046336694E+00
H3	H4	2.7428439340E+00	1.2408936350E-01	3.7046427991E+00	3.7046498213E+00

B1	N5	2.4805227699E+01	2.9028198873E-01	4.7199550915E+00	1.7888146958E+00	(Bonded)
H2	N5	1.3525816178E+01	1.2596808078E-01	3.7607472205E+00	7.7625744223E-01	
H3	N5	1.3525874180E+01	1.2596770895E-01	3.7607201191E+00	7.7625515090E-01	
H4	N5	1.3525844741E+01	1.2597507085E-01	3.7609470348E+00	7.7630051737E-01	
B1	H6	1.8292996340E+00	4.8809007005E-03	7.9362940200E-02	4.0969282191E-01	
H2	H6	9.9323353879E-01	8.7860078914E-03	2.6230418494E-01	7.3747953241E-01	
H3	H6	9.9581866489E-01	3.6242447893E-03	1.0820050955E-01	3.0421169496E-01	
H4	H6	9.9581675775E-01	3.6242770010E-03	1.0820167632E-01	3.0421439875E-01	
N5	H6	4.4698695614E+00	7.2669637534E-01	4.4781460996E+00	6.0997407437E+01	(Bonded)
B1	H7	1.8293056583E+00	4.8793291231E-03	7.9337386515E-02	4.0955973565E-01	
H2	H7	9.9581723920E-01	3.6243131653E-03	1.0820301126E-01	3.0421656429E-01	
H3	H7	9.9324060638E-01	8.7860679131E-03	2.6230486086E-01	7.3748246144E-01	
H4	H7	9.9581963020E-01	3.6242382076E-03	1.0820051816E-01	3.0421027252E-01	
N5	H7	4.4698597333E+00	7.2674367595E-01	4.4784375817E+00	6.1001203300E+01	(Bonded)
H6	H7	3.4841313777E-01	1.2840512567E-02	1.0778063622E+00	1.0778032799E+00	
B1	H8	1.8293063607E+00	4.8693110399E-03	7.9174493518E-02	4.0871980157E-01	
H2	H8	9.9581496045E-01	3.6241796482E-03	1.0819902514E-01	3.0420607239E-01	
H3	H8	9.9581911083E-01	3.6243679781E-03	1.0820418731E-01	3.0422188041E-01	
H4	H8	9.9323638002E-01	8.7860475426E-03	2.6230474991E-01	7.3748248546E-01	
N5	H8	4.4698516478E+00	7.2673712039E-01	4.4783971842E+00	6.1000796459E+01	(Bonded)
H6	H8	3.4841230124E-01	1.2840517150E-02	1.0778067469E+00	1.0778061986E+00	
H7	H8	3.4841331503E-01	1.2840519098E-02	1.0778038281E+00	1.0778063621E+00	

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
B1	N5	5.9744924280E+01	4.6344703326E+01	3.7083881960E+01
B1	H2	5.6247169335E+01	4.3525654790E+01	3.4955191210E+01
B1	H3	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
B1	H4	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
B1	Total	2.2848643234E+02	1.7692166775E+02	1.4194945563E+02
H2	B1	5.6247169335E+01	4.3525654790E+01	3.4955191210E+01
H2	Total	5.6247169335E+01	4.3525654790E+01	3.4955191210E+01
H3	B1	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
H3	Total	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
H4	B1	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
H4	Total	5.6247169361E+01	4.3525654817E+01	3.4955191230E+01
N5	B1	5.9744924280E+01	4.6344703326E+01	3.7083881960E+01
N5	H6	3.2849553079E+01	2.5457237949E+01	2.0402567036E+01
N5	H7	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
N5	H8	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
N5	Total	1.5829358335E+02	1.2271641705E+02	9.8291582978E+01
H6	N5	3.2849553079E+01	2.5457237949E+01	2.0402567036E+01

H6	Total	3.2849553079E+01	2.5457237949E+01	2.0402567036E+01
H7	N5	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
H7	Total	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
H8	N5	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
H8	Total	3.2849552997E+01	2.5457237888E+01	2.0402566991E+01
Total	Total	6.5407018282E+02	5.0658676295E+02	4.0631431330E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta^2 \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta^2 \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N_{IAS}(A B)$	$G_{IAS}(A B)$	$K_{IAS}(A B)$	$L_{IAS}(A B)$	$\Delta^2 \rho_{IAS}(A B)$	$V_{IAS}(A B)$
B1	N5	8.1744191352E-01	7.1107678313E-01	1.8858233965E-01	-5.2249444348E-01	2.0899777739E+00	-8.9965912278E-01
B1	H2	9.3972899466E-01	6.4055557853E-01	3.9149454280E-01	-2.4906103573E-01	9.9624414292E-01	-1.0320501213E+00

B1	H3	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					
B1	H4	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					

B1	Total	3.6366288832E+00	2.6327435203E+00	1.3630659549E+00	-1.2696775653E+00
5.0787102613E+00 -3.9958094751E+00					
H2	B1	9.3972899466E-01	6.4055557853E-01	3.9149454280E-01	-2.4906103573E-01
9.9624414292E-01 -1.0320501213E+00					

H2	Total	9.3972899466E-01	6.4055557853E-01	3.9149454280E-01	-2.4906103573E-01
9.9624414292E-01 -1.0320501213E+00					
H3	B1	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					

H3	Total	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					
H4	B1	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					

H4	Total	9.3972898749E-01	6.4055557930E-01	3.9149453624E-01	-2.4906104306E-01
9.9624417224E-01 -1.0320501155E+00					
N5	B1	8.1744191352E-01	7.1107678313E-01	1.8858233965E-01	-5.2249444348E-01
2.0899777739E+00 -8.9965912278E-01					
N5	H6	8.3468751491E-01	5.4833114915E-01	4.3680877107E-01	-1.1152237808E-01
4.4608951232E-01 -9.8513992021E-01					
N5	H7	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
4.4608945439E-01 -9.8513992892E-01					
N5	H8	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
4.4608945439E-01 -9.8513992892E-01					

N5	Total	3.3215044510E+00	2.3560702248E+00	1.4990086760E+00	-8.5706154876E-01
3.4282461950E+00 -3.8550789008E+00					

H6	N5	8.3468751491E-01	5.4833114915E-01	4.3680877107E-01	-1.1152237808E-01
		4.4608951232E-01	-9.8513992021E-01		

H6	Total	8.3468751491E-01	5.4833114915E-01	4.3680877107E-01	-1.1152237808E-01
		4.4608951232E-01	-9.8513992021E-01		

H7	N5	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
		4.4608945439E-01	-9.8513992892E-01		

H7	Total	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
		4.4608945439E-01	-9.8513992892E-01		

H8	N5	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
		4.4608945439E-01	-9.8513992892E-01		

H8	Total	8.3468751131E-01	5.4833114626E-01	4.3680878266E-01	-1.1152236360E-01
		4.4608945439E-01	-9.8513992892E-01		

Total	Total	1.2281382841E+01	8.5554739239E+00	5.3469845826E+00	-3.2084893412E+00
		1.2833957365E+01	-1.3902458506E+01		

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

$|ESP|_{Int\_IDS}(A)$ = Surface Integral of $|ESP|$ Over Atom A's Part of IDS

$ESP*ESP_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Atom A's Part of IDS

$Area\_ESP+_{IDS}(A)$ = Surface Area of Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Int\_IDS}(A)$ = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

$Area\_ESP-_{IDS}(A)$ = Surface Area of Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Int\_IDS}(A)$ = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

$ESP+_{Min\_IDS}(A)$ = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Avg\_IDS}(A)$ = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Var\_IDS}(A)$ = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+*ESP+_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Positive Regions of Atom A's Part of IDS

$ESP-_{Min\_IDS}(A)$ = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Avg\_IDS}(A)$ = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Var\_IDS}(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-*ESP-_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)

B1	4.5904901916E+00

H2	7.6035950887E+01

H3	7.5808544245E+01

H4	7.5688983446E+01

N5	3.7824378805E+01

H6	3.4922632866E+01

H7	3.5003879615E+01

H8	3.4783702017E+01

Total	3.7465856207E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				
B1	4.4628539713E+00	-1.5369474281E-01	1.5140160259E-02	-5.5473144321E-02	-3.4438667230E-02
	1.9296841024E-02	4.9433784866E-04			
H2	6.2230941033E+01	-2.1532786906E+00	1.7543352070E-02	-5.5447693187E-02	-3.4601416190E-02
	1.3920802394E-02	2.9597328120E-04			
H3	6.2236785836E+01	-2.1435295513E+00	1.8085908665E-02	-5.5400806227E-02	-3.4441520759E-02
	1.3993281085E-02	2.9878509052E-04			
H4	6.1945839313E+01	-2.1441480767E+00	1.7241321254E-02	-5.5380219434E-02	-3.4613270244E-02
	1.3852267149E-02	2.9181429517E-04			
N5	3.6841173257E+01	1.8997953781E+00	6.8899870122E-02	8.4216454824E-03	5.1567179059E-02
	1.5733424027E-02	3.1994522498E-04			
H6	2.8989494430E+01	1.9219600884E+00	8.1427156637E-02	2.9478016354E-02	6.6298503171E-02
	9.5583027982E-03	1.5222799217E-04			
H7	2.8919420331E+01	1.9090123330E+00	8.1437287714E-02	2.3390759942E-02	6.6011431459E-02
	9.9330278963E-03	1.6390450016E-04			
H8	2.9220647325E+01	1.9303296409E+00	8.1412783309E-02	2.4529632088E-02	6.6060468114E-02
	9.7906434609E-03	1.6104738402E-04			
Total	3.1484715550E+02	1.0664463790E+00	8.1437287714E-02	-5.5473144321E-02	3.3871875936E-03
		2.4967607405E-03			

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
ESP-_Int_IDS(A)					
B1	1.6226124354E-01	7.4991997338E-03	6.1981134748E-01	4.2832503638E-03	3.8430426238E+00
	-1.5797799318E-01				
H2	2.2069793662E+00	9.2925187955E-02	3.5535402673E+00	2.6850337803E-02	5.8677400766E+01
	-2.1801290284E+00				
H3	2.1983019123E+00	9.2421841228E-02	3.5677252403E+00	2.7386180506E-02	5.8669060596E+01
	-2.1709157318E+00				

H4	2.1938832247E+00	9.2292658259E-02	3.4891738843E+00	2.4867574034E-02
5.8456665429E+01	-2.1690156507E+00			
N5	1.8997953781E+00	1.0975424590E-01	3.6841173257E+01	1.8997953781E+00
0.0000000000E+00	NULL			
H6	1.9219600884E+00	1.3183608955E-01	2.8989494430E+01	1.9219600884E+00
0.0000000000E+00	NULL			
H7	1.9090123330E+00	1.3075665991E-01	2.8919420331E+01	1.9090123330E+00
0.0000000000E+00	NULL			
H8	1.9303296409E+00	1.3222438850E-01	2.9220647325E+01	1.9303296409E+00
0.0000000000E+00	NULL			

Total	1.4422523187E+01	7.8971027104E-01	1.3520098608E+02	7.7444847831E+00
1.7964616941E+02	-6.6780384041E+00			

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

B1	2.1252851932E-03	6.9105710653E-03	3.1982658969E-03	1.4818887840E-05
3.8784620870E-05				
H2	1.0921238718E-04	7.5559402127E-03	4.2742595589E-03	2.6600399332E-05
2.9740513728E-04				
H3	6.1149851587E-05	7.6760901307E-03	4.4144077780E-03	2.5655511332E-05
3.0175060523E-04				
H4	1.2033392533E-04	7.1270664226E-03	4.4031298044E-03	2.5242832703E-05
2.6530948454E-04				
N5	8.4216454824E-03	5.1567179059E-02	1.5733424027E-02	3.1994522498E-04
1.0975424590E-01				
H6	2.9478016354E-02	6.6298503171E-02	9.5583027982E-03	1.5222799217E-04
1.3183608955E-01				
H7	2.3390759942E-02	6.6011431459E-02	9.9330278963E-03	1.6390450016E-04
1.3075665991E-01				
H8	2.4529632088E-02	6.6060468114E-02	9.7906434609E-03	1.6104738402E-04
1.3222438850E-01				

Total	6.1149851587E-05	5.7281274401E-02	4.5754603974E-04	5.0547463371E-01

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
B1	-2.1407474273E-04	-4.1107530840E-02	1.2960500724E-02	2.5144917216E-04	7.4604151130E-03
H2	-4.1299774394E-04	-3.7154492188E-02	1.1719238000E-02	1.9813754038E-04	9.2627782818E-02
H3	-1.6824239259E-05	-3.7002735510E-02	1.1790995813E-02	2.0096231071E-04	9.2120090623E-02
H4	-7.7878987039E-04	-3.7104676341E-02	1.1708654966E-02	1.9752623577E-04	9.2027348775E-02
N5	NULL	NULL	NULL	NULL	NULL
H6	NULL	NULL	NULL	NULL	NULL
H7	NULL	NULL	NULL	NULL	NULL
H8	NULL	NULL	NULL	NULL	NULL
Total	-1.6824239259E-05	-3.7173285831E-02	2.0034385961E-04	2.8423563733E-01	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
B1	4.7133776276E+00				
H2	5.3057394970E+01				
H3	5.2647407836E+01				
H4	5.2797929435E+01				
N5	3.7373327431E+01				
H6	2.4573033799E+01				
H7	2.4603836138E+01				
H8	2.4445748109E+01				

Total 2.742120535E+02

Atomic Surface Area and Volume Data:

$$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1 9.9966949289E+01	2.3307692253E+02	2.5585823207E+01	3.0740339986E+00	1.2014598763E-01	
H2 9.8813014138E+01	1.3228312022E+02	1.2097965932E+02	1.6548952933E+00	1.3679120132E-02	
H3 9.8815271308E+01	1.3205571361E+02	1.2107557937E+02	1.6549401367E+00	1.3668653459E-02	
H4 9.8814308929E+01	1.3193615281E+02	1.2103101713E+02	1.6549208820E+00	1.3673527012E-02	
N5 9.9906093247E+01	1.9611796216E+02	1.1563759775E+02	8.1061888362E+00	7.0099941489E-02	
H6 9.8850109138E+01	6.7772185945E+01	4.2266182940E+01	5.8882843580E-01	1.3931431581E-02	
H7 9.8854171765E+01	6.7853432612E+01	4.2332163886E+01	5.8885432003E-01	1.3910328837E-02	
H8 9.8850162887E+01	6.7633255014E+01	4.2264202291E+01	5.8882905530E-01	1.3932099114E-02	

Total	1.0287287449E+03	6.3117222589E+02	1.7911490958E+01	2.8378135512E-02
	9.9507012716E+01			

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	1.8138452172E+02	2.3238494520E+01	3.0725017019E+00	1.3221603918E-01	
	9.9917119317E+01				
H2	1.0575659582E+02	8.7549639819E+01	1.6332742875E+00	1.8655408416E-02	
	9.7522034122E+01				
H3	1.0576244065E+02	8.7606663819E+01	1.6333388219E+00	1.8644002074E-02	
	9.7525472520E+01				
H4	1.0547149413E+02	8.7575925059E+01	1.6333045640E+00	1.8650154855E-02	
	9.7523611865E+01				
N5	1.5955759031E+02	9.9716417354E+01	8.0957604497E+00	8.1187839120E-02	
	9.9777566836E+01				
H6	5.4446732379E+01	3.0419758128E+01	5.8113158300E-01	1.9103754230E-02	
	9.7557992975E+01				
H7	5.4376658219E+01	3.0376062932E+01	5.8109221340E-01	1.9129938422E-02	
	9.7551104783E+01				
H8	5.4677885213E+01	3.0423419296E+01	5.8113084223E-01	1.9101430927E-02	
	9.7557819024E+01				
Total	8.2143391845E+02	4.7690638093E+02	1.7811534464E+01	3.7348073282E-02	
	9.8951705949E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	1.4666283326E+02	2.1434821923E+01	3.0699033046E+00	1.4322037830E-01	
	9.9832619975E+01				
H2	8.8012586180E+01	6.7049386945E+01	1.6041943981E+00	2.3925563994E-02	
	9.5785687699E+01				
H3	8.7602599066E+01	6.7067913209E+01	1.6042381034E+00	2.3919606659E-02	
	9.5787889794E+01				

H4	8.7753120665E+01	6.7016563305E+01	1.6041332397E+00	2.3936369765E-02
9.5781810016E+01				
N5	1.3566491041E+02	8.7190568295E+01	8.0776481966E+00	9.2643600731E-02
9.9554339314E+01				
H6	4.4975600835E+01	2.2693689867E+01	5.7003927465E-01	2.5118844842E-02
9.5695861623E+01				
H7	4.5006403129E+01	2.2693953818E+01	5.7003935358E-01	2.5118556164E-02
9.5695601195E+01				
H8	4.4848315100E+01	2.2679265065E+01	5.7001706382E-01	2.5133841956E-02
9.5692084315E+01				

Total	6.8052636864E+02	3.7782616243E+02	1.7670212934E+01	4.6768103143E-02
9.8166596365E+01				

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

B1	N5	-9.9278053759E-02		
B1	H2	6.7474399110E-01		
B1	H3	6.7475111640E-01		
B1	H4	6.7474794180E-01		
B1		1.9249649955E+00	1.9249496754E+00	
H2	B1	-6.7475931125E-01		
H2		-6.7475931125E-01	-6.7477463140E-01	
H3	B1	-6.7476643655E-01		
H3		-6.7476643655E-01	-6.7478175670E-01	
H4	B1	-6.7476326195E-01		
H4		-6.7476326195E-01	-6.7477858210E-01	
N5	B1	9.9262733611E-02		

N5	H6	-4.0435255665E-01
N5	H7	-4.0435085308E-01
N5	H8	-4.0435225384E-01
N5		-1.1137929300E+00 -1.1138082501E+00
H6	N5	4.0433723650E-01
H6		4.0433723650E-01 4.0432191635E-01
H7	N5	4.0433553293E-01
H7		4.0433553293E-01 4.0432021278E-01
H8	N5	4.0433693369E-01
H8		4.0433693369E-01 4.0432161354E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

B1	7.4286008360E-04	-2.6194133899E-06	7.4024067021E-04
H2	3.9211267181E-06	-4.4978003067E-18	3.9211267181E-06
H3	1.8001000134E-01	-7.3439675916E-01	-5.5438675782E-01
H4	-1.8001017209E-01	7.3439330402E-01	5.5438313193E-01
N5	1.3704498930E-04	1.6099870430E-06	1.3865497634E-04
H6	1.1596770295E-06	6.7459797042E-19	1.1596770295E-06
H7	1.3342901218E-01	-1.6280253936E-01	-2.9373527177E-02
H8	-1.3342936359E-01	1.6280310336E-01	2.9373739772E-02

Total	8.8446371665E-04	-3.9005663976E-06	8.8056315025E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

B1	-2.0570285634E-04	-5.2819108716E-06	-2.1098476721E-04
H2	-2.0785868598E-01	8.4799937499E-01	6.4014068901E-01
H3	1.0393856898E-01	-4.2400416215E-01	-3.2006559317E-01
H4	1.0393773422E-01	-4.2400216732E-01	-3.2006443310E-01
N5	2.9259831802E-04	1.3281644378E-06	2.9392648246E-04
H6	-1.5407043577E-01	1.8798897376E-01	3.3918537991E-02
H7	7.7035680041E-02	-9.3994089164E-02	-1.6958409123E-02
H8	7.7035368655E-02	-9.3994414793E-02	-1.6959046138E-02

Total 1.0512560768E-04 -1.0438418738E-05 9.4687188942E-05

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

B1	6.9571948828E-02	5.5063797787E-01	6.2020992670E-01
H2	-6.7354981697E-02	2.3995501148E-01	1.7260002978E-01
H3	-6.7367406471E-02	2.3995754306E-01	1.7259013659E-01
H4	-6.7359302744E-02	2.3995641413E-01	1.7259711138E-01
N5	1.9762364298E-01	8.4527860038E-01	1.0429022434E+00
H6	-7.8723628928E-02	7.0220178355E-02	-8.5034505728E-03
H7	-7.8722370480E-02	7.0219880094E-02	-8.5024903856E-03
H8	-7.8723304055E-02	7.0220123361E-02	-8.5031806943E-03

Total -1.7105540257E-01 2.3264457287E+00 2.1553903262E+00

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

B1	6.9576218771E-02	5.5063797790E-01	6.2021040433E-01
H2	2.1849926066E-01	8.8129526693E-01	6.6300141178E-01
H3	2.1850673710E-01	8.8130457383E-01	6.6300378311E-01
H4	2.1850398238E-01	8.8130042752E-01	6.6300200690E-01
N5	1.9762390711E-01	8.4527860039E-01	1.0429022940E+00

H6	1.7301765497E-01	2.0067567791E-01	3.4968212600E-02
H7	1.7301736591E-01	2.0067482946E-01	3.4966899799E-02
H8	1.7301792304E-01	2.0067552467E-01	3.4967555191E-02

Total	1.7105772147E-01	2.3264457288E+00	2.1553905081E+00

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

B1	N5	-2.3284725536E-19	
B1	H2	4.4976981858E-18	
B1	H3	-5.5674797112E-01	
B1	H4	5.5674535171E-01	
B1		-2.6194133899E-06	
H2	B1	-4.4978003067E-18	
H2		-4.4978003067E-18	
H3	B1	-7.3439675916E-01	
H3		-7.3439675916E-01	
H4	B1	7.3439330402E-01	
H4		7.3439330402E-01	
N5	B1	2.3281132341E-19	
N5	H6	-6.7462353062E-19	
N5	H7	-4.6474744715E-01	
N5	H8	4.6474905714E-01	
N5		1.6099870430E-06	
H6	N5	6.7459797042E-19	
H6		6.7459797042E-19	

H7	N5	-1.6280253936E-01
H7		-1.6280253936E-01
H8	N5	1.6280310336E-01
H8		1.6280310336E-01

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

B1	N5	-1.4591311889E-10
B1	H2	6.4287039746E-01
B1	H3	-3.2143859577E-01
B1	H4	-3.2143708345E-01
B1		-5.2819108716E-06
H2	B1	8.4799937499E-01
H2		8.4799937499E-01
H3	B1	-4.2400416215E-01
H3		-4.2400416215E-01
H4	B1	-4.2400216732E-01
H4		-4.2400216732E-01
N5	B1	1.4589060222E-10
N5	H6	5.3664638457E-01
N5	H7	-2.6832206351E-01
N5	H8	-2.6832299304E-01
N5		1.3281644378E-06
H6	N5	1.8798897376E-01
H6		1.8798897376E-01
H7	N5	-9.3994089164E-02
H7		-9.3994089164E-02
H8	N5	-9.3994414793E-02
H8		-9.3994414793E-02

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	N5	9.6508639890E-02
B1	H2	1.5137561619E-01
B1	H3	1.5137721700E-01
B1	H4	1.5137650479E-01
B1		5.5063797787E-01
H2	B1	2.3995501148E-01
H2		2.3995501148E-01
H3	B1	2.3995754306E-01
H3		2.3995754306E-01
H4	B1	2.3995641413E-01
H4		2.3995641413E-01
N5	B1	2.1418772692E-01
N5	H6	2.1036397082E-01
N5	H7	2.1036308695E-01
N5	H8	2.1036381569E-01
N5		8.4527860038E-01
H6	N5	7.0220178355E-02
H6		7.0220178355E-02
H7	N5	7.0219880094E-02
H7		7.0219880094E-02
H8	N5	7.0220123361E-02
H8		7.0220123361E-02

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

B1	N5	9.6508639890E-02	
B1	H2	6.6045206117E-01	
B1	H3	6.6045903433E-01	
B1	H4	6.6045592697E-01	
B1		5.5063797790E-01	
H2	B1	8.8129526693E-01	
H2		8.8129526693E-01	

B1	N5	9.6508639890E-02
B1	H2	6.6045206117E-01
B1	H3	6.6045903433E-01
B1	H4	6.6045592697E-01
B1		5.5063797790E-01
H2	B1	8.8129526693E-01
H2		8.8129526693E-01

H3	B1	8.8130457383E-01
H3		8.8130457383E-01
H4	B1	8.8130042752E-01
H4		8.8130042752E-01
N5	B1	2.1418772692E-01
N5	H6	5.7640466886E-01
N5	H7	5.7640224475E-01
N5	H8	5.7640424153E-01
N5		8.4527860039E-01
H6	N5	2.0067567791E-01
H6		2.0067567791E-01
H7	N5	2.0067482946E-01
H7		2.0067482946E-01
H8	N5	2.0067552467E-01
H8		2.0067552467E-01

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)

B1	-1.4957087498E-02	-3.8830634081E-03	3.3475715035E-03	-2.1858048048E-02	2.5619651530E-03	3.6815135546E-02
H2	-3.9719372440E-01	-6.8256200693E-08	2.8814416603E-05	5.9000497693E-01	2.3049451767E-01	-1.9281125253E-01

H3 3.4324444189E-01 4.2750842052E-01 -1.9961549515E-01 -1.5044628312E-01 -1.1519879354E-01 -1.9279815877E-01

H4 3.4322845250E-01 -4.2746831756E-01 1.9962556852E-01 -1.5041436218E-01 -1.1521315306E-01 -1.9281409032E-01

N5 6.9363646635E-01 3.2386034990E-04 -1.9800681666E-04 6.9850068603E-01 -1.1157495432E-03 -1.3921371524E+00

H6 -5.6210115791E-02 2.9660300273E-06 -2.6198530605E-06 1.1106220241E-01 1.9835467852E-02 -5.4852086621E-02

H7 6.9248466009E-02 7.2435461313E-02 -1.7174602890E-02 -1.4403755004E-02 -9.9198317863E-03 -5.4844711004E-02

H8 6.9246374789E-02 -7.2433462077E-02 1.7175095459E-02 -1.4396532327E-02 -9.9222576254E-03 -5.4849842462E-02

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
B1	1	-2.3830397153E-02	4.1950343496E-01	9.0567373269E-01	-6.1416267974E-02
B1	2	-1.3291024436E-02	9.0568977459E-01	-4.2215040329E-01	-3.8923889968E-02
B1	3	3.7121421589E-02	6.1179247012E-02	3.9295380354E-02	9.9735298306E-01
H2	1	-3.9719372992E-01	9.999998067E-01	4.4776555296E-05	-1.9148004791E-04
H2	2	-2.5563659098E-01	1.9651557898E-04	-2.6297403687E-01	9.6480289040E-01
H2	3	6.5283032090E-01	7.1537312061E-06	9.6480290937E-01	2.6297404058E-01
H3	1	-3.9725676434E-01	-5.0003325463E-01	8.6600616670E-01	-2.5198309683E-04
H3	2	-2.5560925987E-01	2.2758874063E-01	1.3169081148E-01	9.6481132627E-01
H3	3	6.5286602421E-01	8.3556574212E-01	4.8238039907E-01	-2.6294303793E-01
H4	1	-3.9720208748E-01	5.0002418539E-01	8.6601141585E-01	-2.0405540726E-04
H4	2	-2.5563484126E-01	-2.2763116652E-01	1.3165872914E-01	9.6480569602E-01
H4	3	6.5283692875E-01	8.3555961251E-01	-4.8237973285E-01	2.6296373759E-01

N5	1	-1.3921377666E+00	9.4849168580E-05	5.3367365361E-04	9.9999985310E-01
N5	2	6.9361500578E-01	9.9780929037E-01	-6.6156001432E-02	-5.9335675318E-05
N5	3	6.9852276082E-01	6.6155960048E-02	9.9780914942E-01	-5.3877937133E-04
H6	1	-5.7190517163E-02	3.0080383256E-03	-1.1707964425E-01	9.9311797316E-01
H6	2	-5.6210106961E-02	9.9999547572E-01	3.3673002809E-04	-2.9891720468E-03
H6	3	1.1340062412E-01	1.5558556850E-05	9.9312247156E-01	1.1708012745E-01
H7	1	-5.7182749844E-02	9.9276022448E-02	6.2189998535E-02	9.9311463359E-01
H7	2	-5.6221632375E-02	-5.0040161717E-01	8.6578324738E-01	-4.1940543079E-03
H7	3	1.1340438222E-01	8.6008284072E-01	4.9653979966E-01	-1.1707149294E-01
H8	1	-5.7188227145E-02	-9.8543587894E-02	6.3470401489E-02	9.9310657506E-01
H8	2	-5.6214992230E-02	5.0056392366E-01	8.6568109570E-01	-5.6567561219E-03
H8	3	1.1340321938E-01	8.6007262462E-01	-4.9655588677E-01	1.1707831435E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.1973131525E+01		1.0502363853E+01	3.0750503246E+00	1.9840358486E+00
	2.2927794788E+00				
H2	3.1306065191E+00		1.6867308303E+00	1.6747746314E+00	2.3056687801E+00
	4.0102617959E+00				
H3	3.1306075903E+00		1.6867335131E+00	1.6747817567E+00	2.3056885400E+00
	4.0103192820E+00				
H4	3.1306073428E+00		1.6867325675E+00	1.6747785821E+00	2.3056781440E+00
	4.0102847654E+00				
N5	1.9231840052E+02		1.9196258325E+01	8.1138082501E+00	8.7738154803E+00
	1.3697519242E+01				

H6 2.4907158122E+00 9.0540339668E-01 5.9567808365E-01 5.8225300730E-01 7.8583372257E-01

H7 2.4907173157E+00 9.0540491301E-01 5.9567978722E-01 5.8225533863E-01 7.8583833052E-01

H8 2.4907153431E+00 9.0540326839E-01 5.9567838646E-01 5.8225411470E-01 7.8583676561E-01

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
B1	-9.0677477947E+01	-1.9358299617E+01	-6.9949952163E+00	-4.6480587107E+00	-
6.0610135102E+00					
H2	-2.6890709113E+00	-2.5915886353E+00	-3.5738269914E+00	-6.3766719551E+00	-
1.4074708443E+01					
H3	-2.6890743477E+00	-2.5915977520E+00	-3.5738525819E+00	-6.3767480754E+00	-
1.4074947605E+01					
H4	-2.6890726629E+00	-2.5915927727E+00	-3.5738371204E+00	-6.3766974168E+00	-
1.4074773465E+01					
N5	-1.9105526577E+02	-3.5997692957E+01	-1.9571447718E+01	-2.5071597350E+01	-
4.6192900344E+01					
H6	-1.7392956124E+00	-1.2352669566E+00	-1.2781555474E+00	-1.7781798048E+00	-
3.1592641075E+00					
H7	-1.7392982220E+00	-1.2352701225E+00	-1.2781601458E+00	-1.7781885677E+00	-
3.1592915190E+00					
H8	-1.7392958062E+00	-1.2352679687E+00	-1.2781582808E+00	-1.7781864035E+00	-
3.1592802461E+00					

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

B1	1.5375251623E+00	1.5375251623E+00	3.0750503246E+00	0.0000000000E+00
H2	8.3738731572E-01	8.3738731572E-01	1.6747746314E+00	0.0000000000E+00
H3	8.3739087836E-01	8.3739087836E-01	1.6747817567E+00	0.0000000000E+00
H4	8.3738929106E-01	8.3738929106E-01	1.6747785821E+00	0.0000000000E+00
N5	4.0569041251E+00	4.0569041251E+00	8.1138082501E+00	0.0000000000E+00
H6	2.9783904183E-01	2.9783904183E-01	5.9567808365E-01	0.0000000000E+00
H7	2.9783989361E-01	2.9783989361E-01	5.9567978722E-01	0.0000000000E+00
H8	2.9783919323E-01	2.9783919323E-01	5.9567838646E-01	0.0000000000E+00

Total	9.0001149012E+00	9.0001149012E+00	1.8000229802E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's

underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

BH4

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\bh4\bh4.wfx

Sum File: D:\calc\ellipticity\bh4\bh4.sum

SumViz File: D:\calc\ellipticity\bh4\bh4.sumviz

Wfx Title: bh4_mp2

Total memory allocated for AIMSum = 0.367 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	9.9999999951
Number of Alpha electrons (from MO Occs)	=	4.9999999975
Number of Beta electrons (from MO Occs)	=	4.9999999975
Number of electron pairs ($N*(N-1)/2$)	=	44.9999999534
Number of electron pairs (from Muller 2EDM)	=	44.9998894953
Number of electron pairs (from Muller 2EDM, no SOSI)	=	45.1130498789

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
B1	5.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
H2	1.0	1.3490444800E+00	1.3490444800E+00	1.3490444800E+00
H3	1.0	-1.3490444800E+00	1.3490444800E+00	-1.3490444800E+00
H4	1.0	1.3490444800E+00	-1.3490444800E+00	-1.3490444800E+00
H5	1.0	-1.3490444800E+00	-1.3490444800E+00	1.3490444800E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	Mu_Intra(A)
B1	1.7936330353E+00	-6.0939967342E-04	2.3887366933E+01	-2.3901997248E+01	6.3785370370E-03
H2	-6.9856706570E-01	2.8750291611E-05	8.0585941981E-01	-8.0635298517E-01	7.6107976139E-02
H3	-6.9856863140E-01	2.8081891845E-05	8.0585978307E-01	-8.0635334866E-01	7.6110022325E-02
H4	-6.9856796320E-01	2.7999528487E-05	8.0585926043E-01	-8.0635282570E-01	7.6109000500E-02
H5	-6.9856762490E-01	2.8257691296E-05	8.0585927151E-01	-8.0635283678E-01	7.6108560803E-02
Total	-1.0006382499E+00	-4.9631027018E-04	2.7110804668E+01	-2.7127409244E+01	

Molecular charge q(Mol) from the wfx file: -9.9999999509E-01

Molecular energy E(Mol) from the wfx file: -2.7127576757E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0006124708E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0006124710E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

B1	20	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	8	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	8	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	8	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H5	8	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total	52								

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 5.38402063378397E-14 -2.20281768018062E-13 5.81937534319252E-14

Type = (3,-3) NACP B1

Rho = 6.6960598704E+01 Rho at Nucleus = 6.6960598704E+01

GradRho = 6.7482377601E-18 -3.4041481286E-17 -8.3949573786E-18

HessRho_EigVals = -6.6846734758E+04 -6.6846734758E+04 -6.6846734757E+04

HessRho_EigVec1 = 1.5437121698E-01 5.6409422350E-01 8.1115179491E-01

HessRho_EigVec2 = 6.3955520913E-01 5.6872777568E-01 -5.1722127918E-01

HessRho_EigVec3 = 7.5308609192E-01 -5.9862043414E-01 2.7297420022E-01

DelSqRho = -2.0054020427E+05

Bond Ellipticity = NA

V = -5.0138434230E+04

G = 1.6915811769E+00

K = 5.0136742649E+04

L = 5.0135051068E+04

Vnuc = 5.0000000171E+08

Ven = -3.3480299467E+10

Vrep = 3.3480249328E+10
DelSqV = 1.0684425663E+09
DelSqVen = 1.0044089800E+27
DelSqVrep = -1.0044089800E+27
DelSqG = 5.0053709690E+07
DelSqK = -1.1184962760E+09
Stress_EigVals = -1.6712811410E+04 -1.6712811410E+04 -1.6712811410E+04
Stress_EigVec1 = 7.6283525723E-01 -5.9339265805E-01 2.5684143687E-01
Stress_EigVec2 = 6.2258979758E-01 5.6685681634E-01 -5.3949540657E-01
Stress_EigVec3 = 1.7454029411E-01 5.7145297544E-01 8.0185858017E-01
-DivStress = -1.9586984904E-05 7.6158055419E-05 -2.0096226925E-05

CP# 2 Coords = 1.33981310687500E+00 1.33981310723697E+00 1.33981310760345E+00

Type = (3,-3) NACP H2

Rho = 4.0165975129E-01 Rho at Nucleus = 4.0064761256E-01

GradRho = -9.7417180516E-16 2.4100323053E-16 -4.7129990836E-16

HessRho_EigVals = -8.0866418738E+00 -8.0866418708E+00 -7.8447329831E+00

HessRho_EigVec1 = 2.0344821422E-01 -7.8652817726E-01 5.8307996921E-01

HessRho_EigVec2 = 7.9074362610E-01 -2.1918050190E-01 -5.7156314207E-01

HessRho_EigVec3 = -5.7735027663E-01 -5.7735026973E-01 -5.7735026121E-01

DelSqRho = -2.4018016728E+01

Bond Ellipticity = NA

V = -6.0158169369E+00

G = 5.6563774791E-03

K = 6.0101605594E+00

L = 6.0045041820E+00

Vnuc = 6.5485710201E+01

Ven = -2.6302974072E+01

Vrep = 2.0287157135E+01

DelSqV = 1.5796889608E+03

DelSqVen = 1.5728368830E+03

DelSqVrep = 6.8520778071E+00

DelSqG = 1.2063033352E+02

DelSqK = -1.7003192944E+03

Stress_EigVals = -2.0255563027E+00 -2.0255563023E+00 -1.9647043319E+00

Stress_EigVec1 = 2.1334148190E-01 5.7587160155E-01 -7.8921309583E-01

Stress_EigVec2 = 7.8813201129E-01 -5.7882516154E-01 -2.0930686838E-01

Stress_EigVec3 = -5.7735027919E-01 -5.7735026709E-01 -5.7735026129E-01

-DivStress = 4.6471624693E+00 4.6471622890E+00 4.6471621077E+00

CP# 3 Coords = -1.33981310687104E+00 1.33981310664916E+00 -1.33981310714153E+00

Type = (3,-3) NACP H3

Rho = 4.0165974645E-01 Rho at Nucleus = 4.0064760765E-01

GradRho = -6.5062877080E-16 2.0505820620E-16 6.2007332777E-16

HessRho_EigVals = -8.0866417759E+00 -8.0866417752E+00 -7.8447328796E+00

HessRho_EigVec1 = -8.1169448515E-01 -3.2927016281E-01 4.8242431806E-01

HessRho_EigVec2 = 8.8423594818E-02 7.4715983734E-01 6.5873624870E-01

HessRho_EigVec3 = 5.7735026687E-01 -5.7735027267E-01 5.7735026803E-01

DelSqRho = -2.4018016431E+01

Bond Ellipticity = NA

V = -6.0158168635E+00

G = 5.6563778858E-03

K = 6.0101604856E+00

L = 6.0045041077E+00

Vnuc = 6.5485707822E+01

Ven = -2.6302972800E+01

Vrep = 2.0287155936E+01

DelSqV = 1.5796889407E+03

DelSqVen = 1.5728368064E+03

DelSqVrep = 6.8521342133E+00

DelSqG = 1.2063033201E+02

DelSqK = -1.7003192727E+03

Stress_EigVals = -2.0255562788E+00 -2.0255562783E+00 -1.9647043064E+00

Stress_EigVec1 = -5.2248913544E-01 2.8212807139E-01 8.0461721003E-01

Stress_EigVec2 = 6.2743268566E-01 7.6620520092E-01 1.3877252992E-01

Stress_EigVec3 = -5.7735026484E-01 5.7735027620E-01 -5.7735026653E-01

-DivStress = -4.6471624141E+00 4.6471625239E+00 -4.6471622815E+00

CP# 4 Coords = 1.33981310637019E+00 -1.33981310666111E+00 -1.33981310687707E+00

Type = (3,-3) NACP H4

Rho = 4.0165975410E-01 Rho at Nucleus = 4.0064761523E-01

GradRho = 2.9160895630E-16 -1.6702405172E-16 7.6425129732E-16

HessRho_EigVals = -8.0866419238E+00 -8.0866419233E+00 -7.8447330247E+00

HessRho_EigVec1 = -6.8542022377E-01 -7.2696177243E-01 4.1541524717E-02

HessRho_EigVec2 = -4.4369557778E-01 3.7174353252E-01 -8.1543913341E-01

HessRho_EigVec3 = -5.7735028459E-01 5.7735026410E-01 5.7735025888E-01

DelSqRho = -2.4018016872E+01

Bond Ellipticity = NA

V = -6.0158169734E+00

G = 5.6563777032E-03

K = 6.0101605957E+00

L = 6.0045042180E+00

Vnuc = 6.5485706121E+01

Ven = -2.6302972618E+01

Vrep = 2.0287155644E+01

DelSqV = 1.5796889680E+03

DelSqVen = 1.5728367945E+03

DelSqVrep = 6.8521735427E+00

DelSqG = 1.2063033414E+02

DelSqK = -1.7003193022E+03

Stress_EigVals = -2.0255563154E+00 -2.0255563150E+00 -1.9647043430E+00

Stress_EigVec1 = -6.3589344045E-01 -7.6148888303E-01 1.2559543548E-01

Stress_EigVec2 = 5.1215836305E-01 -2.9462068350E-01 8.0677906766E-01

Stress_EigVec3 = 5.7735027804E-01 -5.7735026966E-01 -5.7735025987E-01

-DivStress = 4.6471627375E+00 -4.6471625950E+00 -4.6471624862E+00

CP# 5 Coords = -1.33981310679041E+00 -1.33981310673384E+00 1.33981310668176E+00

Type = (3,-3) NACP H5

Rho = 4.0165974472E-01 Rho at Nucleus = 4.0064760590E-01

GradRho = 4.9953101026E-16 -6.3039844764E-16 4.2704002481E-16

HessRho_EigVals = -8.0866417402E+00 -8.0866417376E+00 -7.8447328394E+00

HessRho_EigVec1 = -8.1385471732E-01 4.6376375330E-01 -3.5009095992E-01

HessRho_EigVec2 = 6.5629019704E-02 6.7200435193E-01 7.3763336608E-01

HessRho_EigVec3 = -5.7735026705E-01 -5.7735026813E-01 5.7735027238E-01

DelSqRho = -2.4018016317E+01

Bond Ellipticity = NA

V = -6.0158168348E+00

G = 5.6563777457E-03

K = 6.0101604570E+00

L = 6.0045040793E+00

Vnuc = 6.5485706793E+01

Ven = -2.6302972274E+01

Vrep = 2.0287155439E+01

DelSqV = 1.5796889328E+03

DelSqVen = 1.5728367743E+03

DelSqVrep = 6.8521584604E+00

DelSqG = 1.2063033137E+02

DelSqK = -1.7003192641E+03

Stress_EigVals = -2.0255562692E+00 -2.0255562691E+00 -1.9647042965E+00

Stress_EigVec1 = 3.8154141188E-01 -8.1592637693E-01 -4.3438496573E-01

Stress_EigVec2 = -7.2186759324E-01 3.0509237064E-02 -6.9135834723E-01

Stress_EigVec3 = -5.7735026532E-01 -5.7735026966E-01 5.7735027259E-01

-DivStress = -4.6471624295E+00 -4.6471624595E+00 4.6471624843E+00

CP# 6 Coords = 5.73009856115329E-01 5.73009858487432E-01 5.73009859627462E-01

Type = (3,-1) BCP B1 H2

Rho = 1.4383174035E-01

GradRho = 7.4671668051E-18 -1.4873129276E-17 -4.1016318119E-17

HessRho_EigVals = -2.4299839331E-01 -2.4299838826E-01 4.8226419019E-01
HessRho_EigVec1 = 1.9690341417E-01 5.8778570454E-01 -7.8468911744E-01
HessRho_EigVec2 = 7.9239870885E-01 -5.6672271144E-01 -2.2567599464E-01
HessRho_EigVec3 = -5.7735026778E-01 -5.7735026967E-01 -5.7735027012E-01
DelSqRho = -3.7325913876E-03
Bond Ellipticity = 2.0800543510E-08
V = -2.7034282146E-01
G = 1.3470483681E-01
K = 1.3563798466E-01
L = 9.3314784689E-04
Vnuc = 6.8431182259E+00
Ven = -9.8425760382E-01
Vrep = 7.1391478235E-01
DelSqV = -3.5091659235E+00
DelSqVen = 2.5542564154E-02
DelSqVrep = -3.5347084877E+00
DelSqG = 5.2347192468E+00
DelSqK = -1.7255533232E+00
Stress_EigVals = -1.1339414978E-01 -1.1339414761E-01 -4.3554524079E-02
Stress_EigVec1 = 1.7366769904E-01 -7.7776050774E-01 6.0409280985E-01
Stress_EigVec2 = -7.9781337724E-01 2.4850606124E-01 5.4930733894E-01
Stress_EigVec3 = 5.7735027964E-01 5.7735026641E-01 5.7735026152E-01
-DivStress = -2.2152880845E-01 -2.2152880703E-01 -2.2152880687E-01
BPL = 2.3206243744E+00 = 9.9248218743E-01 + 1.3281421870E+00
GBL_I = 2.3206243744E+00
GBL_II = 2.3366135810E+00
GBL_III = 2.3206243744E+00 = 9.9248218743E-01 + 1.3281421870E+00
GBL_IV = 2.3366135810E+00 = 9.9248218743E-01 + 1.3441313936E+00

CP# 7 Coords = -5.73009878426443E-01 5.73009867527289E-01 -5.73009858233808E-01

Type = (3,-1) BCP B1 H3

Rho = 1.4383174497E-01

GradRho = -6.1149028998E-18 -2.9441799838E-17 -3.1731594592E-17
HessRho_EigVals = -2.4299840726E-01 -2.4299840252E-01 4.8226411999E-01
HessRho_EigVec1 = -5.1475966391E-01 2.9149799804E-01 8.0625765457E-01
HessRho_EigVec2 = 6.3378952332E-01 7.6268970264E-01 1.2890018468E-01
HessRho_EigVec3 = 5.7735026504E-01 -5.7735027031E-01 5.7735027222E-01
DelSqRho = -3.7326897872E-03
Bond Ellipticity = 1.9506332549E-08
V = -2.7034281355E-01
G = 1.3470482055E-01
K = 1.3563799300E-01
L = 9.3317244680E-04
Vnuc = 6.8431181436E+00
Ven = -9.8425762365E-01
Vrep = 7.1391481010E-01
DelSqV = -3.5091655246E+00
DelSqVen = 2.5543237207E-02
DelSqVrep = -3.5347087618E+00
DelSqG = 5.2347185919E+00
DelSqK = -1.7255530672E+00
Stress_EigVals = -1.1339414949E-01 -1.1339414809E-01 -4.3554515961E-02
Stress_EigVec1 = -8.1641920851E-01 -3.9847440610E-01 4.1794476150E-01
Stress_EigVec2 = -1.1241204862E-02 -7.1266038043E-01 -7.0141914536E-01
Stress_EigVec3 = -5.7735025010E-01 5.7735026617E-01 -5.7735029130E-01
-DivStress = 2.2152880373E-01 -2.2152880288E-01 2.2152880041E-01
BPL = 2.3206243738E+00 = 9.9248220472E-01 + 1.3281421691E+00
GBL_I = 2.3206243738E+00
GBL_II = 2.3366135810E+00
GBL_III = 2.3206243738E+00 = 9.9248220472E-01 + 1.3281421691E+00
GBL_IV = 2.3366135810E+00 = 9.9248220472E-01 + 1.3441313763E+00

CP# 8 Coords = 5.73009851118200E-01 -5.73009864318943E-01 -5.73009854467689E-01

Type = (3,-1) BCP H4 B1

Rho = 1.4383174130E-01
GradRho = -7.3108832913E-17 6.8203327005E-17 8.4802298112E-17
HessRho_EigVals = -2.4299839921E-01 -2.4299839743E-01 4.8226421118E-01
HessRho_EigVec1 = 6.2372524995E-01 7.6817952004E-01 -1.4445427504E-01
HessRho_EigVec2 = -5.2690937290E-01 2.7670723202E-01 -8.0361658799E-01
HessRho_EigVec3 = 5.7735026226E-01 -5.7735026868E-01 -5.7735027663E-01
DelSqRho = -3.7325854583E-03
Bond Ellipticity = 7.3349122331E-09
V = -2.7034282474E-01
G = 1.3470483919E-01
K = 1.3563798555E-01
L = 9.3314636457E-04
Vnuc = 6.8431182378E+00
Ven = -9.8425761205E-01
Vrep = 7.1391478731E-01
DelSqV = -3.5091660258E+00
DelSqVen = 2.5542523624E-02
DelSqVrep = -3.5347085494E+00
DelSqG = 5.2347193544E+00
DelSqK = -1.7255533287E+00
Stress_EigVals = -1.1339415147E-01 -1.1339415085E-01 -4.3554522416E-02
Stress_EigVec1 = 2.3982489459E-01 7.9582887354E-01 -5.5600397838E-01
Stress_EigVec2 = 7.8048105821E-01 1.8254608188E-01 5.9793498456E-01
Stress_EigVec3 = -5.7735027297E-01 5.7735026806E-01 5.7735026653E-01
-DivStress = -2.2152880924E-01 2.2152881282E-01 2.2152880805E-01
BPL = 2.3206243733E+00 = 1.3281421884E+00 + 9.9248218493E-01
GBL_I = 2.3206243733E+00
GBL_II = 2.3366135810E+00
GBL_III = 2.3206243733E+00 = 1.3281421884E+00 + 9.9248218493E-01
GBL_IV = 2.3366135810E+00 = 1.3441313961E+00 + 9.9248218493E-01

CP# 9 Coords = -5.73009871953238E-01 -5.73009866284241E-01 5.73009857688785E-01

Type = (3,-1) BCP H5 B1

Rho = 1.4383174361E-01

GradRho = -2.6928818520E-17 -4.0215529531E-17 -1.1360577942E-17

HessRho_EigVals = -2.4299840185E-01 -2.4299840000E-01 4.8226414036E-01

HessRho_EigVec1 = -6.6474528020E-02 7.3799669295E-01 6.7152216517E-01

HessRho_EigVec2 = 8.1378609337E-01 -3.4932441498E-01 4.6446167478E-01

HessRho_EigVec3 = -5.7735026749E-01 -5.7735027002E-01 5.7735027006E-01

DelSqRho = -3.7326614991E-03

Bond Ellipticity = 7.6100155066E-09

V = -2.7034281627E-01

G = 1.3470482545E-01

K = 1.3563799082E-01

L = 9.3316537478E-04

Vnuc = 6.8431181663E+00

Ven = -9.8425761761E-01

Vrep = 7.1391480134E-01

DelSqV = -3.5091656375E+00

DelSqVen = 2.5543043713E-02

DelSqVrep = -3.5347086812E+00

DelSqG = 5.2347187762E+00

DelSqK = -1.7255531387E+00

Stress_EigVals = -1.1339415015E-01 -1.1339414797E-01 -4.3554518153E-02

Stress_EigVec1 = 8.1045844143E-01 -4.9106532720E-01 3.1939311067E-01

Stress_EigVec2 = 9.9115007621E-02 6.5232010494E-01 7.5143509098E-01

Stress_EigVec3 = -5.7735026629E-01 -5.7735026207E-01 5.7735027921E-01

-DivStress = 2.2152880445E-01 2.2152880309E-01 -2.2152880066E-01

BPL = 2.3206243735E+00 = 1.3281421736E+00 + 9.9248219995E-01

GBL_I = 2.3206243735E+00

GBL_II = 2.3366135810E+00

GBL_III = 2.3206243735E+00 = 1.3281421736E+00 + 9.9248219995E-01

GBL_IV = 2.3366135810E+00 = 1.3441313811E+00 + 9.9248219995E-01

Number of NACPs = 5

Number of NNACPs = 0

Number of BCPs = 4

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H3	B1	H2	109.47122071	109.47122064	109.47122063	109.47122064	109.47122064
H4	B1	H2	109.47122109	109.47122065	109.47122063	109.47122116	109.47122116
H4	B1	H3	109.47122196	109.47122062	109.47122063	109.47122148	109.47122148
H5	B1	H2	109.47122119	109.47122063	109.47122063	109.47122106	109.47122106
H5	B1	H3	109.47121901	109.47122063	109.47122063	109.47121943	109.47121943
H5	B1	H4	109.47121985	109.47122063	109.47122063	109.47122002	109.47122002

Total time for electron density critical point search, analysis and connectivity = 1 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$E_e(A) = E(A) - W(A) = -T(A)$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A) = V_{ee}(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
B1	-2.3887366933E+01	2.3887366933E+01	-5.8246339655E+01	-5.2875574124E+01		
H2	-8.0585941981E-01	8.0585941981E-01	-6.6054578521E+00	-1.6613622119E+00		
H3	-8.0585978307E-01	8.0585978307E-01	-6.6054644518E+00	-1.6613629699E+00		
H4	-8.0585926043E-01	8.0585926043E-01	-6.6054604714E+00	-1.6613625400E+00		
H5	-8.0585927151E-01	8.0585927151E-01	-6.6054592637E+00	-1.6613623739E+00		
Total	-2.7110804668E+01	2.7110804668E+01	-8.4668181694E+01	-5.9521024220E+01		

More Virial-Based Atomic Energy Components:

$E(A) = E_e(A) + W(A)$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$E_e(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
B1	-2.3887366930E+01	-2.3887366933E+01	2.6394313183E-09			
H2	-8.0585941892E-01	-8.0585941981E-01	8.9357156680E-10			
H3	-8.0585978218E-01	-8.0585978307E-01	8.9365114124E-10			
H4	-8.0585925954E-01	-8.0585926043E-01	8.9373330116E-10			
H5	-8.0585927062E-01	-8.0585927151E-01	8.9365973574E-10			
Total	-2.7110804662E+01	-2.7110804668E+01	6.2140470633E-09			

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	E_IQA(A) VeeX(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2

B1 4.2796977991E+00			2.3887366933E+01	-3.3647498462E+01	-2.9123169827E+01	
H2 1.4630397946E+00			8.0585941981E-01	-2.1714682568E+00	-3.3027289261E+00	
H3 1.4630397946E+00			8.0585978307E-01	-2.1714682523E+00	-3.3027322259E+00	
H4 1.4630397946E+00			8.0585926043E-01	-2.1714682591E+00	-3.3027302357E+00	
H5 1.4630397946E+00			8.0585927151E-01	-2.1714682511E+00	-3.3027296318E+00	

Total 1.0131856978E+01			2.7110804668E+01	-4.2333371481E+01	-4.2334090846E+01	

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

B1	2.3887366933E+01	-5.2875574124E+01				
H2	8.0585941981E-01	-1.6613622119E+00				

H3	8.0585978307E-01 -1.6613629699E+00
H4	8.0585926043E-01 -1.6613625400E+00
H5	8.0585927151E-01 -1.6613623739E+00

Total	2.7110804668E+01 -5.9521024220E+01

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$	$VeeX(A,A')$

B1	-7.2097113998E+00	-2.6853827654E+00		4.2796977991E+00			
H2	-1.3407871508E+00	-2.4720478201E+00		1.4630397946E+00			
H3	-1.3407867674E+00	-2.4720507410E+00		1.4630397946E+00			
H4	-1.3407869891E+00	-2.4720489657E+00		1.4630397946E+00			
H5	-1.3407870641E+00	-2.4720484449E+00		1.4630397946E+00			

Total	-1.2572859371E+01	-1.2573578737E+01	1.0131856978E+01

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$

B1	3.2063669647E+00	2.2598685575E+00	7.0480658714E+01	9.4649840720E-01	2.9519341286E+01
H2	1.6985670656E+00	1.2509582055E+00	7.3647854757E+01	4.4760886019E-01	2.6352145243E+01
H3	1.6985686314E+00	1.2509596845E+00	7.3647873944E+01	4.4760894688E-01	2.6352126056E+01
H4	1.6985679630E+00	1.2509588930E+00	7.3647856328E+01	4.4760906998E-01	2.6352143672E+01
H5	1.6985676248E+00	1.2509585969E+00	7.3647853554E+01	4.4760902798E-01	2.6352146446E+01

Total	1.0000638250E+01	7.2637039373E+00	7.2632403613E+01	2.7369343122E+00	2.7367596387E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

DI_Bond(A,A')/2 = Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

DI_NonBond(A,A')/2 = Non-Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
B1	3.2063669647E+00	2.2598685575E+00	9.4649840720E-01	9.4658662552E-01	-
	8.8218315106E-05				
H2	1.6985670656E+00	1.2509582055E+00	4.4760886019E-01	2.3652689640E-01	
	2.1108196378E-01				
H3	1.6985686314E+00	1.2509596845E+00	4.4760894688E-01	2.3689722129E-01	
	2.1071172560E-01				
H4	1.6985679630E+00	1.2509588930E+00	4.4760906998E-01	2.3662592307E-01	
	2.1098314691E-01				
H5	1.6985676248E+00	1.2509585969E+00	4.4760902798E-01	2.3653658476E-01	
	2.1107244323E-01				
Total	1.0000638250E+01	7.2637039373E+00	2.7369343122E+00	1.8931732510E+00	
	8.4376106120E-01				

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A')$ = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$D2(A,A)$	$D2(A,A')$	$D2(A,Mol)$
B1	4.0104602774E+00	1.0418188752E+01	1.4428649029E+01
H2	8.1708593551E-01	6.8264388317E+00	7.6435247672E+00
H3	8.1708785549E-01	6.8264439580E+00	7.6435318135E+00
H4	8.1708711596E-01	6.8264416896E+00	7.6435288056E+00
H5	8.1708668965E-01	6.8264405938E+00	7.6435272834E+00
Total	7.2788078741E+00	3.7723953825E+01	4.5002761699E+01

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A)$ = Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A)$ = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	

B1	H2	5.2097024302E+00	4.7305379281E-01	7.3767880909E+00	1.3925084337E+01	(Bonded)
B1	H3	5.2093371256E+00	4.7379444258E-01	7.3883377635E+00	1.3946873674E+01	(Bonded)
H2	H3	2.8147480332E+00	1.4076940556E-01	4.1437694280E+00	4.1437656083E+00	
B1	H4	5.2096062808E+00	4.7325184614E-01	7.3798765293E+00	1.3930906989E+01	(Bonded)
H2	H4	2.8147463181E+00	1.4077056530E-01	4.1438035668E+00	4.1438013776E+00	
H3	H4	2.8147488417E+00	1.4077083708E-01	4.1438077474E+00	4.1438093779E+00	
B1	H5	5.2096945349E+00	4.7307316951E-01	7.3770902507E+00	1.3925650136E+01	(Bonded)
H2	H5	2.8147461422E+00	1.4076976823E-01	4.1437801038E+00	4.1437787395E+00	
H3	H5	2.8147483507E+00	1.4077067022E-01	4.1438028356E+00	4.1438052911E+00	
H4	H5	2.8147474579E+00	1.4077018541E-01	4.1437901950E+00	4.1437910199E+00	

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

B1	H2	6.1540379514E+01	4.6129863078E+01	3.6199370515E+01
B1	H3	6.1538913792E+01	4.6139564199E+01	3.6196305421E+01
B1	H4	6.1530182634E+01	4.6141800002E+01	3.6192450491E+01
B1	H5	6.1534328811E+01	4.6140484584E+01	3.6191515622E+01

B1	Total	2.4614380475E+02	1.8455171186E+02	1.4477964205E+02

H2	B1	6.1540379514E+01	4.6129863078E+01	3.6199370514E+01

H2	Total	6.1540379514E+01	4.6129863078E+01	3.6199370514E+01
H3	B1	6.1538913792E+01	4.6139564199E+01	3.6196305421E+01

H3	Total	6.1538913792E+01	4.6139564199E+01	3.6196305421E+01
H4	B1	6.1530182633E+01	4.6141800002E+01	3.6192450490E+01

H4	Total	6.1530182633E+01	4.6141800002E+01	3.6192450490E+01
H5	B1	6.1534328811E+01	4.6140484584E+01	3.6191515622E+01

H5	Total	6.1534328811E+01	4.6140484584E+01	3.6191515622E+01

Total	Total	4.9228760950E+02	3.6910342373E+02	2.8955928410E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	N_IAS(A B)	G_IAS(A B)	K_IAS(A B)	L_IAS(A B)	DelSqRho_IAS(A B)
V_IAS(A B)						

B1	H2	9.0406663560E-01	5.7314465839E-01	3.4159990135E-01	-2.3154475704E-01	9.2617902816E-01 -9.1474455974E-01
B1	H3	9.0406638237E-01	5.7314446055E-01	3.4159973714E-01	-2.3154472342E-01	9.2617889367E-01 -9.1474419769E-01
B1	H4	9.0406639335E-01	5.7314441806E-01	3.4159971188E-01	-2.3154470618E-01	9.2617882471E-01 -9.1474412994E-01
B1	H5	9.0406643586E-01	5.7314446793E-01	3.4159975753E-01	-2.3154471040E-01	9.2617884162E-01 -9.1474422546E-01

B1	Total	3.6162658472E+00	2.2925780049E+00	1.3663991079E+00	-9.2617889704E-01	3.7047155882E+00 -3.6589771128E+00

H2	B1	9.0406663560E-01	5.7314465839E-01	3.4159990135E-01	-2.3154475704E-01	9.2617902816E-01 -9.1474455974E-01

H2	Total	9.0406663560E-01	5.7314465839E-01	3.4159990135E-01	-2.3154475704E-01	9.2617902816E-01 -9.1474455974E-01

H3	B1	9.0406638237E-01	5.7314446055E-01	3.4159973714E-01	-2.3154472342E-01	9.2617889367E-01 -9.1474419769E-01

H3	Total	9.0406638237E-01	5.7314446055E-01	3.4159973714E-01	-2.3154472342E-01	9.2617889367E-01 -9.1474419769E-01

H4	B1	9.0406639335E-01	5.7314441806E-01	3.4159971188E-01	-2.3154470618E-01	9.2617882471E-01 -9.1474412994E-01

H4	Total	9.0406639335E-01	5.7314441806E-01	3.4159971188E-01	-2.3154470618E-01	9.2617882471E-01 -9.1474412994E-01

H5	B1	9.0406643586E-01	5.7314446793E-01	3.4159975753E-01	-2.3154471041E-01	9.2617884162E-01 -9.1474422546E-01

H5 Total 9.0406643586E-01 5.7314446793E-01 3.4159975753E-01 -2.3154471041E-01
9.2617884162E-01 -9.1474422546E-01

Total Total 7.2325316944E+00 4.5851560099E+00 2.7327982158E+00 -1.8523577941E+00
7.4094311763E+00 -7.3179542257E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP_-Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP*ESP_-Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1	6.9761899659E+00				

H2	8.7837752970E+01				

H3	8.7463678978E+01				

H4	8.7452602243E+01				

H5	8.8233292929E+01				

Total	3.5796351709E+02				

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1	6.6333263128E+00	-1.4533533091E+00	-2.1631463748E-01	-2.2051550542E-01	-
	2.1909872069E-01	1.2079083065E-03	2.0251932651E-06		

H2	6.9905572539E+01	-1.4361796430E+01	-1.8849806191E-01	-2.2017759456E-01	-
	2.0544565918E-01	8.2289753993E-03	8.7782928633E-05		

H3	6.9315084246E+01	-1.4232514033E+01	-1.8847696945E-01	-2.2013700919E-01	-
	2.0533068939E-01	8.1891174113E-03	8.6962654952E-05		

H4	6.9407861012E+01	-1.4252828742E+01	-1.8849482812E-01	-2.2015638101E-01	-
	2.0534891198E-01	8.1956281438E-03	8.7099064840E-05		

H5	6.9810998870E+01	-1.4341243516E+01	-1.8850083587E-01	-2.2011400217E-01	-
	2.0542957052E-01	8.2249244228E-03	8.7712387833E-05		

Total	2.8507284298E+02	-5.8641736030E+01	-1.8847696945E-01	-2.2051550542E-01	-
	2.0570790054E-01	8.9678462530E-05			

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)	ESP-_Int_IDS(A)

B1	1.4533533091E+00	3.1844128449E-01	0.0000000000E+00	NULL	6.6333263128E+00	-1.4533533091E+00

H2	1.4361796430E+01	2.9567052505E+00	0.0000000000E+00	NULL	6.9905572539E+01	-1.4361796430E+01

H3	1.4232514033E+01	2.9283997419E+00	0.0000000000E+00	NULL	6.9315084246E+01	-1.4232514033E+01

H4	1.4252828742E+01	2.9328482345E+00	0.0000000000E+00	NULL	6.9407861012E+01	-1.4252828742E+01

H5	1.4341243516E+01	2.9522387856E+00	0.0000000000E+00	NULL	6.9810998870E+01	-1.4341243516E+01

Total	5.8641736030E+01	1.2088633297E+01	0.0000000000E+00	NULL	2.8507284298E+02	-5.8641736030E+01

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

B1	NULL	NULL	NULL	NULL	NULL

H2	NULL	NULL	NULL	NULL	NULL

H3	NULL	NULL	NULL	NULL	NULL

H4	NULL	NULL	NULL	NULL	NULL

H5	NULL	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL	NULL

0.001 IsoDensity Surface:

Atom A	ESP- _Max_IDS(A)	ESP- _Avg_IDS(A)	ESP- _MAD_IDS(A)	ESP- _Var_IDS(A)	ESP-*ESP- _Int_IDS(A)

B1	-2.1631463748E-01	-2.1909872069E-01	1.2079083065E-03	2.0251932651E-06	3.1844128449E-01
H2	-1.8849806191E-01	-2.0544565918E-01	8.2289753993E-03	8.7782928633E-05	2.9567052505E+00
H3	-1.8847696945E-01	-2.0533068939E-01	8.1891174113E-03	8.6962654952E-05	2.9283997419E+00
H4	-1.8849482812E-01	-2.0534891198E-01	8.1956281438E-03	8.7099064840E-05	2.9328482345E+00
H5	-1.8850083587E-01	-2.0542957052E-01	8.2249244228E-03	8.7712387833E-05	2.9522387856E+00

Total	-1.8847696945E-01	-2.0570790054E-01	8.9678462530E-05	1.2088633297E+01	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

B1	7.2264018126E+00						
H2	5.8187891736E+01						
H3	5.7439967401E+01						
H4	5.7783038235E+01						
H5	5.7953092027E+01						

Total	2.3859039121E+02						

Atomic Surface Area and Volume Data:

Area(A) = Area_IAS(A|Total) + Area_IDS(A)

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A)) = \text{Average Number of Electrons in Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A) = \text{Average Electron Density in Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	2.5311999472E+02	3.4346962882E+01	3.2045201336E+00	9.3298500499E-02	9.9942401131E+01
H2	1.4937813248E+02	1.4445654152E+02	1.6702752989E+00	1.1562476031E-02	9.8334374464E+01
H3	1.4900259277E+02	1.4460629798E+02	1.6703414044E+00	1.1550958898E-02	9.8338175657E+01
H4	1.4898278488E+02	1.4452188093E+02	1.6703043779E+00	1.1557449759E-02	9.8336034477E+01
H5	1.4976762174E+02	1.4455000530E+02	1.6703111481E+00	1.1555247920E-02	9.8336452645E+01
Total	8.5025112659E+02	6.1248168861E+02	9.8857523629E+00	1.6140486396E-02	9.8851214455E+01

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	1.9118503817E+02	3.0288800227E+01	3.2018879278E+00	1.0571194315E-01	9.9860308039E+01
H2	1.1603543562E+02	1.0048521938E+02	1.6420095189E+00	1.6340806429E-02	9.6670278852E+01
H3	1.1545464845E+02	1.0051976442E+02	1.6420546378E+00	1.6335639536E-02	9.6672846033E+01
H4	1.1554966101E+02	1.0056778004E+02	1.6420978872E+00	1.6328270213E-02	9.6675430290E+01

H5	1.1595148345E+02	1.0052333711E+02	1.6420475493E+00	1.6334988437E-02
9.6672485995E+01				

Total	6.5417626670E+02	4.3238490118E+02	9.7700975210E+00	2.2595834162E-02
9.7694739847E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	1.5200604386E+02	2.7188764446E+01	3.1974392452E+00	1.1760149129E-01	9.9721562766E+01
H2	9.4387262250E+01	7.4019510156E+01	1.6045482878E+00	2.1677369715E-02	9.4464818034E+01
H3	9.3636272822E+01	7.3984619370E+01	1.6044912013E+00	2.1686821058E-02	9.4461370099E+01
H4	9.3975488725E+01	7.4021729893E+01	1.6045594466E+00	2.1676870412E-02	9.4465425074E+01
H5	9.4144607649E+01	7.4013477741E+01	1.6045378639E+00	2.1678995676E-02	9.4464173247E+01
Total	5.2814967531E+02	3.2322810161E+02	9.6155760448E+00	2.9748576925E-02	9.6149623702E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
B1	H2	4.7620301017E-01		
B1	H3	4.7620457587E-01		
B1	H4	4.7620390767E-01		

B1	H5	4.7620356937E-01
B1		1.9048150631E+00 1.7936330353E+00
H2	B1	-5.8738503793E-01
H2		-5.8738503793E-01 -6.9856706570E-01
H3	B1	-5.8738660363E-01
H3		-5.8738660363E-01 -6.9856863140E-01
H4	B1	-5.8738593543E-01
H4		-5.8738593543E-01 -6.9856796320E-01
H5	B1	-5.8738559713E-01
H5		-5.8738559713E-01 -6.9856762490E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

B1	5.6482829061E-03	7.2385867333E-07	5.6490067648E-03
H2	4.3941767426E-02	-4.5583112699E-01	-4.1188935956E-01
H3	-4.3941915196E-02	4.5583232892E-01	4.1189041372E-01
H4	4.3941522724E-02	-4.5583182641E-01	-4.1189030369E-01
H5	-4.3942864475E-02	4.5583155164E-01	4.1188868717E-01

Total	5.6467933851E-03	1.6510201181E-06	5.6484444052E-03

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

B1	-1.8827109965E-03	-6.0273039282E-08	-1.8827712695E-03
H2	4.3940760781E-02	-4.5583112559E-01	-4.1189036481E-01

H3	4.3942380723E-02	-4.5583233532E-01	-4.1188995460E-01
H4	-4.3943312491E-02	4.5583181866E-01	4.1188850617E-01
H5	-4.3940436248E-02	4.5583155497E-01	4.1189111873E-01

Total	-1.8833182315E-03	-1.4755600264E-07	-1.8834657875E-03

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

B1	2.2886752168E-03	1.0888132094E-06	2.2897640300E-03
H2	4.3940353314E-02	-4.5583112493E-01	-4.1189077161E-01
H3	-4.3942129712E-02	4.5583234078E-01	4.1189021107E-01
H4	-4.3939820496E-02	4.5583182445E-01	4.1189200395E-01
H5	4.3940593437E-02	-4.5583156002E-01	-4.1189096659E-01

Total	2.2876717598E-03	2.5690937676E-06	2.2902408536E-03

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

B1	6.3785370370E-03	1.3088614988E-06	6.3795865379E-03
H2	7.6107976139E-02	7.8952266962E-01	7.1341469349E-01
H3	7.6110022325E-02	7.8952476397E-01	7.1341474164E-01
H4	7.6109000500E-02	7.8952387744E-01	7.1341487699E-01
H5	7.6108560803E-02	7.8952341390E-01	7.1341485312E-01

Total	6.3770373353E-03	3.0574307827E-06	6.3794647690E-03

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

B1	H2	-2.7286901834E-01	
B1	H3	2.7286992612E-01	
B1	H4	-2.7286953023E-01	
B1	H5	2.7286934631E-01	
B1		7.2385867333E-07	
H2	B1	-4.5583112699E-01	
H2		-4.5583112699E-01	
H3	B1	4.5583232892E-01	
H3		4.5583232892E-01	
H4	B1	-4.5583182641E-01	
H4		-4.5583182641E-01	
H5	B1	4.5583155164E-01	
H5		4.5583155164E-01	

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

B1	H2	-2.7286901947E-01	
B1	H3	-2.7286992093E-01	
B1	H4	2.7286953652E-01	
B1	H5	2.7286934361E-01	
B1		-6.0273039282E-08	
H2	B1	-4.5583112559E-01	
H2		-4.5583112559E-01	
H3	B1	-4.5583233532E-01	
H3		-4.5583233532E-01	
H4	B1	4.5583181866E-01	
H4		4.5583181866E-01	
H5	B1	4.5583155497E-01	
H5		4.5583155497E-01	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	H2	-2.7286902001E-01	
B1	H3	2.7286991651E-01	
B1	H4	2.7286953183E-01	
B1	H5	-2.7286933951E-01	
B1		1.0888132094E-06	
H2	B1	-4.5583112493E-01	
H2		-4.5583112493E-01	
H3	B1	4.5583234078E-01	
H3		4.5583234078E-01	
H4	B1	4.5583182445E-01	
H4		4.5583182445E-01	
H5	B1	-4.5583156002E-01	
H5		-4.5583156002E-01	
Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

B1	H2	4.7262300519E-01	
B1	H3	4.7262456736E-01	
B1	H4	4.7262389475E-01	
B1	H5	4.7262356615E-01	
B1		1.3088614988E-06	
H2	B1	7.8952266962E-01	
H2		7.8952266962E-01	
H3	B1	7.8952476397E-01	
H3		7.8952476397E-01	
H4	B1	7.8952387744E-01	
H4		7.8952387744E-01	
H5	B1	7.8952341390E-01	
H5		7.8952341390E-01	

Atomic Traceless Quadrupole Moment Tensors:

$Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$
B1	8.9659819701E-03	1.3352258509E-02	1.3213984319E-03	1.6358661871E-02	-3.3188719856E-02	-2.5324643841E-02
H2	-1.1411459796E-05	3.5340119710E-01	3.5341403120E-01	1.0458299811E-05	3.5339891611E-01	9.5315999656E-07
H3	-2.2994100198E-06	-3.5340205292E-01	3.5340993777E-01	5.7441719774E-06	-3.5340089498E-01	-3.4447619605E-06
H4	-3.2005631577E-06	-3.5340725187E-01	-3.5340813394E-01	-5.6822065707E-06	3.5340193652E-01	8.8827697335E-06
H5	-1.3622730073E-05	3.5341542047E-01	-3.5340010697E-01	7.2771668068E-07	-3.5340303518E-01	1.2895013394E-05

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
B1	1	-4.4784174451E-02	-1.4431490118E-01	4.9622136058E-01	8.5611773174E-01

B1	2	5.9005914145E-03	9.2424579022E-01	-2.4145575327E-01	2.9575131188E-01
B1	3	3.8883583036E-02	3.5347267018E-01	8.3394453084E-01	-4.2378484036E-01
H2	1	-3.5342005916E-01	-7.6371046564E-01	1.3172712068E-01	6.3197649510E-01
H2	2	-3.5338937046E-01	2.8881918326E-01	-8.0580017022E-01	5.1698120378E-01
H2	3	7.0680942962E-01	5.7734721274E-01	5.7735089101E-01	5.7735270380E-01
H3	1	-3.5341281656E-01	-7.1506307139E-01	-1.6192215935E-02	6.9887238898E-01
H3	2	-3.5339577389E-01	-3.9414563096E-01	-8.1633596938E-01	-4.2219048626E-01
H3	3	7.0680859045E-01	5.7735086865E-01	-5.7735032453E-01	5.7734961438E-01
H4	1	-3.5341234873E-01	7.8040471592E-01	5.9811022004E-01	1.8229822834E-01
H4	2	-3.5339919953E-01	-2.4007237557E-01	5.5582001422E-01	-7.9588275913E-01
H4	3	7.0681154826E-01	-5.7735061606E-01	5.7734588981E-01	5.7735430167E-01
H5	1	-3.5342205859E-01	7.3661677249E-01	-6.7334534379E-01	6.3259611846E-02
H5	2	-3.5339031655E-01	-3.5223426983E-01	-4.6180995410E-01	-8.1404089912E-01
H5	3	7.0681237514E-01	-5.7734456752E-01	-5.7735397660E-01	5.7735226341E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.1963051359E+01	1.0575114825E+01	3.2063669647E+00	2.2424824060E+00	2.8845482241E+00
H2	3.0436329290E+00	1.6613622119E+00	1.6985670657E+00	2.4648555448E+00	4.6739743785E+00
H3	3.0436332861E+00	1.6613629699E+00	1.6985686314E+00	2.4648588051E+00	4.6739805423E+00
H4	3.0436330537E+00	1.6613625400E+00	1.6985679632E+00	2.4648578592E+00	4.6739795777E+00

H5 3.0436329321E+00 1.6613623739E+00 1.6985676249E+00 2.4648572515E+00
4.6739795115E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
B1	-9.0702193444E+01	-1.9503279651E+01	-7.3113926474E+00	-5.4140313082E+00	-8.2171892554E+00
H2	-2.6215797932E+00	-2.5685468432E+00	-3.6830920077E+00	-7.0458018269E+00	-1.7290330008E+01
H3	-2.6215804655E+00	-2.5685483109E+00	-3.6830952200E+00	-7.0458085865E+00	-1.7290345936E+01
H4	-2.6215802786E+00	-2.5685480873E+00	-3.6830951182E+00	-7.0458090572E+00	-1.7290347751E+01
H5	-2.6215800656E+00	-2.5685476730E+00	-3.6830943997E+00	-7.0458088373E+00	-1.7290351664E+01

Atomic Electronic Spin Populations:

$$N\_alpha(A) = \text{Average number of Alpha electrons in Atom A}$$

$$N\_beta(A) = \text{Average number of Beta electrons in Atom A}$$

$$N\_total(A) = N\_alpha(A) + N\_beta(A)$$

$$N\_spin(A) = N\_alpha(A) - N\_beta(A)$$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)

B1	1.6031834824E+00	1.6031834824E+00	3.2063669647E+00	0.0000000000E+00
H2	8.4928353283E-01	8.4928353283E-01	1.6985670657E+00	0.0000000000E+00
H3	8.4928431569E-01	8.4928431569E-01	1.6985686314E+00	0.0000000000E+00
H4	8.4928398159E-01	8.4928398159E-01	1.6985679632E+00	0.0000000000E+00
H5	8.4928381246E-01	8.4928381246E-01	1.6985676249E+00	0.0000000000E+00

Total	5.0003191250E+00	5.0003191250E+00	1.0000638250E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed

to be the Hartree-Fock exchange functional and the atomic energies $E_{\text{IQA}}(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

BMe3

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\bme3\bme3.wfn

Sum File: D:\calc\ellipticity\bme3\bme3.sum

Wfn Title: bme3.wfn

Total memory allocated for AIMSum = 1.019 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	31.9999998000
Number of Alpha electrons (from MO Occs)	=	15.9999999000
Number of Beta electrons (from MO Occs)	=	15.9999999000
Number of electron pairs ($N*(N-1)/2$)	=	495.9999937000
Number of electron pairs (from Muller 2EDM)	=	495.9999096000

Number of electron pairs (from Muller 2EDM, no SOSI) = 496.3708167130

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
B1	5.0	6.9927000000E-03	-2.6974300000E-03	-1.7586810000E-02
C2	6.0	-1.9407609700E+00	-2.2617374800E+00	-1.0373630000E-02
H3	1.0	-2.8674525500E+00	-2.2862435300E+00	1.8506749900E+00
H4	1.0	-3.4673820500E+00	-1.9383575300E+00	-1.3749426000E+00
H5	1.0	-1.1229482000E+00	-4.1298624500E+00	-3.4173377000E-01
C6	6.0	-9.9450753000E-01	2.8047933000E+00	1.7986950000E-02
H7	1.0	-7.5893350000E-01	3.5304324000E+00	-1.9191305600E+00
H8	1.0	-2.9894561100E+00	3.0133454800E+00	5.1616224000E-01
H9	1.0	1.5073255000E-01	4.0428082400E+00	1.2188696600E+00
C10	6.0	2.9388757900E+00	-5.4322783000E-01	-1.4332500000E-02
H11	1.0	3.4097361300E+00	-1.2945845900E+00	1.8685134800E+00
H12	1.0	3.4584076500E+00	-2.0365646000E+00	-1.3515648400E+00
H13	1.0	4.1306888100E+00	1.1135457600E+00	-3.3859945000E-01

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
B1	2.0539703512E+00	1.5029121138E-04	2.3857421654E+01	-2.3884076120E+01	4.6059948241E-03

C2 -7.0162741200E-01 -1.1448115462E-04 3.8215341746E+01 -3.8258037454E+01
1.0754335500E+00

H3 1.3941900760E-02 3.0456895855E-05 6.0141013453E-01 -6.0208205398E-01 1.6336533510E-
01

H4 9.3365516200E-03 2.8328056424E-05 6.0598170384E-01 -6.0665873084E-01 1.6309477006E-
01

H5 -6.1311612000E-03 4.0592047966E-05 6.1664686215E-01 -6.1733580469E-01 1.6279552836E-
01

C6 -7.0218412300E-01 -2.0127779889E-04 3.8216498410E+01 -3.8259195411E+01
1.0759703720E+00

H7 1.5639240600E-02 2.9428324250E-05 5.9939607940E-01 -6.0006574867E-01 1.6346176002E-
01

H8 -4.5625974000E-03 3.8214111721E-05 6.1543792182E-01 -6.1612551368E-01 1.6295475156E-
01

H9 5.9889127700E-03 2.9399171204E-05 6.0873472757E-01 -6.0941483036E-01 1.6289628026E-
01

C10 -7.0242233380E-01 -1.1427943778E-04 3.8216023224E+01 -3.8258719694E+01
1.0764209641E+00

H11 1.5688749890E-02 3.1632796953E-05 5.9960521161E-01 -6.0027511453E-01 1.6325197760E-
01

H12 7.1910167700E-03 3.1697636996E-05 6.0805003963E-01 -6.0872937746E-01 1.6288997321E-
01

H13 -4.8627530000E-03 3.5979556469E-05 6.1581731385E-01 -6.1650532959E-01 1.6283817601E-
01

Total -3.3656790001E-05 1.5981417928E-05 1.4397636503E+02 -1.4413722118E+02

Molecular charge q(Mol) from the wfn file: 2.0000000007E-07

Molecular energy E(Mol) from the wfn file: -1.4413721018E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0011172400E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	
B1	78	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
C2	69	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H3	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H5	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C6	68	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H7	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H9	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C10	68	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H11	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H12	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H13	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 418

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = $(-1/4)\text{DelSqRho}$

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 6.99269414693709E-03 -2.69744403227059E-03 -1.75868380835341E-02

Type = (3,-3) NACP B1

Rho = 6.7229468615E+01 Rho at Nucleus = 6.7229468615E+01

GradRho = 1.5994150449E-14 8.7985174702E-15 9.8809849192E-15

HessRho_EigVals = -6.7121564046E+04 -6.7119153427E+04 -6.7119149866E+04

HessRho_EigVec1 = 1.6432628915E-02 -3.5770777407E-02 9.9922490971E-01

HessRho_EigVec2 = 1.2502417165E-01 9.9158995058E-01 3.3441387678E-02

HessRho_EigVec3 = 9.9201760328E-01 -1.2437773672E-01 -2.0766641509E-02

DelSqRho = -2.0135986734E+05

Bond Ellipticity = NA

V = -5.0343034738E+04

G = 1.5339517142E+00

K = 5.0341500786E+04

L = 5.0339966835E+04

Vnuc = 1.5656775879E+08

Ven = -1.0525967226E+10

Vrep = 1.0525916883E+10

DelSqV = 1.0727904747E+09

DelSqVen = 3.1520764985E+13

DelSqVrep = -3.1519692195E+13

DelSqG = 5.0261697899E+07

DelSqK = -1.1230521726E+09

Stress_EigVals = -1.6781251728E+04 -1.6781249951E+04 -1.6780533059E+04

Stress_EigVec1 = 9.9708783697E-01 -7.4230591192E-02 -1.7483268964E-02

Stress_EigVec2 = 7.4753948478E-02 9.9670525416E-01 3.1471948084E-02

Stress_EigVec3 = 1.5089484724E-02 -3.2687240028E-02 9.9935171576E-01

-DivStress = 2.0408701099E+00 4.9023679946E+00 9.8017036626E+00

CP# 2 Coords = -1.94076316959274E+00 -2.26173926701324E+00 -1.03732204980710E-02

Type = (3,-3) NACP C2

Rho = 1.1939495956E+02 Rho at Nucleus = 1.1939495882E+02

GradRho = -8.3163476106E-12 6.1226336501E-12 1.3427106649E-13

HessRho_EigVals = -1.8101063708E+05 -1.8101033812E+05 -1.8100933244E+05
HessRho_EigVec1 = 3.6363324627E-02 1.1605203748E-02 9.9927124839E-01
HessRho_EigVec2 = 7.2339182434E-01 -6.9019495087E-01 -1.8308421001E-02
HessRho_EigVec3 = 6.8947949723E-01 7.2353040644E-01 -3.3492892566E-02
DelSqRho = -5.4303030763E+05
Bond Ellipticity = NA
V = -1.3577297394E+05
G = 7.6985156714E+00
K = 1.3576527542E+05
L = 1.3575757691E+05
Vnuc = 2.0953846722E+06
Ven = -2.5017836820E+08
Vrep = 2.5004259523E+08
DelSqV = 4.6013157359E+09
DelSqVen = 1.1378573967E+12
DelSqVrep = -1.1332560810E+12
DelSqG = 2.0584239716E+08
DelSqK = -4.8071581331E+09
Stress_EigVals = -4.5257842134E+04 -4.5257607853E+04 -4.5257523953E+04
Stress_EigVec1 = 6.6813900672E-01 7.4391994112E-01 -1.3167721961E-02
Stress_EigVec2 = 7.4382506777E-01 -6.6826640756E-01 -1.2011539466E-02
Stress_EigVec3 = 1.7735169983E-02 1.7691036315E-03 9.9984115439E-01
-DivStress = 3.2931160459E+03 2.6754030848E+03 -6.1310820164E+02

CP# 3 Coords = -2.85523910270754E+00 -2.28566500465710E+00 1.82673483190368E+00

Type = (3,-3) NACP H3

Rho = 4.1286759324E-01 Rho at Nucleus = 4.1002471105E-01

GradRho = 1.5352302762E-16 1.6050528961E-15 6.2406677048E-16

HessRho_EigVals = -8.2510211155E+00 -8.2449928358E+00 -7.6569732766E+00

HessRho_EigVec1 = -5.3519582059E-01 8.0580051431E-01 -2.5347774015E-01

HessRho_EigVec2 = 7.1366662622E-01 5.9186181364E-01 3.7467257728E-01

HessRho_EigVec3 = -4.5193515048E-01 -1.9624593811E-02 8.9183490349E-01

DelSqRho = -2.4152987228E+01

Bond Ellipticity = NA

V = -6.0606737566E+00

G = 1.1213474819E-02

K = 6.0494602818E+00

L = 6.0382468070E+00

Vnuc = 4.4833738801E+01

Ven = -1.8510397835E+01

Vrep = 1.2449724078E+01

DelSqV = 1.5657391101E+03

DelSqVen = 1.0828687206E+03

DelSqVrep = 4.8287038950E+02

DelSqG = 1.1896483724E+02

DelSqK = -1.6847039474E+03

Stress_EigVals = -2.0702364102E+00 -2.0698726910E+00 -1.9205646555E+00

Stress_EigVec1 = 3.9359635295E-01 8.9388855948E-01 2.1458134629E-01

Stress_EigVec2 = 8.0180888163E-01 -4.4798944873E-01 3.9548447653E-01

Stress_EigVec3 = -4.4964922805E-01 -1.6391981679E-02 8.9305479935E-01

-DivStress = -6.1812213889E+00 -2.8955559474E-01 1.2122927446E+01

CP# 4 Coords = -3.44737037079156E+00 -1.94240112814465E+00 -1.35719134341279E+00

Type = (3,-3) NACP H4

Rho = 4.1697085116E-01 Rho at Nucleus = 4.1406377496E-01

GradRho = 1.7771721594E-13 -3.6741009540E-14 1.5843663187E-13

HessRho_EigVals = -8.3344339406E+00 -8.3291981780E+00 -7.7276623096E+00

HessRho_EigVec1 = -2.9643710532E-01 8.0297612473E-01 5.1706323183E-01

HessRho_EigVec2 = -6.0491782420E-01 -5.7681447625E-01 5.4896218991E-01

HessRho_EigVec3 = 7.3905308913E-01 -1.5004800266E-01 6.5672378390E-01

DelSqRho = -2.4391294428E+01

Bond Ellipticity = NA

V = -6.1198977058E+00

G = 1.1037049410E-02

K = 6.1088606564E+00
L = 6.0978236070E+00
Vnuc = 4.4564676627E+01
Ven = -1.8582171145E+01
Vrep = 1.2462273439E+01
DelSqV = 1.5806548848E+03
DelSqVen = 1.0869901487E+03
DelSqVrep = 4.9366473608E+02
DelSqG = 1.2011953401E+02
DelSqK = -1.7007744188E+03
Stress_EigVals = -2.0911364147E+00 -2.0905656185E+00 -1.9381956727E+00
Stress_EigVec1 = 3.5305836558E-01 9.1758539011E-01 -1.8272066754E-01
Stress_EigVec2 = -5.7569778692E-01 3.6701004892E-01 7.3066796982E-01
Stress_EigVec3 = 7.3751057526E-01 -1.5277655528E-01 6.5782784642E-01
-DivStress = -1.0230613744E+01 2.0702715113E+00 -9.0778046091E+00

CP# 5 Coords = -1.13364092437943E+00 -4.10525759218485E+00 -3.37363207067250E-01

Type = (3,-3) NACP H5

Rho = 4.2408313487E-01 Rho at Nucleus = 4.2110133954E-01

GradRho = -1.8388068845E-16 -4.7965104111E-16 2.9487927399E-16

HessRho_EigVals = -8.4718884584E+00 -8.4698719013E+00 -7.8500136699E+00

HessRho_EigVec1 = 3.8828790057E-01 4.9235172741E-03 9.2152496724E-01

HessRho_EigVec2 = 8.3364709110E-01 4.2432412860E-01 -3.5352731350E-01

HessRho_EigVec3 = -3.9276587655E-01 9.0549698667E-01 1.6065544920E-01

DelSqRho = -2.4791774030E+01

Bond Ellipticity = NA

V = -6.2194151213E+00

G = 1.0735806939E-02

K = 6.2086793143E+00

L = 6.1979435074E+00

Vnuc = 4.4360891535E+01

Ven = -1.8812705948E+01

Vrep = 1.2593290826E+01
DelSqV = 1.6059783134E+03
DelSqVen = 1.0997851987E+03
DelSqVrep = 5.0619311469E+02
DelSqG = 1.2199435932E+02
DelSqK = -1.7279726727E+03
Stress_EigVals = -2.1256828417E+00 -2.1249466497E+00 -1.9687856299E+00
Stress_EigVec1 = 9.0967837501E-01 4.0958577092E-01 -6.8736819040E-02
Stress_EigVec2 = 1.2814337011E-01 -1.1937614336E-01 9.8454487612E-01
Stress_EigVec3 = -3.9505003573E-01 9.0442735068E-01 1.6107959714E-01
-DivStress = 5.5580677322E+00 -1.2785537414E+01 -2.2716359945E+00

CP# 6 Coords = -9.94508163146452E-01 2.80479606867106E+00 1.79863006875338E-02

Type = (3,-3) NACP C6

Rho = 1.1939608793E+02 Rho at Nucleus = 1.1939608716E+02

GradRho = -9.5870811290E-12 -1.4891646943E-11 1.6669998715E-13

HessRho_EigVals = -1.8101238058E+05 -1.8101204895E+05 -1.8101103846E+05

HessRho_EigVec1 = -5.7682475262E-02 2.8395176093E-02 9.9793108280E-01

HessRho_EigVec2 = 9.5097970380E-01 3.0577256878E-01 4.6268122219E-02

HessRho_EigVec3 = -3.0382615917E-01 9.5168106536E-01 -4.4640954785E-02

DelSqRho = -5.4303546799E+05

Bond Ellipticity = NA

V = -1.3577426310E+05

G = 7.6980488931E+00

K = 1.3576656505E+05

L = 1.3575886700E+05

Vnuc = 2.0594412046E+06

Ven = -2.4588922315E+08

Vrep = 2.4575344888E+08

DelSqV = 4.6013592320E+09

DelSqVen = 1.1183496028E+12

DelSqVrep = -1.1137482436E+12

DelSqG = 2.0584436667E+08

DelSqK = -4.8072035987E+09

Stress_EigVals = -4.5258275421E+04 -4.5258040646E+04 -4.5257947028E+04

Stress_EigVec1 = -3.2274506456E-01 9.4640221909E-01 -1.2588208891E-02

Stress_EigVec2 = 9.4509432436E-01 3.2296298380E-01 4.9916221437E-02

Stress_EigVec3 = -5.1306348241E-02 -4.2131693338E-03 9.9867407488E-01

-DivStress = 9.4788689157E+02 -4.1451457297E+03 9.7214505704E+02

CP# 7 Coords = -7.61836857608065E-01 3.52069006273361E+00 -1.89432632381189E+00

Type = (3,-3) NACP H7

Rho = 4.1116703435E-01 Rho at Nucleus = 4.0835102081E-01

GradRho = 2.7929047963E-16 8.1618739545E-16 -3.6776137691E-16

HessRho_EigVals = -8.2171880699E+00 -8.2108575100E+00 -7.6284677916E+00

HessRho_EigVec1 = 9.6750684644E-01 1.7543632400E-01 1.8207854985E-01

HessRho_EigVec2 = -2.2802533727E-01 9.1655220120E-01 3.2853692036E-01

HessRho_EigVec3 = -1.0924718605E-01 -3.5938024249E-01 9.2677445673E-01

DelSqRho = -2.4056513372E+01

Bond Ellipticity = NA

V = -6.0366723211E+00

G = 1.1271989111E-02

K = 6.0254003320E+00

L = 6.0141283429E+00

Vnuc = 4.4944848204E+01

Ven = -1.8479839946E+01

Vrep = 1.2443167624E+01

DelSqV = 1.5597331033E+03

DelSqVen = 1.0812163418E+03

DelSqVrep = 4.7851676147E+02

DelSqG = 1.1850767837E+02

DelSqK = -1.6782407816E+03

Stress_EigVals = -2.0617449934E+00 -2.0614717446E+00 -1.9134555831E+00

Stress_EigVec1 = 5.4871505368E-01 -8.0054751741E-01 -2.4090550477E-01

Stress_EigVec2 = 8.2860689759E-01 4.8252465834E-01 2.8386715793E-01

Stress_EigVec3 = -1.1100630218E-01 -3.5537814572E-01 9.2810773859E-01

-DivStress = 1.4660231042E+00 4.9083753043E+00 -1.2510582033E+01

CP# 8 Coords = -2.96324260004763E+00 3.01051847489082E+00 5.09590164753612E-01

Type = (3,-3) NACP H8

Rho = 4.2332890049E-01 Rho at Nucleus = 4.2035415538E-01

GradRho = 1.6115581092E-15 1.4376520807E-15 -8.2746309804E-16

HessRho_EigVals = -8.4575476029E+00 -8.4547169646E+00 -7.8369441505E+00

HessRho_EigVec1 = 2.6115531968E-01 4.9651597268E-01 8.2781023663E-01

HessRho_EigVec2 = -3.3449508748E-02 8.6171045509E-01 -5.0629657509E-01

HessRho_EigVec3 = 9.6471707219E-01 -1.0453219817E-01 -2.4164848475E-01

DelSqRho = -2.4749208718E+01

Bond Ellipticity = NA

V = -6.2088208778E+00

G = 1.0759349143E-02

K = 6.1980615286E+00

L = 6.1873021795E+00

Vnuc = 4.4384544388E+01

Ven = -1.8789260374E+01

Vrep = 1.2580439497E+01

DelSqV = 1.6032771578E+03

DelSqVen = 1.0984823529E+03

DelSqVrep = 5.0479480493E+02

DelSqG = 1.2179425662E+02

DelSqK = -1.7250714145E+03

Stress_EigVals = -2.1220180346E+00 -2.1212881522E+00 -1.9655146910E+00

Stress_EigVec1 = 8.2743051539E-02 9.9264983495E-01 -8.8317000566E-02

Stress_EigVec2 = 2.4951858635E-01 6.5162713021E-02 9.6617508553E-01

Stress_EigVec3 = 9.6482851455E-01 -1.0198100803E-01 -2.4229282183E-01

-DivStress = -1.3599034454E+01 1.4647972218E+00 3.4100136348E+00

CP# 9 Coords = 1.35822660094290E-01 4.02648406538988E+00 1.20316277267373E+00

Type = (3,-3) NACP H9

Rho = 4.1907966212E-01 Rho at Nucleus = 4.1614444044E-01

GradRho = -3.1414107426E-14 -3.7031142042E-14 -3.3164443414E-14

HessRho_EigVals = -8.3761162342E+00 -8.3712007383E+00 -7.7635760832E+00

HessRho_EigVec1 = -8.0213518787E-01 1.8646218396E-01 5.6728387455E-01

HessRho_EigVec2 = 2.3336136857E-01 -7.7656692221E-01 5.8522327960E-01

HessRho_EigVec3 = 5.4965590330E-01 6.0181032666E-01 5.7939858361E-01

DelSqRho = -2.4510893056E+01

Bond Ellipticity = NA

V = -6.1496147565E+00

G = 1.0945746305E-02

K = 6.1386690102E+00

L = 6.1277232639E+00

Vnuc = 4.4465822801E+01

Ven = -1.8634721996E+01

Vrep = 1.2485107239E+01

DelSqV = 1.5881599929E+03

DelSqVen = 1.0898970273E+03

DelSqVrep = 4.9826296563E+02

DelSqG = 1.2068457826E+02

DelSqK = -1.7088445712E+03

Stress_EigVals = -2.1015395507E+00 -2.1009082861E+00 -1.9471669198E+00

Stress_EigVec1 = 6.4064658058E-01 -7.4972261754E-01 1.6579492014E-01

Stress_EigVec2 = 5.3454356695E-01 2.8046944694E-01 -7.9724529749E-01

Stress_EigVec3 = -5.5121242170E-01 -5.9937708171E-01 -5.8044119434E-01

-DivStress = 7.6621969255E+00 8.3854177041E+00 8.0715277124E+00

CP# 10 Coords = 2.93887845789105E+00 -5.43228753515804E-01 -1.43318961054401E-02

Type = (3,-3) NACP C10

Rho = 1.1939565821E+02 Rho at Nucleus = 1.1939565746E+02

GradRho = 1.3932743848E-11 -9.3339502794E-12 -1.1352030427E-13

HessRho_EigVals = -1.8101170774E+05 -1.8101138199E+05 -1.8101038418E+05

HessRho_EigVec1 = -7.5614852269E-02 -9.9681237207E-02 9.9214214963E-01

HessRho_EigVec2 = 2.1468349597E-01 9.7002871351E-01 1.1382131398E-01

HessRho_EigVec3 = 9.7375222242E-01 -2.2160312702E-01 5.1948661383E-02

DelSqRho = -5.4303347391E+05

Bond Ellipticity = NA

V = -1.3577376504E+05

G = 7.6982789840E+00

K = 1.3576606676E+05

L = 1.3575836848E+05

Vnuc = 2.0782330673E+06

Ven = -2.4813200499E+08

Vrep = 2.4799623123E+08

DelSqV = 4.6013424228E+09

DelSqVen = 1.1285500928E+12

DelSqVrep = -1.1239487504E+12

DelSqG = 2.0584359639E+08

DelSqK = -4.8071860192E+09

Stress_EigVals = -4.5258106788E+04 -4.5257874822E+04 -4.5257783425E+04

Stress_EigVec1 = 9.7991660355E-01 -1.9776703043E-01 2.5527470905E-02

Stress_EigVec2 = 1.9365690160E-01 9.7434858908E-01 1.1463782718E-01

Stress_EigVec3 = -4.7544237915E-02 -1.0739193933E-01 9.9307931043E-01

-DivStress = -3.9942055186E+03 1.3826804003E+03 -9.0410938486E+02

CP# 11 Coords = 3.40327213199802E+00 -1.28482564882255E+00 1.84436780542049E+00

Type = (3,-3) NACP H11

Rho = 4.1147909068E-01 Rho at Nucleus = 4.0865536979E-01

GradRho = 1.5638532136E-15 -1.0755285551E-16 -4.1286418728E-16

HessRho_EigVals = -8.2236695464E+00 -8.2175522323E+00 -7.6336095911E+00

HessRho_EigVec1 = 3.5850706759E-01 8.9491037174E-01 2.6572186405E-01

HessRho_EigVec2 = -9.0288993302E-01 2.6007385217E-01 3.4227380892E-01

HessRho_EigVec3 = 2.3719707279E-01 -3.6262517558E-01 9.0124387970E-01

DelSqRho = -2.4074831370E+01

Bond Ellipticity = NA

V = -6.0412145274E+00

G = 1.1253342485E-02

K = 6.0299611849E+00

L = 6.0187078425E+00

Vnuc = 4.4904052641E+01

Ven = -1.8477078749E+01

Vrep = 1.2435864221E+01

DelSqV = 1.5608473841E+03

DelSqVen = 1.0810574952E+03

DelSqVrep = 4.7978988894E+02

DelSqG = 1.1859689372E+02

DelSqK = -1.6794442778E+03

Stress_EigVals = -2.0634076254E+00 -2.0630791675E+00 -1.9147277345E+00

Stress_EigVec1 = 9.7224433678E-01 1.0694238628E-01 -2.0809679386E-01

Stress_EigVec2 = -2.1128552308E-02 9.2592195269E-01 3.7712348350E-01

Stress_EigVec3 = 2.3301187497E-01 -3.6225938711E-01 9.0248191260E-01

-DivStress = 3.2573984730E+00 -4.9245721307E+00 1.2187709652E+01

CP# 12 Coords = 3.45145980791816E+00 -2.01703172856461E+00 -1.33409345561910E+00

Type = (3,-3) NACP H12

Rho = 4.1858972186E-01 Rho at Nucleus = 4.1565963399E-01

GradRho = -5.5529799509E-14 1.5847566315E-13 1.4098444634E-13

HessRho_EigVals = -8.3661848152E+00 -8.3611050982E+00 -7.7547168558E+00

HessRho_EigVec1 = 5.7189007064E-01 6.5068727336E-01 -4.9954761473E-01

HessRho_EigVec2 = 7.7928767276E-01 -2.4072216159E-01 5.7858755950E-01

HessRho_EigVec3 = -2.5622737985E-01 7.2017977839E-01 6.4473918495E-01

DelSqRho = -2.4482006769E+01

Bond Ellipticity = NA

V = -6.1424483066E+00

G = 1.0973307130E-02

K = 6.1314749995E+00
L = 6.1205016923E+00
Vnuc = 4.4467060610E+01
Ven = -1.8613454533E+01
Vrep = 1.2471006226E+01
DelSqV = 1.5863156446E+03
DelSqVen = 1.0886428789E+03
DelSqVrep = 4.9767276570E+02
DelSqG = 1.2054328956E+02
DelSqK = -1.7068589341E+03
Stress_EigVals = -2.0990445615E+00 -2.0984464097E+00 -1.9449573354E+00
Stress_EigVec1 = 9.6716644327E-01 1.7409890947E-01 1.8514491823E-01
Stress_EigVec2 = -2.0899348262E-02 -6.7155288465E-01 7.4066182591E-01
Stress_EigVec3 = -2.5328302009E-01 7.2021267195E-01 6.4586486117E-01
-DivStress = 3.5631681884E+00 -1.0024344064E+01 -8.9675736243E+00

CP# 13 Coords = 4.11495203489820E+00 1.09180614468357E+00 -3.34309528047708E-01

Type = (3,-3) NACP H13

Rho = 4.2358331384E-01 Rho at Nucleus = 4.2060563613E-01

GradRho = -9.1581047607E-10 -1.2647785553E-09 2.4951313173E-10

HessRho_EigVals = -8.4622276963E+00 -8.4596383490E+00 -7.8410840584E+00

HessRho_EigVec1 = -3.0633910263E-01 3.9293652304E-01 8.6703935497E-01

HessRho_EigVec2 = 7.5521190868E-01 -4.5415605797E-01 4.7264918068E-01

HessRho_EigVec3 = 5.7949230123E-01 7.9958937204E-01 -1.5762458230E-01

DelSqRho = -2.4762950104E+01

Bond Ellipticity = NA

V = -6.2122437313E+00

G = 1.0753102671E-02

K = 6.2014906286E+00

L = 6.1907375259E+00

Vnuc = 4.4369894872E+01

Ven = -1.8794347104E+01

Vrep = 1.2582103373E+01
DelSqV = 1.6041346392E+03
DelSqVen = 1.0987294971E+03
DelSqVrep = 5.0540514208E+02
DelSqG = 1.2185577390E+02
DelSqK = -1.7259904131E+03
Stress_EigVals = -2.1232101843E+00 -2.1224815675E+00 -1.9665519794E+00
Stress_EigVec1 = -8.1555400652E-01 5.7502761696E-01 -6.4922277997E-02
Stress_EigVec2 = 3.8940657303E-02 1.6646967350E-01 9.8527735842E-01
Stress_EigVec3 = 5.7736928188E-01 8.0101878101E-01 -1.5815696256E-01
-DivStress = 8.1668808354E+00 1.1285212980E+01 -2.2270896320E+00

CP# 14 Coords = -6.23540867116620E-01 -7.48403809956117E-01 -2.64186388703348E-02

Type = (3,-1) BCP B1 C2
Rho = 1.7795844689E-01
GradRho = 1.6851971207E-14 1.9900747716E-14 3.4520997172E-16
HessRho_EigVals = -3.8300964519E-01 -2.9661217200E-01 4.9787007560E-01
HessRho_EigVec1 = 2.3401638732E-02 -2.5516399951E-02 9.9940045859E-01
HessRho_EigVec2 = 7.6231919010E-01 -6.4628898769E-01 -3.4351081474E-02
HessRho_EigVec3 = 6.4677802661E-01 7.6266601978E-01 4.3274199386E-03
DelSqRho = -1.8175174159E-01
Bond Ellipticity = 2.9128094306E-01
V = -3.2525670592E-01
G = 1.3990938526E-01
K = 1.8534732066E-01
L = 4.5437935398E-02
Vnuc = 1.3640218095E+01
Ven = -2.4273920275E+00
Vrep = 2.1021353216E+00
DelSqV = -3.6663383688E+00
DelSqVen = 2.4791333945E+00
DelSqVrep = -6.1454717633E+00

DelSqG = 5.9836043908E+00

DelSqK = -2.3172660219E+00

Stress_EigVals = -1.4177697614E-01 -1.1400081311E-01 -6.9478916663E-02

Stress_EigVec1 = 7.5959600120E-01 -6.4932869811E-01 -3.7231126366E-02

Stress_EigVec2 = 3.4627480484E-02 -1.6787573024E-02 9.9925928316E-01

Stress_EigVec3 = 6.4947274967E-01 7.6032257575E-01 -9.7328434822E-03

-DivStress = 3.3216689472E-01 3.9349614621E-01 5.0210657429E-03

BPL = 2.9830997052E+00 = 9.7659152969E-01 + 2.0065081755E+00

GBL_I = 2.9827964897E+00

GBL_II = 2.9827937134E+00

GBL_III = 2.9829591937E+00 = 9.7659027067E-01 + 2.0063689230E+00

GBL_IV = 2.9829564132E+00 = 9.7659028542E-01 + 2.0063661278E+00

CP# 15 Coords = -2.52439851592722E+00 -2.27195333743770E+00 1.17082912509472E+00

Type = (3,-1) BCP H3 C2

Rho = 2.5930923194E-01

GradRho = -8.6736173799E-18 -1.2359904766E-16 -8.5001450323E-17

HessRho_EigVals = -6.3837660468E-01 -6.1788564705E-01 4.3542207662E-01

HessRho_EigVec1 = -5.6007150175E-01 7.8471460032E-01 -2.6559915094E-01

HessRho_EigVec2 = 6.9669921078E-01 6.1961213187E-01 3.6151212391E-01

HessRho_EigVec3 = -4.4825229796E-01 -1.7429919295E-02 8.9373713993E-01

DelSqRho = -8.2084017510E-01

Bond Ellipticity = 3.3163025759E-02

V = -3.1133854093E-01

G = 5.3064248580E-02

K = 2.5827429236E-01

L = 2.0521004378E-01

Vnuc = 1.1042348854E+01

Ven = -2.8633830003E+00

Vrep = 2.5520444593E+00

DelSqV = -2.0816962706E+00

DelSqVen = 9.0640035671E+00

DelSqVrep = -1.1145699838E+01

DelSqG = 1.4513130739E+00

DelSqK = 6.3038319671E-01

Stress_EigVals = -2.0263925784E-01 -2.0028965999E-01 9.1590376894E-02

Stress_EigVec1 = 5.7504851408E-01 7.6207038127E-01 2.9760366334E-01

Stress_EigVec2 = 6.8574808244E-01 -6.4736797888E-01 3.3266239245E-01

Stress_EigVec3 = -4.4617123830E-01 -1.2784126995E-02 8.9485629696E-01

-DivStress = 6.4879821120E-02 9.2497056113E-04 -1.3210504637E-01

BPL = 2.0523467703E+00 = 7.3474958885E-01 + 1.3175971814E+00

GBL_I = 2.0522681768E+00

GBL_II = 2.0791488155E+00

GBL_III = 2.0523122814E+00 = 7.3474880055E-01 + 1.3175634808E+00

GBL_IV = 2.0791951138E+00 = 7.6163027771E-01 + 1.3175648361E+00

CP# 16 Coords = -2.90741243563937E+00 -2.05228580381129E+00 -8.76743401861072E-01

Type = (3,-1) BCP C2 H4

Rho = 2.6296953976E-01

GradRho = -3.0184188482E-16 1.3010426070E-16 -1.9428902931E-16

HessRho_EigVals = -6.5334389603E-01 -6.3456161471E-01 4.4283277702E-01

HessRho_EigVec1 = -3.4550664855E-01 7.5300290937E-01 5.6001051266E-01

HessRho_EigVec2 = -5.7997394308E-01 -6.4048892951E-01 5.0339264648E-01

HessRho_EigVec3 = 7.3773666112E-01 -1.5086599900E-01 6.5801524996E-01

DelSqRho = -8.4507273371E-01

Bond Ellipticity = 2.9598829940E-02

V = -3.1546926406E-01

G = 5.2100540318E-02

K = 2.6336872375E-01

L = 2.1126818343E-01

Vnuc = 1.1012112680E+01

Ven = -2.8958502033E+00

Vrep = 2.5803809392E+00

DelSqV = -2.1521342084E+00

DelSqVen = 9.3060361664E+00

DelSqVrep = -1.1458170375E+01

DelSqG = 1.4832383101E+00

DelSqK = 6.6889589831E-01

Stress_EigVals = -2.0578256587E-01 -2.0328325118E-01 9.3596552994E-02

Stress_EigVec1 = 4.5519956711E-01 8.3265626014E-01 -3.1539959821E-01

Stress_EigVec2 = -4.9928217495E-01 5.3199602260E-01 6.8388415811E-01

Stress_EigVec3 = 7.3723175724E-01 -1.5383037535E-01 6.5789478774E-01

-DivStress = 1.0727255002E-01 -2.4068783306E-02 9.7310113721E-02

BPL = 2.0459637958E+00 = 1.3148963244E+00 + 7.3106747139E-01

GBL_I = 2.0459132831E+00

GBL_II = 2.0729676765E+00

GBL_III = 2.0459357048E+00 = 1.3148683767E+00 + 7.3106732811E-01

GBL_IV = 2.0729908422E+00 = 1.3148694393E+00 + 7.5812140295E-01

CP# 17 Coords = -1.41924419331216E+00 -3.44483469020435E+00 -2.20449959786864E-01

Type = (3,-1) BCP C2 H5

Rho = 2.6831563775E-01

GradRho = 1.3376105779E-13 -8.9176929730E-14 -3.1745981711E-14

HessRho_EigVals = -6.7122468072E-01 -6.5952617706E-01 4.5020072901E-01

HessRho_EigVec1 = 2.7334743115E-01 -5.1866884299E-02 9.6051601142E-01

HessRho_EigVec2 = 8.7880597679E-01 4.1948793161E-01 -2.2744214737E-01

HessRho_EigVec3 = -3.9112815937E-01 9.0627793835E-01 1.6024687642E-01

DelSqRho = -8.8055012877E-01

Bond Ellipticity = 1.7737739704E-02

V = -3.2177676342E-01

G = 5.0819615615E-02

K = 2.7095714781E-01

L = 2.2013753219E-01

Vnuc = 1.0987148846E+01

Ven = -2.9480238497E+00

Vrep = 2.6262470863E+00

DelSqV = -2.2042066341E+00

DelSqVen = 9.6747353312E+00

DelSqVrep = -1.1878941965E+01

DelSqG = 1.5256218685E+00

DelSqK = 6.7858476560E-01

Stress_EigVals = -2.0997716010E-01 -2.0721145066E-01 9.5411847338E-02

Stress_EigVec1 = 9.0520566585E-01 4.1101021376E-01 -1.0804307796E-01

Stress_EigVec2 = 1.6367721638E-01 -1.0255973472E-01 9.8116831872E-01

Stress_EigVec3 = -3.9218933099E-01 9.0584331151E-01 1.6011066064E-01

-DivStress = -6.2547540261E-02 1.3644289733E-01 2.4856226091E-02

BPL = 2.0388863261E+00 = 1.3099168699E+00 + 7.2896945619E-01

GBL_I = 2.0388547239E+00

GBL_II = 2.0660368275E+00

GBL_III = 2.0388659546E+00 = 1.3098965835E+00 + 7.2896937115E-01

GBL_IV = 2.0660481074E+00 = 1.3098972561E+00 + 7.5615085133E-01

CP# 18 Coords = -3.27412525062607E-01 9.13721117762028E-01 1.10555819333039E-02

Type = (3,-1) BCP C6 B1

Rho = 1.7813706577E-01

GradRho = 6.6821548295E-15 -1.8138268665E-14 -7.6154360595E-16

HessRho_EigVals = -3.8350743297E-01 -2.9724072418E-01 5.0107061315E-01

HessRho_EigVec1 = 1.1656269806E-02 -2.0319243193E-02 9.9972559222E-01

HessRho_EigVec2 = 9.3992122877E-01 3.4136771569E-01 -4.0207451293E-03

HessRho_EigVec3 = -3.4119234323E-01 9.3971017396E-01 2.3077562227E-02

DelSqRho = -1.7967754401E-01

Bond Ellipticity = 2.9022506598E-01

V = -3.2627021873E-01

G = 1.4067541636E-01

K = 1.8559480236E-01

L = 4.4919386002E-02

Vnuc = 1.3647431858E+01

Ven = -2.4311134666E+00

Vrep = 2.1048432478E+00
DelSqV = -3.6829553061E+00
DelSqVen = 2.4521370384E+00
DelSqVrep = -6.1350923445E+00
DelSqG = 6.0122262475E+00
DelSqK = -2.3292709414E+00
Stress_EigVals = -1.4214341125E-01 -1.1435173766E-01 -6.9775069815E-02
Stress_EigVec1 = 9.4065816601E-01 3.3932312054E-01 -4.6941005429E-03
Stress_EigVec2 = 6.7780017968E-03 -4.9564783047E-03 9.9996474539E-01
Stress_EigVec3 = -3.3928789162E-01 9.4065682010E-01 6.9622845127E-03
-DivStress = 1.7720912481E-01 -4.8492845498E-01 -1.5764234156E-02
BPL = 2.9814346113E+00 = 2.0054866616E+00 + 9.7594794973E-01
GBL_I = 2.9809879636E+00
GBL_II = 2.9809851395E+00
GBL_III = 2.9812460582E+00 = 2.0053002506E+00 + 9.7594580754E-01
GBL_IV = 2.9812432268E+00 = 2.0052974313E+00 + 9.7594579555E-01

CP# 19 Coords = -8.42523510803186E-01 3.25785837583475E+00 -1.21119853786107E+00

Type = (3,-1) BCP C6 H7
Rho = 2.5776446965E-01
GradRho = 1.4521023273E-13 -1.6122389881E-13 -3.7659458885E-13
HessRho_EigVals = -6.3210807768E-01 -6.1097172090E-01 4.3223808133E-01
HessRho_EigVec1 = 9.6345066944E-01 1.9165385744E-01 1.8716732217E-01
HessRho_EigVec2 = -2.4425864806E-01 9.1539022250E-01 3.1999758342E-01
HessRho_EigVec3 = -1.1000236545E-01 -3.5401912304E-01 9.2874643478E-01
DelSqRho = -8.1084171725E-01
Bond Ellipticity = 3.4594656449E-02
V = -3.0950823674E-01
G = 5.3398903717E-02
K = 2.5610933303E-01
L = 2.0271042931E-01
Vnuc = 1.1049100260E+01

Ven = -2.8480654686E+00
Vrep = 2.5385572318E+00
DelSqV = -2.0510144088E+00
DelSqVen = 8.9590714288E+00
DelSqVrep = -1.1010085838E+01
DelSqG = 1.4374979467E+00
DelSqK = 6.1351646209E-01
Stress_EigVals = -2.0128932764E-01 -1.9894729288E-01 9.0728383772E-02
Stress_EigVec1 = 3.6057559472E-01 -8.8689546652E-01 -2.8879347630E-01
Stress_EigVec2 = 9.2586543874E-01 3.0283847548E-01 2.2596912868E-01
Stress_EigVec3 = -1.1295321971E-01 -3.4886285160E-01 9.3034202363E-01
-DivStress = -1.6952965977E-02 -5.0433300080E-02 1.3733430186E-01
BPL = 2.0552235848E+00 = 1.3188431065E+00 + 7.3638047826E-01
GBL_I = 2.0551349642E+00
GBL_II = 2.0819393542E+00
GBL_III = 2.0551893814E+00 = 1.3188101289E+00 + 7.3637925255E-01
GBL_IV = 2.0819968037E+00 = 1.3188116122E+00 + 7.6318519150E-01

CP# 20 Coords = -2.25985458096364E+00 2.93365836926829E+00 3.33642012318467E-01

Type = (3,-1) BCP C6 H8
Rho = 2.6776793803E-01
GradRho = -6.1686766806E-15 -1.1102230246E-15 1.6306400674E-15
HessRho_EigVals = -6.6987726995E-01 -6.5661613116E-01 4.4951980373E-01
HessRho_EigVec1 = 2.6324177914E-01 3.4827797297E-01 8.9967006133E-01
HessRho_EigVec2 = 1.1274121019E-02 9.3138734188E-01 -3.6385507223E-01
HessRho_EigVec3 = 9.6466401400E-01 -1.0592484571E-01 -2.4125353293E-01
DelSqRho = -8.7697359738E-01
Bond Ellipticity = 2.0196181849E-02
V = -3.2103481205E-01
G = 5.0895706351E-02
K = 2.7013910570E-01
L = 2.1924339935E-01

Vnuc = 1.0996216058E+01
Ven = -2.9444341001E+00
Vrep = 2.6233992880E+00
DelSqV = -2.1997813883E+00
DelSqVen = 9.6433911542E+00
DelSqVrep = -1.1843172543E+01
DelSqG = 1.5209898619E+00
DelSqK = 6.7879152636E-01
Stress_EigVals = -2.0953745407E-01 -2.0675478322E-01 9.5257425242E-02
Stress_EigVec1 = 6.6764076327E-02 9.8476963331E-01 -1.6053450541E-01
Stress_EigVec2 = 2.5398149871E-01 1.3882027460E-01 9.5719503220E-01
Stress_EigVec3 = 9.6490204499E-01 -1.0467903647E-01 -2.4084505995E-01
-DivStress = 1.4620612709E-01 -1.2862211450E-02 -3.7150711721E-02
BPL = 2.0396190412E+00 = 1.3104962765E+00 + 7.2912276473E-01
GBL_I = 2.0395860734E+00
GBL_II = 2.0667589284E+00
GBL_III = 2.0395980402E+00 = 1.3104753252E+00 + 7.2912271504E-01
GBL_IV = 2.0667710083E+00 = 1.3104760524E+00 + 7.5629495589E-01

CP# 21 Coords = -2.65139862458882E-01 3.58724312962164E+00 7.80216876162168E-01

Type = (3,-1) BCP H9 C6
Rho = 2.6471929140E-01
GradRho = -5.2041704279E-17 2.4286128664E-17 -1.1102230246E-16
HessRho_EigVals = -6.6026767063E-01 -6.4225601816E-01 4.4587263941E-01
HessRho_EigVec1 = -7.7291103701E-01 1.0182000948E-01 6.2629163696E-01
HessRho_EigVec2 = 3.1764299743E-01 -7.9236606700E-01 5.2082525097E-01
HessRho_EigVec3 = 5.4928267317E-01 6.0148873766E-01 5.8008606553E-01
DelSqRho = -8.5665104939E-01
Bond Ellipticity = 2.8044349850E-02
V = -3.1747582831E-01
G = 5.1656532984E-02
K = 2.6581929533E-01

L = 2.1416276235E-01
Vnuc = 1.1005131463E+01
Ven = -2.9132706028E+00
Vrep = 2.5957947745E+00
DelSqV = -2.1785237167E+00
DelSqVen = 9.4275574167E+00
DelSqVrep = -1.1606081133E+01
DelSqG = 1.4977708300E+00
DelSqK = 6.8075288667E-01
Stress_EigVals = -2.0723408156E-01 -2.0462235976E-01 9.4380613005E-02
Stress_EigVec1 = 5.4122022594E-01 -7.8596142266E-01 2.9890685692E-01
Stress_EigVec2 = 6.3497704377E-01 1.4896569074E-01 -7.5803256979E-01
Stress_EigVec3 = -5.5125749057E-01 -6.0006155107E-01 -5.7969070548E-01
-DivStress = -8.2361692627E-02 -8.6634577852E-02 -8.6245324824E-02
BPL = 2.0432806404E+00 = 7.2978545671E-01 + 1.3134951837E+00
GBL_I = 2.0432358163E+00
GBL_II = 2.0703562775E+00
GBL_III = 2.0432529684E+00 = 7.2978543115E-01 + 1.3134675373E+00
GBL_IV = 2.0703738010E+00 = 7.5690534283E-01 + 1.3134684582E+00

CP# 22 Coords = 9.68459496691176E-01 -1.71711271981157E-01 -3.04946660802675E-02

Type = (3,-1) BCP C10 B1
Rho = 1.7814754035E-01
GradRho = -8.2399365109E-14 1.4281978378E-14 1.6341095144E-15
HessRho_EigVals = -3.8350322909E-01 -2.9748178988E-01 4.9939358342E-01
HessRho_EigVec1 = 2.5195858866E-03 -2.9851669434E-02 9.9955116403E-01
HessRho_EigVec2 = 1.7490003608E-01 9.8416045857E-01 2.8951151334E-02
HessRho_EigVec3 = 9.8458297216E-01 -1.7474858974E-01 -7.7007348626E-03
DelSqRho = -1.8159143555E-01
Bond Ellipticity = 2.8916539481E-01
V = -3.2580185291E-01
G = 1.4020199701E-01

K = 1.8559985590E-01

L = 4.5397858887E-02

Vnuc = 1.3638534703E+01

Ven = -2.4296714112E+00

Vrep = 2.1038695583E+00

DelSqV = -3.6738408545E+00

DelSqVen = 2.4766410954E+00

DelSqVrep = -6.1504819499E+00

DelSqG = 5.9966622526E+00

DelSqK = -2.3228213981E+00

Stress_EigVals = -1.4196767428E-01 -1.1420756418E-01 -6.9626614457E-02

Stress_EigVec1 = 1.7687195240E-01 9.8371437996E-01 3.1973913069E-02

Stress_EigVec2 = -1.2427293674E-02 -3.0251432700E-02 9.9946506352E-01

Stress_EigVec3 = 9.8415541193E-01 -1.7717468634E-01 6.8742775271E-03

-DivStress = -5.0823265943E-01 8.9004554149E-02 7.3936663910E-03

BPL = 2.9816618844E+00 = 2.0053657738E+00 + 9.7629611065E-01

GBL_I = 2.9812981774E+00

GBL_II = 2.9812953824E+00

GBL_III = 2.9814969433E+00 = 2.0052025725E+00 + 9.7629437080E-01

GBL_IV = 2.9814941428E+00 = 2.0051997749E+00 + 9.7629436784E-01

CP# 23 Coords = 3.23040001018158E+00 -1.01862471574942E+00 1.18052471644894E+00

Type = (3,-1) BCP H11 C10

Rho = 2.5811533377E-01

GradRho = -1.5431406153E-13 -6.6995020642E-15 1.1228171171E-13

HessRho_EigVals = -6.3352832719E-01 -6.1296063393E-01 4.3312515122E-01

HessRho_EigVec1 = 3.3572664019E-01 9.0132272709E-01 2.7368771384E-01

HessRho_EigVec2 = -9.1288615573E-01 2.3969859607E-01 3.3042919017E-01

HessRho_EigVec3 = 2.3222077803E-01 -3.6077960680E-01 9.0327824372E-01

DelSqRho = -8.1336380990E-01

Bond Ellipticity = 3.3554672384E-02

V = -3.0986615266E-01

G = 5.3262600093E-02

K = 2.5660355257E-01

L = 2.0334095247E-01

Vnuc = 1.1042899157E+01

Ven = -2.8503416017E+00

Vrep = 2.5404754490E+00

DelSqV = -2.0604150985E+00

DelSqVen = 8.9818945304E+00

DelSqVrep = -1.1042309629E+01

DelSqG = 1.4408079935E+00

DelSqK = 6.1960710500E-01

Stress_EigVals = -2.0159415923E-01 -1.9926481103E-01 9.0992817598E-02

Stress_EigVec1 = 9.5410032722E-01 -1.0418454208E-01 -2.8078131489E-01

Stress_EigVec2 = 1.9560310719E-01 9.2672978819E-01 3.2079794909E-01

Stress_EigVec3 = 2.2678622105E-01 -3.6099512583E-01 9.0457201431E-01

-DivStress = -3.2348510345E-02 5.2854387196E-02 -1.3324140131E-01

BPL = 2.0544393391E+00 = 7.3582407279E-01 + 1.3186152663E+00

GBL_I = 2.0543592724E+00

GBL_II = 2.0811908670E+00

GBL_III = 2.0544086901E+00 = 7.3582290943E-01 + 1.3185857806E+00

GBL_IV = 2.0812430281E+00 = 7.6265577743E-01 + 1.3185872507E+00

CP# 24 Coords = 3.26432002551868E+00 -1.49153267067865E+00 -8.63331976310390E-01

Type = (3,-1) BCP C10 H12

Rho = 2.6435832977E-01

GradRho = -6.9388939039E-17 -8.6736173799E-17 -2.0469737017E-16

HessRho_EigVals = -6.5893471807E-01 -6.4055560653E-01 4.4538199093E-01

HessRho_EigVec1 = 4.9082107748E-01 6.7210469425E-01 -5.5440955066E-01

HessRho_EigVec2 = 8.3276520867E-01 -1.7484060236E-01 5.2529312864E-01

HessRho_EigVec3 = -2.5611867782E-01 7.1951792454E-01 6.4552085879E-01

DelSqRho = -8.5410833366E-01

Bond Ellipticity = 2.8692452852E-02

V = -3.1711422711E-01
G = 5.1793571846E-02
K = 2.6532065526E-01
L = 2.1352708341E-01
Vnuc = 1.0997027316E+01
Ven = -2.9071557738E+00
Vrep = 2.5900415467E+00
DelSqV = -2.1752276989E+00
DelSqVen = 9.3926526763E+00
DelSqVrep = -1.1567880375E+01
DelSqG = 1.4951396101E+00
DelSqK = 6.8008808889E-01
Stress_EigVals = -2.0695699407E-01 -2.0440308856E-01 9.4245855519E-02
Stress_EigVec1 = 9.4511359391E-01 4.2455666856E-02 3.2397192929E-01
Stress_EigVec2 = -2.0603059501E-01 -6.9212438581E-01 6.9174795156E-01
Stress_EigVec3 = -2.5359749316E-01 7.2052852193E-01 6.4538899940E-01
-DivStress = -3.5214196179E-02 1.0596847905E-01 9.5699645981E-02
BPL = 2.0437232685E+00 = 1.3138006827E+00 + 7.2992258576E-01
GBL_I = 2.0436744906E+00
GBL_II = 2.0707869020E+00
GBL_III = 2.0436933323E+00 = 1.3137707827E+00 + 7.2992254959E-01
GBL_IV = 2.0708061571E+00 = 1.3137717199E+00 + 7.5703443722E-01

CP# 25 Coords = 3.69188365153954E+00 5.09293316139684E-01 -2.19609270982882E-01

Type = (3,-1) BCP H13 C10
Rho = 2.6797054691E-01
GradRho = 1.2143064332E-17 -1.1796119637E-16 -3.4694469520E-18
HessRho_EigVals = -6.7039559794E-01 -6.5766715027E-01 4.4982905737E-01
HessRho_EigVec1 = -1.7546950925E-01 3.1153720481E-01 9.3389240351E-01
HessRho_EigVec2 = 7.9487659359E-01 -5.1484708407E-01 3.2109761910E-01
HessRho_EigVec3 = 5.8084563551E-01 7.9867205413E-01 -1.5729366696E-01
DelSqRho = -8.7823369084E-01

$$\text{Bond Ellipticity} = 1.9353935597\text{E-}02$$

$$V = -3.2131903793\text{E-}01$$

$$G = 5.0880307610\text{E-}02$$

$$K = 2.7043873032\text{E-}01$$

$$L = 2.1955842271\text{E-}01$$

$$V_{\text{nuc}} = 1.0989141890\text{E+}01$$

$$V_{\text{en}} = -2.9447663625\text{E+}00$$

$$V_{\text{rep}} = 2.6234473245\text{E+}00$$

$$\text{DelSqV} = -2.2021652235\text{E+}00$$

$$\text{DelSqVen} = 9.6510346417\text{E+}00$$

$$\text{DelSqVrep} = -1.1853199865\text{E+}01$$

$$\text{DelSqG} = 1.5227170211\text{E+}00$$

$$\text{DelSqK} = 6.7944820234\text{E-}01$$

$$\text{Stress\_EigVals} = -2.0970300633\text{E-}01 \ -2.0694209930\text{E-}01 \ 9.5326067699\text{E-}02$$

$$\text{Stress\_EigVec1} = 8.1454163121\text{E-}01 \ -5.6506548099\text{E-}01 \ 1.3123617344\text{E-}01$$

$$\text{Stress\_EigVec2} = -1.6260160957\text{E-}02 \ 2.0389995820\text{E-}01 \ 9.7885668727\text{E-}01$$

$$\text{Stress\_EigVec3} = 5.7987717509\text{E-}01 \ 7.9945344408\text{E-}01 \ -1.5689694888\text{E-}01$$

$$-\text{DivStress} = -8.5306166063\text{E-}02 \ -1.2286652932\text{E-}01 \ 2.4313099088\text{E-}02$$

$$\text{BPL} = 2.0393653728\text{E+}00 = 7.2901597920\text{E-}01 + 1.3103493936\text{E+}00$$

$$\text{GBL\_I} = 2.0393317192\text{E+}00$$

$$\text{GBL\_II} = 2.0665105995\text{E+}00$$

$$\text{GBL\_III} = 2.0393434785\text{E+}00 = 7.2901591279\text{E-}01 + 1.3103275657\text{E+}00$$

$$\text{GBL\_IV} = 2.0665224476\text{E+}00 = 7.5619418518\text{E-}01 + 1.3103282624\text{E+}00$$

$$\text{Number of NACPs} = 13$$

$$\text{Number of NNACPs} = 0$$

$$\text{Number of BCPs} = 12$$

$$\text{Number of RCPs} = 0$$

$$\text{Number of CCPs} = 0$$

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H3	C2	B1	108.47677697	107.57565464	107.58596841	107.68795822	107.68805184
H4	C2	B1	111.16631292	111.16536095	111.17118971	110.93029278	110.93040353
H4	C2	H3	104.91647345	105.24616894	105.23732864	105.44363199	105.44349371
H5	C2	B1	113.89092617	115.20809246	115.21017303	114.74516081	114.74529752
H5	C2	H3	108.37036457	108.02432921	108.01885557	108.24843435	108.24831199
H5	C2	H4	109.58632626	109.09121046	109.08616557	109.32349246	109.32338560
C6	B1	C2	119.73368650	119.59508116	119.59508422	119.73856634	119.73856606
H7	C6	B1	107.45964166	106.19637674	106.20869097	106.40416063	106.40424888
H8	C6	B1	113.77064167	114.97120346	114.97363237	114.50508317	114.50521803
H8	C6	H7	107.52804060	107.36313356	107.35696810	107.57751785	107.57738619
H9	C6	B1	112.15726969	112.59311983	112.59719683	112.27512859	112.27524960
H9	C6	H7	105.34824065	105.59440771	105.58578325	105.79740375	105.79726533
H9	C6	H8	110.08156556	109.50384327	109.49884904	109.74393022	109.74382791
C10	B1	C2	120.23586309	120.32183866	120.32183692	120.23402536	120.23402416
C10	B1	C6	120.02929564	120.07522735	120.07522616	120.02579460	120.02579612
H11	C10	B1	107.95923551	106.78275049	106.79446702	106.93904709	106.93913514
H12	C10	B1	111.76942114	112.12954371	112.13386440	111.83567537	111.83579361
H12	C10	H11	105.22321768	105.50068606	105.49212154	105.69910171	105.69896337
H13	C10	B1	113.73054222	114.93582066	114.93808752	114.49502857	114.49516366
H13	C10	H11	107.68346618	107.51871471	107.51283588	107.72863296	107.72850353
H13	C10	H12	110.01297241	109.40340697	109.39854755	109.64598051	109.64587926

Total time for electron density critical point search, analysis and connectivity = 15 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
B1	-2.3857421654E+01	2.3857421654E+01	-7.6088570108E+01	-5.2156274108E+01		
C2	-3.8215341746E+01	3.8215341746E+01	-1.3564163506E+02	-9.1894649324E+01		
H3	-6.0141013453E-01	6.0141013453E-01	-8.3143108704E+00	-1.2415990707E+00		
H4	-6.0598170384E-01	6.0598170384E-01	-8.3221914272E+00	-1.2496175933E+00		
H5	-6.1664686215E-01	6.1664686215E-01	-8.4228806878E+00	-1.2694757172E+00		
C6	-3.8216498410E+01	3.8216498410E+01	-1.3567240457E+02	-9.1897078329E+01		
H7	-5.9939607940E-01	5.9939607940E-01	-8.3058015612E+00	-1.2383448259E+00		
H8	-6.1543792182E-01	6.1543792182E-01	-8.4209612470E+00	-1.2673727228E+00		
H9	-6.0873472757E-01	6.0873472757E-01	-8.3416012943E+00	-1.2545780761E+00		
C10	-3.8216023224E+01	3.8216023224E+01	-1.3562066411E+02	-9.1897297968E+01		

H11 -5.9960521161E-01 5.9960521161E-01 -8.3029272477E+00 -1.2386275774E+00
H12 -6.0805003963E-01 6.0805003963E-01 -8.3214313161E+00 -1.2531659445E+00
H13 -6.1581731385E-01 6.1581731385E-01 -8.4174764023E+00 -1.2679600105E+00

Total -1.4397636503E+02 1.4397636503E+02 -5.5819285590E+02 -3.3912604127E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$$V_{nn}(A) = \text{Contribution of Atom A to Nuclear Repulsion Energy of Molecule}$$

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$$V_{eeC}(A) = \text{Coulomb Part of } V_{ee}(A)$$

$$V_{eeX}(A) = \text{Exchange-Correlation Part of } V_{ee}(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

B1	-2.3857421654E+01					
C2	-3.8215341746E+01					
H3	-6.0141013453E-01					
H4	-6.0598170384E-01					
H5	-6.1664686215E-01					
C6	-3.8216498410E+01					
H7	-5.9939607940E-01					
H8	-6.1543792182E-01					
H9	-6.0873472757E-01					

C10	-3.8216023224E+01
H11	-5.9960521161E-01
H12	-6.0805003963E-01
H13	-6.1581731385E-01

Total	-1.4397636503E+02

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
$VeeC(A)$	$VeeX(A)$					

B1			2.3857421654E+01	-4.9084840806E+01	-3.8044285054E+01	
2.0448087919E+01						
C2			3.8215341746E+01	-6.3687414559E+01	-6.7820817532E+01	
1.9316486038E+01						
H3			6.0141013453E-01	-4.3396631361E+00	-4.1571554352E+00	
3.7898854168E+00						
H4			6.0598170384E-01	-4.3270158685E+00	-4.1610957136E+00	
3.7736170780E+00						

H5 3.7582487202E+00	6.1664686215E-01 -4.3181403416E+00 -4.2114403439E+00
C6 1.9326783038E+01	3.8216498410E+01 -6.3697362921E+01 -6.7836202284E+01
H7 3.7932758377E+00	5.9939607940E-01 -4.3415413137E+00 -4.1529007806E+00
H8 3.7638347077E+00	6.1543792182E-01 -4.3229802364E+00 -4.2104806235E+00
H9 3.7689517488E+00	6.0873472757E-01 -4.3241736973E+00 -4.1708006472E+00
C10 1.9303682936E+01	3.8216023224E+01 -6.3674305328E+01 -6.7810332053E+01
H11 3.7915701907E+00	5.9960521161E-01 -4.3400933239E+00 -4.1514636239E+00
H12 3.7640945647E+00	6.0805003963E-01 -4.3188681514E+00 -4.1607156581E+00
H13 3.7606065092E+00	6.1581731385E-01 -4.3200184093E+00 -4.2087382011E+00

Total 1.1235912470E+02	1.4397636503E+02 -2.7909641809E+02 -2.7909642795E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

B1	2.3857421654E+01 -5.2156274108E+01
C2	3.8215341746E+01 -9.1894649324E+01
H3	6.0141013453E-01 -1.2415990707E+00
H4	6.0598170384E-01 -1.2496175933E+00
H5	6.1664686215E-01 -1.2694757172E+00
C6	3.8216498410E+01 -9.1897078329E+01
H7	5.9939607940E-01 -1.2383448259E+00
H8	6.1543792182E-01 -1.2673727228E+00
H9	6.0873472757E-01 -1.2545780761E+00
C10	3.8216023224E+01 -9.1897297968E+01
H11	5.9960521161E-01 -1.2386275774E+00
H12	6.0805003963E-01 -1.2531659445E+00
H13	6.1581731385E-01 -1.2679600105E+00

Total 1.4397636503E+02 -3.3912604127E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$$VeeC(A,A') = \text{Coulomb Part of } Vee(A,A')$$

$VeeX(A,A') = \text{Exchange-Correlation Part of } Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Inter(A)	Vne(A,A')/2	Ven(A,A')/2	Vee(A,A')	Vnn(A)	VeeC(A,A')
VeeX(A,A')						
B1	-2.3006703752E+01	-1.1966148000E+01		2.0448087919E+01		
C2	-1.7740089897E+01	-2.1873492870E+01		1.9316486038E+01		
H3	-3.7188636008E+00	-3.5363558999E+00		3.7898854168E+00		
H4	-3.7022070718E+00	-3.5362869169E+00		3.7736170780E+00		
H5	-3.6834024830E+00	-3.5767024853E+00		3.7582487202E+00		
C6	-1.7748823757E+01	-2.1887663119E+01		1.9326783038E+01		
H7	-3.7223689007E+00	-3.5337283676E+00		3.7932758377E+00		
H8	-3.6892938750E+00	-3.5767942621E+00		3.7638347077E+00		
H9	-3.6968846593E+00	-3.5435116091E+00		3.7689517488E+00		
C10	-1.7725656344E+01	-2.1861683069E+01		1.9303682936E+01		
H11	-3.7207795352E+00	-3.5321498352E+00		3.7915701907E+00		
H12	-3.6922851792E+00	-3.5341326858E+00		3.7640945647E+00		
H13	-3.6860384041E+00	-3.5747581959E+00		3.7606065092E+00		
Total	-1.0953339746E+02	-1.0953340732E+02		1.1235912470E+02		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other

Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	Li(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
B1	2.9460296489E+00	2.1895528518E+00	7.4322159409E+01	7.5647679700E-01	2.5677840591E+01
C2	6.7016274119E+00	5.0092249871E+00	7.4746396349E+01	1.6924024248E+00	2.5253603651E+01
H3	9.8605809881E-01	4.9460790279E-01	5.0160117683E+01	4.9145019602E-01	4.9839882317E+01
H4	9.9066344859E-01	4.9899632078E-01	5.0369913363E+01	4.9166712782E-01	4.9630086637E+01
H5	1.0061311610E+00	5.1374296119E-01	5.1061231489E+01	4.9238819979E-01	4.8938768511E+01
C6	6.7021841228E+00	5.0094434359E+00	7.4743446974E+01	1.6927406869E+00	2.5256553026E+01
H7	9.8436075955E-01	4.9311235073E-01	5.0094677785E+01	4.9124840881E-01	4.9905322215E+01
H8	1.0045625973E+00	5.1221845508E-01	5.0989202310E+01	4.9234414224E-01	4.9010797690E+01
H9	9.9401108727E-01	5.0220549086E-01	5.0523127689E+01	4.9180559640E-01	4.9476872311E+01
C10	6.7024223340E+00	5.0103690342E+00	7.4754600420E+01	1.6920532998E+00	2.5245399580E+01
H11	9.8431124973E-01	4.9311264178E-01	5.0097227063E+01	4.9119860795E-01	4.9902772937E+01
H12	9.9280898303E-01	5.0104668465E-01	5.0467581702E+01	4.9176229838E-01	4.9532418298E+01
H13	1.0048627532E+00	5.1250714723E-01	5.1002701175E+01	4.9235560596E-01	4.8997298825E+01
Total	3.2000033656E+01	2.1740140264E+01	6.7937866872E+01	1.0259893392E+01	3.2062133128E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

DI_Bond(A,A')/2 = Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

DI_NonBond(A,A')/2 = Non-Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
B1	2.9460296489E+00	2.1895528518E+00	7.5647679700E-01	6.9592180061E-01	6.0554996390E-02
C2	6.7016274119E+00	5.0092249871E+00	1.6924024248E+00	1.5429068183E+00	1.4949560652E-01
H3	9.8605809881E-01	4.9460790279E-01	4.9145019602E-01	4.3664566231E-01	5.4804533709E-02
H4	9.9066344859E-01	4.9899632078E-01	4.9166712782E-01	4.3668425554E-01	5.4982872274E-02
H5	1.0061311610E+00	5.1374296119E-01	4.9238819979E-01	4.3775861654E-01	5.4629583248E-02
C6	6.7021841228E+00	5.0094434359E+00	1.6927406869E+00	1.5426253158E+00	1.5011537105E-01
H7	9.8436075955E-01	4.9311235073E-01	4.9124840881E-01	4.3644521726E-01	5.4803191550E-02
H8	1.0045625973E+00	5.1221845508E-01	4.9234414224E-01	4.3754254278E-01	5.4801599460E-02

H9	9.9401108727E-01	5.0220549086E-01	4.9180559640E-01	4.3683311557E-01	5.4972480834E-02
C10	6.7024223340E+00	5.0103690342E+00	1.6920532998E+00	1.5433191381E+00	1.4873416170E-01
H11	9.8431124973E-01	4.9311264178E-01	4.9119860795E-01	4.3653990469E-01	5.4658703258E-02
H12	9.9280898303E-01	5.0104668465E-01	4.9176229838E-01	4.3694954141E-01	5.4812756967E-02
H13	1.0048627532E+00	5.1250714723E-01	4.9235560596E-01	4.3753061546E-01	5.4824990500E-02

Total	3.2000033656E+01	2.1740140264E+01	1.0259893392E+01	9.2577025444E+00	1.0021908475E+00

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

B1	3.2447689200E+00	4.2418689156E+01	4.5663458076E+01
C2	1.9951292491E+01	8.3923925233E+01	1.0387521772E+02
H3	2.3885133572E-01	1.5045042042E+01	1.5283893377E+01
H4	2.4120887380E-01	1.5114067705E+01	1.5355276579E+01
H5	2.4927847595E-01	1.5345747270E+01	1.5595025746E+01
C6	1.9954914290E+01	8.3928932380E+01	1.0388384667E+02
H7	2.3792687710E-01	1.5019657877E+01	1.5257584754E+01

H8 2.4846377842E-01 1.5322249296E+01 1.5570713074E+01
H9 2.4292627537E-01 1.5164238320E+01 1.5407164595E+01
C10 1.9956048054E+01 8.3931490806E+01 1.0388753886E+02
H11 2.3787799728E-01 1.5018939532E+01 1.5256817529E+01
H12 2.4231149607E-01 1.5146220331E+01 1.5388531827E+01
H13 2.4862100276E-01 1.5326744569E+01 1.5575365572E+01

Total 6.5294489867E+01 4.3070594452E+02 4.9600043438E+02

Diatomic Electron Pair Contributions and Delocalization Data:

 $2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$
B1	C2	1.9511374767E+01	4.6363656774E-01	7.8688374354E+00	3.4591341717E+00 (Bonded)
B1	H3	2.8967354797E+00	1.6441829735E-02	2.7905064943E-01	8.3371505975E-01
C2	H3	6.1715483224E+00	8.7329132462E-01	6.5155168360E+00	4.4281940672E+01 (Bonded)
B1	H4	2.9116522785E+00	1.3743226204E-02	2.3324996423E-01	6.9363749231E-01
C2	H4	6.2023730676E+00	8.7336851108E-01	6.5160927145E+00	4.4079980559E+01 (Bonded)
H3	H4	9.5865589151E-01	3.6391650353E-02	1.8453096423E+00	1.8367312534E+00
B1	H5	2.9591398156E+00	9.9048305495E-03	1.6810473298E-01	4.9222362519E-01
C2	H5	6.3049575519E+00	8.7551723308E-01	6.5321240593E+00	4.3509100356E+01 (Bonded)

H3	H5	9.7474503836E-01	3.4717482785E-02	1.7604177090E+00	1.7252960713E+00	
H4	H5	9.7942326897E-01	3.4628193400E-02	1.7477274169E+00	1.7208588077E+00	
B1	C6	1.9513028698E+01	4.6360888044E-01	7.8683675268E+00	3.4586402876E+00	(Bonded)
C2	C6	4.4853441328E+01	1.2419901881E-01	9.2663327257E-01	9.2655630262E-01	
H3	C6	6.6043579887E+00	8.7698906464E-03	4.4469441795E-01	6.5425617125E-02	
H4	C6	6.6345883797E+00	1.0040912980E-02	5.0677720038E-01	7.4907767348E-02	
H5	C6	6.7387045441E+00	9.1434967793E-03	4.5438890743E-01	6.8212814001E-02	
B1	H7	2.8911869461E+00	1.7538073327E-02	2.9765609002E-01	8.9083565944E-01	
C2	H7	6.5937205042E+00	6.1970904205E-03	4.6235712906E-02	3.1477740048E-01	
H3	H7	9.6994171657E-01	1.3903650731E-03	7.0501174059E-02	7.0622739664E-02	
H4	H7	9.7469850365E-01	9.4344212899E-04	4.7616682049E-02	4.7921563301E-02	
H5	H7	9.9003009619E-01	7.3187526275E-04	3.6370768103E-02	3.7175154315E-02	
C6	H7	6.1609218364E+00	8.7289043452E-01	6.5119848883E+00	4.4337933327E+01	(Bonded)
B1	H8	2.9543029841E+00	1.0336423525E-02	1.7542972673E-01	5.1447383927E-01	
C2	H8	6.7266390108E+00	1.1130456828E-02	8.3042939750E-02	5.5399518445E-01	
H3	H8	9.8932731446E-01	2.4595407831E-03	1.2471581472E-01	1.2241849287E-01	
H4	H8	9.9350486023E-01	3.3571735056E-03	1.6944066677E-01	1.6709628223E-01	
H5	H8	1.0101967661E+00	1.0499325149E-03	5.2176721863E-02	5.2258192654E-02	
C6	H8	6.2952209473E+00	8.7508508555E-01	6.5283575438E+00	4.3555527943E+01	(Bonded)
H7	H8	9.7134770733E-01	3.5008587962E-02	1.7782397166E+00	1.7424791673E+00	
B1	H9	2.9220507979E+00	1.2670673008E-02	2.1504659691E-01	6.3735068804E-01	
C2	H9	6.6577292164E+00	7.5254676074E-03	5.6146568175E-02	3.7854042595E-01	
H3	H9	9.7986264136E-01	5.8008309184E-04	2.9414245090E-02	2.9178904505E-02	
H4	H9	9.8416428575E-01	1.1323317951E-03	5.7150175307E-02	5.6957704479E-02	
H5	H9	9.9948866338E-01	1.2337317593E-03	6.1310682302E-02	6.2058249405E-02	
C6	H9	6.2252122114E+00	8.7366623114E-01	6.5177725286E+00	4.3946503330E+01	(Bonded)
H7	H9	9.6040897071E-01	3.6113076294E-02	1.8343415228E+00	1.8165328715E+00	
H8	H9	9.8134166171E-01	3.4409395755E-02	1.7126556298E+00	1.7308356112E+00	
B1	C10	1.9513235839E+01	4.6459815305E-01	7.8851574565E+00	3.4658973271E+00	(Bonded)
C2	C10	4.4855806201E+01	1.2266207790E-01	9.1516634957E-01	9.1505780882E-01	
H3	C10	6.6059788686E+00	5.9979109639E-03	3.0413577917E-01	4.4744352601E-02	

H4	C10	6.6363849667E+00	6.9197132734E-03	3.4924642083E-01	5.1620988119E-02
H5	C10	6.7380912507E+00	1.0849427140E-02	5.3916564562E-01	8.0936612161E-02
C6	C10	4.4858977975E+01	1.2378115108E-01	9.2343890299E-01	9.2340608299E-01
H7	C10	6.5935125814E+00	8.1779162457E-03	4.1539223127E-01	6.1007169037E-02
H8	C10	6.7285148019E+00	8.9759724077E-03	4.4676023334E-01	6.6960659598E-02
H9	C10	6.6572155074E+00	1.0133208332E-02	5.0971304352E-01	7.5593627398E-02
B1	H11	2.8911863797E+00	1.7247491346E-02	2.9272433414E-01	8.7611979193E-01
C2	H11	6.5922621077E+00	8.4502906923E-03	6.3046557000E-02	4.2924891363E-01
H3	H11	9.7000330157E-01	1.1695559527E-03	5.9304616743E-02	5.9409864158E-02
H4	H11	9.7462692297E-01	9.8850834531E-04	4.9891229292E-02	5.0213199614E-02
H5	H11	9.8971830739E-01	1.2558261257E-03	6.2408668691E-02	6.3792125004E-02
C6	H11	6.5939718292E+00	6.1268011037E-03	4.5707496180E-02	3.1122275121E-01
H7	H11	9.6826401801E-01	1.3067028013E-03	6.6373165967E-02	6.6376504467E-02
H8	H11	9.8834589681E-01	9.1273757687E-04	4.5429601864E-02	4.6364276397E-02
H9	H11	9.7809851265E-01	6.3556580423E-04	3.1969754280E-02	3.2284798350E-02
C10	H11	6.1607297991E+00	8.7307980938E-01	6.5131661799E+00	4.4349783141E+01
(Bonded)					
B1	H12	2.9183334596E+00	1.3022480030E-02	2.2101746387E-01	6.5584015920E-01
C2	H12	6.6486226311E+00	9.6265287254E-03	7.1822321160E-02	4.8481273286E-01
H3	H12	9.7841823866E-01	1.0981992535E-03	5.5686336069E-02	5.5307681148E-02
H4	H12	9.8333158358E-01	4.1597469084E-04	2.0994753134E-02	2.0949381903E-02
H5	H12	9.9647421142E-01	4.8436866102E-03	2.4070850790E-01	2.4393849638E-01
C6	H12	6.6503679730E+00	7.2412600576E-03	5.4021643728E-02	3.6468546223E-01
H7	H12	9.7692463841E-01	7.1513241192E-04	3.6324711493E-02	3.6015609455E-02
H8	H12	9.9683074354E-01	1.0160541923E-03	5.0571970078E-02	5.1170678833E-02
H9	H12	9.8631176411E-01	1.1027451257E-03	5.5469458029E-02	5.5536621070E-02
C10	H12	6.2172755598E+00	8.7389908282E-01	6.5192779511E+00	4.4011441161E+01
(Bonded)					
H11	H12	9.5912454491E-01	3.6217011836E-02	1.8397133958E+00	1.8239667678E+00
B1	H13	2.9552562098E+00	1.0198508295E-02	1.7308903016E-01	5.0745777285E-01
C2	H13	6.7297007916E+00	9.0299607972E-03	6.7371402812E-02	4.4931314095E-01
H3	H13	9.9056558628E-01	5.7493939016E-04	2.9153423660E-02	2.8607856562E-02
H4	H13	9.9478394617E-01	1.3937085547E-03	7.0342181127E-02	6.9348204534E-02

H5	H13	1.0105547827E+00	9.3789163849E-04	4.6608815772E-02	4.6667648667E-02
C6	H13	6.7292086633E+00	1.1133053398E-02	8.3055412936E-02	5.5395890446E-01
H7	H13	9.8836710888E-01	1.5607081772E-03	7.9275212977E-02	7.7657778250E-02
H8	H13	1.0089269541E+00	1.0411663227E-03	5.1821873795E-02	5.1806394427E-02
H9	H13	9.9661574999E-01	4.4579357253E-03	2.2423973849E-01	2.2181813940E-01
C10	H13	6.2974839441E+00	8.7506123092E-01	6.5279475637E+00	4.3541330801E+01
(Bonded)					
H11	H13	9.7157967579E-01	3.5036073217E-02	1.7797253270E+00	1.7433262953E+00
H12	H13	9.8046136695E-01	3.4350802257E-02	1.7299804315E+00	1.7092285562E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

B1	C2	7.0622365283E+01	5.3779322024E+01	4.1770391490E+01
B1	C6	7.0813154049E+01	5.3934917697E+01	4.1876322761E+01
B1	C10	7.0325002490E+01	5.3604408344E+01	4.1678309409E+01

B1	Total	2.1176052182E+02	1.6131864807E+02	1.2532502366E+02

C2	B1	7.0622365283E+01	5.3779322024E+01	4.1770391490E+01
C2	H3	4.4751547261E+01	3.4358182200E+01	2.7225557087E+01
C2	H4	4.5478803251E+01	3.4916764413E+01	2.7546888248E+01
C2	H5	4.6562278222E+01	3.5646068749E+01	2.7992690554E+01

C2	Total	2.0741499402E+02	1.5870033739E+02	1.2453552738E+02
H3	C2	4.4751547261E+01	3.4358182200E+01	2.7225557087E+01
H3	Total	4.4751547261E+01	3.4358182200E+01	2.7225557087E+01
H4	C2	4.5478803251E+01	3.4916764413E+01	2.7546888248E+01
H4	Total	4.5478803251E+01	3.4916764413E+01	2.7546888248E+01
H5	C2	4.6562278222E+01	3.5646068749E+01	2.7992690554E+01
H5	Total	4.6562278222E+01	3.5646068749E+01	2.7992690554E+01
C6	B1	7.0813154049E+01	5.3934917697E+01	4.1876322761E+01
C6	H7	4.4367639633E+01	3.4058470920E+01	2.7068735508E+01
C6	H8	4.6559030407E+01	3.5636959979E+01	2.7960856906E+01
C6	H9	4.5800326607E+01	3.5193968721E+01	2.7749171489E+01
C6	Total	2.0754015070E+02	1.5882431732E+02	1.2465508666E+02
H7	C6	4.4367639633E+01	3.4058470920E+01	2.7068735508E+01
H7	Total	4.4367639633E+01	3.4058470920E+01	2.7068735508E+01
H8	C6	4.6559030407E+01	3.5636959979E+01	2.7960856906E+01
H8	Total	4.6559030407E+01	3.5636959979E+01	2.7960856906E+01
H9	C6	4.5800326607E+01	3.5193968721E+01	2.7749171489E+01

H9	Total	4.5800326607E+01	3.5193968721E+01	2.7749171489E+01
C10	B1	7.0325002490E+01	5.3604408344E+01	4.1678309409E+01
C10	H11	4.4395625494E+01	3.4066364856E+01	2.7058615833E+01
C10	H12	4.5720190684E+01	3.5160545797E+01	2.7756367641E+01
C10	H13	4.6582482576E+01	3.5663493971E+01	2.8004076650E+01
C10	Total	2.0702330124E+02	1.5849481297E+02	1.2449736953E+02
H11	C10	4.4395625494E+01	3.4066364856E+01	2.7058615833E+01
H11	Total	4.4395625494E+01	3.4066364856E+01	2.7058615833E+01
H12	C10	4.5720190684E+01	3.5160545797E+01	2.7756367641E+01
H12	Total	4.5720190684E+01	3.5160545797E+01	2.7756367641E+01
H13	C10	4.6582482576E+01	3.5663493971E+01	2.8004076650E+01
H13	Total	4.6582482576E+01	3.5663493971E+01	2.8004076650E+01
Total	Total	1.2439568919E+03	9.5203893534E+02	7.4737596715E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

DelSqRho_IAS(A|B) = Integral of Laplacian of Electron Density $\text{DelSqRho}(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	N_IAS(A B)	G_IAS(A B)	K_IAS(A B)	L_IAS(A B)	DelSqRho_IAS(A B)	V_IAS(A B)
B1	C2	1.0215827535E+00	7.6565197848E-01	4.3868329490E-01	-3.2696868358E-01	1.3078747343E+00	-1.2043352734E+00
B1	C6	1.0236658737E+00	7.6868038161E-01	4.3935472110E-01	-3.2932566052E-01	1.3173026421E+00	-1.2080351027E+00
B1	C10	1.0207805769E+00	7.6510521629E-01	4.3957109983E-01	-3.2553411646E-01	1.3021364658E+00	-1.2046763161E+00
B1	Total	3.0660292041E+00	2.2994375764E+00	1.3176091158E+00	-9.8182846056E-01	3.9273138422E+00	-3.6170466922E+00
C2	B1	1.0215827535E+00	7.6565197848E-01	4.3868329490E-01	-3.2696868358E-01	1.3078747343E+00	-1.2043352734E+00
C2	H3	9.5813074759E-01	5.3391300981E-01	3.8111419205E-01	-1.5279881775E-01	6.1119527101E-01	-9.1502720186E-01
C2	H4	9.6358919441E-01	5.3710163613E-01	3.8578790866E-01	-1.5131372746E-01	6.0525490986E-01	-9.2288954479E-01
C2	H5	9.7358764925E-01	5.4358640137E-01	3.9374656657E-01	-1.4983983480E-01	5.9935933920E-01	-9.3733296794E-01
C2	Total	3.9168903447E+00	2.3802530258E+00	1.5993319622E+00	-7.8092106359E-01	3.1236842544E+00	-3.9795849880E+00
H3	C2	9.5813074759E-01	5.3391300981E-01	3.8111419205E-01	-1.5279881775E-01	6.1119527101E-01	-9.1502720186E-01
H3	Total	9.5813074759E-01	5.3391300981E-01	3.8111419205E-01	-1.5279881775E-01	6.1119527101E-01	-9.1502720186E-01
H4	C2	9.6358919441E-01	5.3710163613E-01	3.8578790866E-01	-1.5131372746E-01	6.0525490986E-01	-9.2288954479E-01

H4	Total	9.6358919441E-01	5.3710163613E-01	3.8578790866E-01	-1.5131372746E-01

6.0525490986E-01 -9.2288954479E-01

H5 C2 9.7358764925E-01 5.4358640137E-01 3.9374656657E-01 -1.4983983480E-01

5.9935933920E-01 -9.3733296794E-01

H5	Total	9.7358764925E-01	5.4358640137E-01	3.9374656657E-01	-1.4983983480E-01

5.9935933920E-01 -9.3733296794E-01

C6 B1 1.0236658737E+00 7.6868038161E-01 4.3935472110E-01 -3.2932566052E-01

1.3173026421E+00 -1.2080351027E+00

C6 H7 9.5556492374E-01 5.3213924118E-01 3.7913953119E-01 -1.5299970999E-01

6.1199883995E-01 -9.1127877237E-01

C6 H8 9.7256345673E-01 5.4267875594E-01 3.9282169521E-01 -1.4985706073E-01

5.9942824290E-01 -9.3550045115E-01

C6 H9 9.6668222523E-01 5.3908906350E-01 3.8816208523E-01 -1.5092697827E-01

6.0370791306E-01 -9.2725114873E-01

C6	Total	3.9184764794E+00	2.3825874422E+00	1.5994780327E+00	-7.8310940951E-01

3.1324376380E+00 -3.9820654749E+00

H7 C6 9.5556492374E-01 5.3213924118E-01 3.7913953119E-01 -1.5299970999E-01

6.1199883995E-01 -9.1127877237E-01

H7	Total	9.5556492374E-01	5.3213924118E-01	3.7913953119E-01	-1.5299970999E-01

6.1199883995E-01 -9.1127877237E-01

H8 C6 9.7256345673E-01 5.4267875594E-01 3.9282169521E-01 -1.4985706073E-01

5.9942824290E-01 -9.3550045115E-01

H8	Total	9.7256345673E-01	5.4267875594E-01	3.9282169521E-01	-1.4985706073E-01

5.9942824290E-01 -9.3550045115E-01

H9 C6 9.6668222523E-01 5.3908906350E-01 3.8816208523E-01 -1.5092697827E-01

6.0370791306E-01 -9.2725114873E-01

H9	Total	9.6668222523E-01	5.3908906350E-01	3.8816208523E-01	-1.5092697827E-01
6.0370791306E-01 -9.2725114873E-01					
C10	B1	1.0207805769E+00	7.6510521629E-01	4.3957109983E-01	-3.2553411646E-01
1.3021364658E+00 -1.2046763161E+00					
C10	H11	9.5565435594E-01	5.3197892399E-01	3.7955542920E-01	-1.5242349479E-01
6.0969397917E-01 -9.1153435319E-01					
C10	H12	9.6614245141E-01	5.3896704103E-01	3.8761515147E-01	-1.5135188956E-01
6.0540755825E-01 -9.2658219251E-01					
C10	H13	9.7311002590E-01	5.4326971974E-01	3.9309175823E-01	-1.5017796151E-01
6.0071184603E-01 -9.3636147797E-01					

C10	Total	3.9156874102E+00	2.3793209010E+00	1.5998334387E+00	-7.7948746232E-01
3.1179498493E+00 -3.9791543398E+00					
H11	C10	9.5565435594E-01	5.3197892399E-01	3.7955542920E-01	-1.5242349479E-01
6.0969397917E-01 -9.1153435319E-01					

H11	Total	9.5565435594E-01	5.3197892399E-01	3.7955542920E-01	-1.5242349479E-01
6.0969397917E-01 -9.1153435319E-01					
H12	C10	9.6614245141E-01	5.3896704103E-01	3.8761515147E-01	-1.5135188956E-01
6.0540755825E-01 -9.2658219251E-01					

H12	Total	9.6614245141E-01	5.3896704103E-01	3.8761515147E-01	-1.5135188956E-01
6.0540755825E-01 -9.2658219251E-01					
H13	C10	9.7311002590E-01	5.4326971974E-01	3.9309175823E-01	-1.5017796151E-01
6.0071184603E-01 -9.3636147797E-01					

H13	Total	9.7311002590E-01	5.4326971974E-01	3.9309175823E-01	-1.5017796151E-01
6.0071184603E-01 -9.3636147797E-01					

Total	Total	2.3502108469E+01	1.4284322738E+01	9.5972868673E+00	-4.6870358708E+00
1.8748143483E+01 -2.3881609605E+01					

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1 1.8134755175E+00

C2 2.7707109751E+01

H3 5.0102743042E+01

H4 4.9057814943E+01

H5 4.8161785009E+01

C6 2.7440214711E+01

H7 5.0793968401E+01

H8 4.7982243293E+01

H9 4.8216876875E+01

C10 2.8233467305E+01

H11 5.0573991630E+01

H12 4.8637631737E+01

H13 4.8152347611E+01

Total 5.2687366983E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

B1 2.5934143296E+00 6.2472630286E-02 3.2813229340E-02 3.1143648789E-03 2.4088950837E-02 6.7015242971E-03 6.4936136470E-05

C2 2.7972924862E+01 5.8166476350E-02 3.0372704611E-02 -1.0756889164E-02 2.0793848565E-03 8.7501546973E-03 1.1394009489E-04

H3 4.1912138649E+01 2.6426169822E-01 1.8713412310E-02 -8.5978172427E-03 6.3051351409E-03 5.6643214104E-03 4.3501188715E-05

H4 4.1371656322E+01 1.7074824143E-01 1.3081823127E-02 -9.1300217538E-03 4.1271792479E-03 4.8379328095E-03 3.2261606588E-05

H5 4.0838931528E+01 6.5671628983E-02 9.9472166608E-03 -9.6213366934E-03 1.6080643280E-03 4.0566671347E-03 2.3519885276E-05

C6 2.7752439506E+01 5.5201295769E-02 3.1080270727E-02 -1.0716210797E-02 1.9890610250E-03 8.6487453525E-03 1.1236380652E-04

H7 4.2314239756E+01 2.9581813238E-01 2.1702266293E-02 -8.5433851144E-03 6.9909830376E-03 5.9055579823E-03 4.7166794816E-05

H8 4.1028664160E+01 7.8927903375E-02 1.0218945406E-02 -9.5038134790E-03 1.9237258876E-03 3.9835968973E-03 2.3403376820E-05

H9 4.0828343865E+01 1.4047318999E-01 1.2135442695E-02 -9.1000166852E-03 3.4405801630E-03 4.4458116395E-03 2.7946602392E-05

C10 2.8214145418E+01 4.9470361571E-02 2.9822998800E-02 -1.0701995066E-02 1.7533886225E-03 8.4356226572E-03 1.0740928177E-04

H11 4.2307769074E+01 2.8141835055E-01 2.1348019251E-02 -8.6163463339E-03 6.6516943982E-03 5.9248491173E-03 4.7294187486E-05

H12 4.0973561252E+01 1.5020596796E-01 1.2455308117E-02 -9.0612046225E-03 3.6659241562E-03 4.6170728266E-03 2.9665862157E-05

H13 4.1106586971E+01 7.2672492666E-02 1.0039186430E-02 -9.6153842811E-03 1.7679038330E-03 3.9390463581E-03 2.2969184777E-05

Total	4.5921481569E+02	1.7455083695E+00	3.2813229340E-02	-1.0756889164E-02
	3.8010715462E-03	5.4002938527E-05		

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
B1	6.2472630286E-02	1.6733064265E-03	2.5934143296E+00	6.2472630286E-02	0.0000000000E+00
	NULL				
C2	2.3708523412E-01	3.3081882032E-03	1.3279655489E+01	1.4762585524E-01	1.4693269372E+01
	-8.9459378888E-02				
H3	3.2451205239E-01	3.4894335727E-03	3.3193568239E+01	2.9438687531E-01	8.7185704101E+00
	-3.0125177085E-02				
H4	2.4808026473E-01	2.0394246988E-03	3.0576220187E+01	2.0941425308E-01	1.0795436136E+01
	-3.8666011650E-02				
H5	1.7403869410E-01	1.0661311883E-03	2.5670343124E+01	1.1985516154E-01	1.5168588404E+01
	-5.4183532559E-02				
C6	2.3310666010E-01	3.2281684890E-03	1.3122173772E+01	1.4415397793E-01	1.4630265734E+01
	-8.8952682163E-02				

H7	3.4967915216E-01 8.1460575276E+00	4.0638866100E-03 -2.6930509891E-02	3.4168182228E+01	3.2274864227E-01
H8	1.8037551255E-01 1.3606684707E+01	1.1120449387E-03 -5.0723804587E-02	2.7421979453E+01	1.2965170796E-01
H9	2.2024459926E-01 1.1463053276E+01	1.6243227632E-03 -3.9885704634E-02	2.9365290588E+01	1.8035889462E-01
C10	2.3117766150E-01 1.5272831636E+01	3.1172018643E-03 -9.0853649966E-02	1.2941313782E+01	1.4032401154E-01
H11	3.4025843268E-01 8.8115062106E+00	3.8728204286E-03 -2.9420041067E-02	3.3496262863E+01	3.1083839162E-01
H12	2.3075544704E-01 1.1234586491E+01	1.7661597065E-03 -4.0274739542E-02	2.9738974761E+01	1.9048070750E-01
H13	1.7648357646E-01 1.3990672125E+01	1.0726627700E-03 -5.1905541896E-02	2.7115914846E+01	1.2457803456E-01

Total	3.0082699174E+00 1.4653152203E+02	3.1433751660E-02 -6.3138077393E-01	3.1268329366E+02	2.3768891435E+00

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A) ESP+*ESP+_Int_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)

B1	3.1143648789E-03 1.6733064265E-03	2.4088950837E-02	6.7015242971E-03	6.4936136470E-05
C2	8.0392840042E-05 2.5963423015E-03	1.1116693152E-02	7.3145976631E-03	7.1931908803E-05
H3	5.7592936799E-05 3.3385523135E-03	8.8687926887E-03	4.0682058043E-03	2.1922805674E-05
H4	1.3445943323E-05 1.8372505402E-03	6.8489254655E-03	3.1239253937E-03	1.3179782427E-05
H5	5.5047520575E-06 7.7278676211E-04	4.6690128356E-03	2.4773578559E-03	8.3045821953E-06
C6	1.2001666989E-05 2.5226429386E-03	1.0985525755E-02	7.1768817936E-03	7.1560986589E-05
H7	1.0208526851E-05 3.9332015336E-03	9.4458827255E-03	4.4111467380E-03	2.5888287032E-05

H8	1.8740917359E-05	4.7280214831E-03	2.4610788355E-03	8.1531087835E-06
8.3657044211E-04				
H9	3.7331862121E-06	6.1419073679E-03	2.7364756851E-03	1.0610773779E-05
1.4193360791E-03				
C10	6.0401002497E-05	1.0843104023E-02	7.0422799503E-03	6.8060653613E-05
2.4023421287E-03				
H11	1.0010826524E-05	9.2797931783E-03	4.3584170661E-03	2.5118421896E-05
3.7258892486E-03				
H12	5.0286339589E-05	6.4050865583E-03	2.8199926705E-03	1.1341318940E-05
1.5573246170E-03				
H13	2.4657260883E-06	4.5942773928E-03	2.4532937276E-03	8.0500476415E-06
7.9063045418E-04				

Total	2.4657260883E-06	7.6015866266E-03	2.9864234032E-05	2.7406175786E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

B1	NULL	NULL	NULL	NULL	NULL
C2	-2.9980421097E-05	-6.0884597308E-03	3.0198820276E-03	1.1377731638E-05	
7.1184590170E-04					
H3	-5.7322834785E-06	-3.4552886159E-03	1.9700563517E-03	5.3667144385E-06	
1.5088125914E-04					
H4	-1.6979241871E-05	-3.5816998187E-03	2.0602005598E-03	5.8991698754E-06	
2.0217415856E-04					
H5	-6.4753613636E-06	-3.5720879964E-03	2.1666401125E-03	6.5791276840E-06	
2.9334442615E-04					
C6	-2.7842274861E-05	-6.0800455563E-03	2.9962017764E-03	1.1256746361E-05	
7.0552555046E-04					
H7	-1.8279236654E-05	-3.3059562617E-03	1.9156118426E-03	5.1133923960E-06	
1.3068507642E-04					
H8	-9.2056836006E-06	-3.7278591869E-03	2.1311609264E-03	6.3485924421E-06	
2.7547449662E-04					
H9	-1.0926822074E-05	-3.4795009386E-03	2.0332670573E-03	5.7754540412E-06	
2.0498668408E-04					

C10	-4.2263454654E-06	-5.9487102414E-03	3.0310335032E-03	1.1418818837E-05
	7.1485973561E-04			
H11	-2.7725554117E-05	-3.3388208966E-03	2.0005926901E-03	5.5271971573E-06
	1.4693117997E-04			
H12	-3.8475485510E-05	-3.5848884669E-03	2.0233597397E-03	5.7371617851E-06
	2.0883508958E-04			
H13	-2.5831518272E-05	-3.7100106009E-03	2.1388563329E-03	6.3944179649E-06
	2.8203231586E-04			

Total	-4.2263454654E-06	-4.3088392530E-03	8.9199756730E-06	4.0275758742E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

B1	3.4071492950E+00
C2	2.8958320435E+01
H3	3.5652217234E+01
H4	3.5187790996E+01
H5	3.5610415377E+01
C6	2.8795457784E+01
H7	3.5641640081E+01
H8	3.5667500009E+01
H9	3.5412392767E+01
C10	2.8805613670E+01
H11	3.5691461316E+01
H12	3.5209039330E+01
H13	3.5328958476E+01

Total	4.0936795677E+02

Atomic Surface Area and Volume Data:

$$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$$

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an

Isosurface of the Electron Density Distribution (IsoDensity Surface)

N(Vol(A)) = Average Number of Electrons in Vol(A)

$\text{N(Vol(A))}/\text{Vol(A)}$ = Average Electron Density in Vol(A)

$$\%N(\text{Vol(A)}) = 100 * \text{N(Vol(A))} / \text{N(A)}$$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
B1	2.1357399734E+02	2.1295006694E+01	2.9457116910E+00	1.3832875159E-01	
	9.9989207244E+01				
C2	2.3512210377E+02	1.0900337980E+02	6.6958610584E+00	6.1428013251E-02	
	9.9913955921E+01				
H3	9.4854290303E+01	7.1270840276E+01	9.7466725900E-01	1.3675540449E-02	
	9.8844810438E+01				
H4	9.4536618194E+01	7.1132271096E+01	9.7952252852E-01	1.3770437994E-02	
	9.8875408205E+01				
H5	9.4724063231E+01	7.1596157039E+01	9.9518037028E-01	1.3899913228E-02	
	9.8911594100E+01				
C6	2.3498036541E+02	1.0900926870E+02	6.6964566582E+00	6.1430158538E-02	
	9.9914543309E+01				
H7	9.5161608034E+01	7.1459642745E+01	9.7282410816E-01	1.3613615613E-02	
	9.8828005776E+01				
H8	9.4541273700E+01	7.1542906055E+01	9.9358780497E-01	1.3887998961E-02	
	9.8907505370E+01				
H9	9.4017203482E+01	7.1073981742E+01	9.8297711530E-01	1.3830336942E-02	
	9.8889954843E+01				
C10	2.3525676854E+02	1.0932824612E+02	6.6966106484E+00	6.1252337672E-02	
	9.9913289776E+01				
H11	9.4969617124E+01	7.1443831499E+01	9.7279557761E-01	1.3616229102E-02	
	9.8830078139E+01				

H12	9.4357822421E+01	7.0949780261E+01	9.8175589521E-01	1.3837335247E-02
9.8886685334E+01				
H13	9.4734830187E+01	7.1496160558E+01	9.9392016048E-01	1.3901727767E-02
9.8911036110E+01				

Total	1.7708305617E+03	9.9060147259E+02	3.1881870876E+01	3.2184356432E-02
9.9630741699E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	1.6391206239E+02	2.0141154573E+01	2.9449382881E+00	1.4621496883E-01	
9.9962954864E+01					
C2	1.8667326224E+02	9.5384597220E+01	6.6869213479E+00	7.0104833933E-02	
9.9780559807E+01					
H3	7.6270320849E+01	5.1346943551E+01	9.6183931660E-01	1.8732163009E-02	
9.7543878737E+01					
H4	7.6288420735E+01	5.1399874807E+01	9.6676786197E-01	1.8808759080E-02	
9.7587920858E+01					
H5	7.6485000277E+01	5.1917540104E+01	9.8246572453E-01	1.8923580019E-02	
9.7647877575E+01					
C6	1.8657675683E+02	9.5303385058E+01	6.6874404689E+00	7.0170020350E-02	
9.9780017173E+01					
H7	7.6372710676E+01	5.1368756846E+01	9.5992611947E-01	1.8686964186E-02	
9.7517714954E+01					
H8	7.6665624139E+01	5.1960118217E+01	9.8091833984E-01	1.8878293074E-02	
9.7646313169E+01					
H9	7.6022312586E+01	5.1471572874E+01	9.7031441720E-01	1.8851462332E-02	
9.7616055763E+01					
C10	1.8670895839E+02	9.5451523039E+01	6.6874985891E+00	7.0061727421E-02	
9.9777338044E+01					
H11	7.6374133930E+01	5.1338326187E+01	9.5987241082E-01	1.8696994665E-02	
9.7517163470E+01					
H12	7.6134107049E+01	5.1417773469E+01	9.6914973474E-01	1.8848535620E-02	
9.7616938516E+01					
H13	7.6770080942E+01	5.1895077233E+01	9.8124563061E-01	1.8908260339E-02	
9.7649716609E+01					

Total	1.4112537510E+03	7.7039664318E+02	3.1739298250E+01	4.1198645569E-02
	9.9185202713E+01			

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

B1	1.2873217296E+02	1.8935636456E+01	2.9431716092E+00	1.5543029758E-01
	9.9902986733E+01			
C2	1.5349384782E+02	8.4565113820E+01	6.6712925313E+00	7.8889417042E-02
	9.9547350534E+01			
H3	6.2877774321E+01	3.8610319023E+01	9.4373737384E-01	2.4442620463E-02
	9.5708090078E+01			
H4	6.2734679244E+01	3.8712299337E+01	9.4865324473E-01	2.4505215680E-02
	9.5759386932E+01			
H5	6.3603105931E+01	3.9185810901E+01	9.6425381644E-01	2.4607218641E-02
	9.5837784737E+01			
C6	1.5345054444E+02	8.4516144371E+01	6.6718202263E+00	7.8941370029E-02
	9.9546955199E+01			
H7	6.2710375589E+01	3.8647375378E+01	9.4193938229E-01	2.4372661095E-02
	9.5690464425E+01			
H8	6.3628356915E+01	3.9141785952E+01	9.6258287788E-01	2.4592206372E-02
	9.5821094710E+01			
H9	6.3161564256E+01	3.8813593393E+01	9.5223236794E-01	2.4533476154E-02
	9.5796956410E+01			
C10	1.5330298320E+02	8.4645321917E+01	6.6718973602E+00	7.8821808567E-02
	9.9544568037E+01			
H11	6.2750077149E+01	3.8618973624E+01	9.4186155571E-01	2.4388570366E-02
	9.5687370799E+01			
H12	6.2965406971E+01	3.8767151229E+01	9.5109094101E-01	2.4533423552E-02
	9.5797978974E+01			
H13	6.3333035126E+01	3.9130457651E+01	9.6298514721E-01	2.4609606047E-02
	9.5832504920E+01			

Total	1.1567439239E+03	6.2228998305E+02	3.1527518434E+01	5.0663708709E-02
	9.8523391484E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
B1	C2	6.8446935065E-01		
B1	C6	6.8510779686E-01		
B1	C10	6.8439454997E-01		
B1		2.0539716975E+00	2.0539703512E+00	
C2	B1	-6.8447069692E-01		
C2	H3	-1.3944593303E-02		
C2	H4	-9.3392441632E-03		
C2	H5	6.1284686568E-03		
C2		-7.0162606573E-01	-7.0162741200E-01	
H3	C2	1.3943247032E-02		
H3		1.3943247032E-02	1.3941900760E-02	
H4	C2	9.3378978916E-03		
H4		9.3378978916E-03	9.3365516200E-03	
H5	C2	-6.1298149284E-03		
H5		-6.1298149284E-03	-6.1311612000E-03	
C6	B1	-6.8510914313E-01		
C6	H7	-1.5641933143E-02		
C6	H8	4.5599048568E-03		
C6	H9	-5.9916053132E-03		
C6		-7.0218277673E-01	-7.0218412300E-01	
H7	C6	1.5640586872E-02		
H7		1.5640586872E-02	1.5639240600E-02	
H8	C6	-4.5612511284E-03		

H8		-4.5612511284E-03 -4.5625974000E-03
H9	C6	5.9902590416E-03
H9		5.9902590416E-03 5.9889127700E-03
C10	B1	-6.8439589624E-01
C10	H11	-1.5691442433E-02
C10	H12	-7.1937093132E-03
C10	H13	4.8600604568E-03
C10		-7.0242098753E-01 -7.0242233380E-01
H11	C10	1.5690096162E-02
H11		1.5690096162E-02 1.5688749890E-02
H12	C10	7.1923630416E-03
H12		7.1923630416E-03 7.1910167700E-03
H13	C10	-4.8614067284E-03
H13		-4.8614067284E-03 -4.8627530000E-03

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

B1	-9.6528336746E-04	2.6618926159E-03	1.6966092484E-03
C2	-7.2312373379E-01	8.8123608032E-01	1.5811234653E-01
H3	7.4796928404E-02	-4.7832871423E-03	7.0013641262E-02
H4	1.2250817166E-01	-5.2289390813E-03	1.1727923258E-01
H5	-5.0401985144E-02	-1.8162396030E-03	-5.2218224747E-02
C6	-3.4416442362E-01	4.6955015644E-01	1.2538573282E-01
H7	-1.2259477731E-02	1.3073968256E-03	-1.0952080905E-02
H8	1.5526835302E-01	3.3278957976E-03	1.5859624882E-01

H9	-7.9502549576E-02	2.4911834789E-03	-7.7011366097E-02
C10	1.0535962105E+00	-1.3452889020E+00	-2.9169269151E-01
H11	-4.5713879488E-02	2.8138009652E-03	-4.2900078523E-02
H12	-5.4404994502E-02	1.3959486572E-03	-5.3009045845E-02
H13	-1.0563135521E-01	-2.1332103498E-03	-1.0776456556E-01

Total	-9.9980188445E-03	5.5337769206E-03	-4.4642419239E-03

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

B1	9.3283562405E-06	-1.7601782734E-03	-1.7508499171E-03
C2	-7.9536251740E-01	1.0448967903E+00	2.4953427294E-01
H3	1.2396355189E-02	-1.9925168503E-04	1.2197103504E-02
H4	-1.2672199859E-02	1.0638505878E-03	-1.1608349271E-02
H5	1.5280440440E-01	4.1990933884E-03	1.5700349779E-01
C6	1.0188313457E+00	-1.2844035106E+00	-2.6557216494E-01
H7	-6.3277591986E-02	4.2632177039E-03	-5.9014374282E-02
H8	-3.0902416967E-02	-3.6347292374E-04	-3.1265889891E-02
H9	-1.0670837885E-01	2.7289530215E-03	-1.0397942583E-01
C10	-2.1661929823E-01	2.3486759906E-01	1.8248300831E-02
H11	5.6246208004E-02	-4.3298369637E-03	5.1916371040E-02
H12	1.1286439069E-01	-3.9200675049E-03	1.0894432319E-01
H13	-1.2126748528E-01	-2.9375168962E-03	-1.2420500218E-01

Total	6.3421437672E-03	-5.8943307821E-03	4.4781298513E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

B1	4.5037017355E-03	-4.7439435091E-03	-2.4024177364E-04
C2	3.2370543993E-02	-1.3147390075E-03	3.1055804985E-02
H3	-1.4470653956E-01	9.4792588378E-03	-1.3522728072E-01
H4	1.0691616926E-01	-4.6521332419E-03	1.0226403602E-01

H5	2.4755563892E-02	7.4344731042E-04	2.5499011202E-02
C6	-3.5295606724E-02	-2.0847957035E-02	-5.6143563759E-02
H7	1.5021783698E-01	-1.1072472291E-02	1.3914536469E-01
H8	-3.8613860628E-02	-8.3252059447E-04	-3.9446381222E-02
H9	-9.3956716732E-02	2.6276438045E-03	-9.1329072927E-02
C10	4.1148473552E-02	2.5779151659E-03	4.3726388718E-02
H11	-1.4627991488E-01	1.0794609858E-02	-1.3548530502E-01
H12	1.0409067807E-01	-3.5115480045E-03	1.0057913007E-01
H13	2.5543793346E-02	5.7845965689E-04	2.6122253003E-02

Total	3.0694122304E-02	-2.0173979050E-02	1.0520143254E-02

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

B1	4.6059948241E-03	5.7174207358E-03	2.4498315215E-03
C2	1.0754335500E+00	1.3668899225E+00	2.9703759109E-01
H3	1.6336533510E-01	1.0619599109E-02	1.5276484134E-01
H4	1.6309477006E-01	7.0792602502E-03	1.5603558963E-01
H5	1.6279552836E-01	4.6350647766E-03	1.6741278591E-01
C6	1.0759703720E+00	1.3677003929E+00	2.9900210123E-01
H7	1.6346176002E-01	1.1936664287E-02	1.5153902785E-01
H8	1.6295475156E-01	3.4496512209E-03	1.6639213624E-01
H9	1.6289628026E-01	4.5340590735E-03	1.5837762173E-01
C10	1.0764209641E+00	1.3656396540E+00	2.9551586054E-01
H11	1.6325197760E-01	1.1966142486E-02	1.5130100527E-01
H12	1.6288997321E-01	5.4448665075E-03	1.5746423689E-01
H13	1.6283817601E-01	3.6761674998E-03	1.6650061939E-01

Total	3.2898515353E-02	2.1733735369E-02	1.1436931692E-02

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B) = \text{Contribution of Bond Between Atom A and Atom B to Mu\_Bond}(A)$

$\text{Mu\_Bond}(A) = \text{Sum of Mu\_Bond}(A|B) \text{ Over All B}$

$= \text{Total Bonding Dipole Moment Contribution of Atom A}$

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

B1	C2	4.3158090125E-01	
B1	C6	2.2910362700E-01	
B1	C10	-6.5802263563E-01	
B1		2.6618926159E-03	
C2	B1	9.0159856182E-01	
C2	H3	-8.1385882144E-03	
C2	H4	-9.0277940583E-03	
C2	H5	-3.1960992199E-03	
C2		8.8123608032E-01	
H3	C2	-4.7832871423E-03	
H3		-4.7832871423E-03	
H4	C2	-5.2289390813E-03	
H4		-5.2289390813E-03	
H5	C2	-1.8162396030E-03	
H5		-1.8162396030E-03	
C6	B1	4.5703288722E-01	
C6	H7	2.3773238671E-03	
C6	H8	5.7698621632E-03	
C6	H9	4.3700831921E-03	
C6		4.6955015644E-01	
H7	C6	1.3073968256E-03	
H7		1.3073968256E-03	
H8	C6	3.3278957976E-03	
H8		3.3278957976E-03	
H9	C6	2.4911834789E-03	
H9		2.4911834789E-03	

C10	B1	-1.3485448250E+00
C10	H11	4.5744355189E-03
C10	H12	2.3411512280E-03
C10	H13	-3.6596637315E-03
C10		-1.3452889020E+00
H11	C10	2.8138009652E-03
H11		2.8138009652E-03
H12	C10	1.3959486572E-03
H12		1.3959486572E-03
H13	C10	-2.1332103498E-03
H13		-2.1332103498E-03

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

B1	C2	5.1041316166E-01	
B1	C6	-6.2784549226E-01	
B1	C10	1.1567215232E-01	
B1		-1.7601782734E-03	
C2	B1	1.0358325518E+00	
C2	H3	-1.4245597721E-04	
C2	H4	1.9561203443E-03	
C2	H5	7.2505741707E-03	
C2		1.0448967903E+00	
H3	C2	-1.9925168503E-04	
H3		-1.9925168503E-04	
H4	C2	1.0638505878E-03	
H4		1.0638505878E-03	
H5	C2	4.1990933884E-03	
H5		4.1990933884E-03	
C6	B1	-1.2955908424E+00	
C6	H7	7.0868136257E-03	
C6	H8	-5.8761245523E-04	

C6	H9	4.6881305565E-03
C6		-1.2844035106E+00
H7	C6	4.2632177039E-03
H7		4.2632177039E-03
H8	C6	-3.6347292374E-04
H8		-3.6347292374E-04
H9	C6	2.7289530215E-03
H9		2.7289530215E-03
C10	B1	2.5426440769E-01
C10	H11	-7.4596628657E-03
C10	H12	-6.8218293641E-03
C10	H13	-5.1153164023E-03
C10		2.3486759906E-01
H11	C10	-4.3298369637E-03
H11		-4.3298369637E-03
H12	C10	-3.9200675049E-03
H12		-3.9200675049E-03
H13	C10	-2.9375168962E-03
H13		-2.9375168962E-03

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

B1	C2	6.0451161719E-03	
B1	C6	-1.9623126034E-02	
B1	C10	8.8340663531E-03	
B1		-4.7439435091E-03	
C2	B1	-1.0982338404E-02	
C2	H3	1.6471392028E-02	
C2	H4	-8.0912388350E-03	
C2	H5	1.2874462026E-03	
C2		-1.3147390075E-03	
H3	C2	9.4792588378E-03	

H3		9.4792588378E-03
H4	C2	-4.6521332419E-03
H4		-4.6521332419E-03
H5	C2	7.4344731042E-04
H5		7.4344731042E-04
C6	B1	-4.7487436369E-03
C6	H7	-1.9226837222E-02
C6	H8	-1.4393570517E-03
C6	H9	4.5669808755E-03
C6		-2.0847957035E-02
H7	C6	-1.1072472291E-02
H7		-1.1072472291E-02
H8	C6	-8.3252059447E-04
H8		-8.3252059447E-04
H9	C6	2.6276438045E-03
H9		2.6276438045E-03
C10	B1	-1.1061320140E-02
C10	H11	1.8749033228E-02
C10	H12	-6.1074554396E-03
C10	H13	9.9765751735E-04
C10		2.5779151659E-03
H11	C10	1.0794609858E-02
H11		1.0794609858E-02
H12	C10	-3.5115480045E-03
H12		-3.5115480045E-03
H13	C10	5.7845965689E-04
H13		5.7845965689E-04

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

B1	C2	6.6844611851E-01	
B1	C6	6.6862807384E-01	

B1	C10	6.6817054451E-01
B1		5.7174207358E-03
C2	B1	1.3732988217E+00
C2	H3	1.8372905790E-02
C2	H4	1.2279886736E-02
C2	H5	8.0276642775E-03
C2		1.3668899225E+00
H3	C2	1.0619599109E-02
H3		1.0619599109E-02
H4	C2	7.0792602502E-03
H4		7.0792602502E-03
H5	C2	4.6350647766E-03
H5		4.6350647766E-03
C6	B1	1.3738476049E+00
C6	H7	2.0628763067E-02
C6	H8	5.9756461159E-03
C6	H9	7.8697845928E-03
C6		1.3677003929E+00
H7	C6	1.1936664287E-02
H7		1.1936664287E-02
H8	C6	3.4496512209E-03
H8		3.4496512209E-03
H9	C6	4.5340590735E-03
H9		4.5340590735E-03
C10	B1	1.3723504971E+00
C10	H11	2.0690535937E-02
C10	H12	9.4508918570E-03
C10	H13	6.3682745737E-03
C10		1.3656396540E+00
H11	C10	1.1966142486E-02
H11		1.1966142486E-02
H12	C10	5.4448665075E-03

H12 5.4448665075E-03
H13 C10 3.6761674998E-03
H13 3.6761674998E-03

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
B1	1.7723699848E-01	-4.3331621193E-03	2.8836544442E-03	1.7160749445E-01	-1.4649538118E-02	-3.4884449293E-01
C2	-2.4792973506E-01	-2.3169953869E+00	1.0834451582E-01	-4.7285144046E-01	1.8399658901E-01	7.2078117552E-01
H3	-1.1082596124E-01	7.8127584217E-03	-2.5673492068E-01	-1.9182760645E-01	1.2317903322E-02	3.0265356769E-01
H4	1.0438916489E-01	-7.8563948729E-02	3.2588926283E-01	-1.6015758495E-01	-8.4844153978E-02	5.5768420061E-02
H5	-5.6263445738E-02	-2.4287404927E-01	-5.6774942362E-02	2.9722221297E-01	1.0287276321E-01	-2.4095876723E-01
C6	1.5373522179E+00	1.3517570701E+00	-9.3960309094E-02	-2.2500187260E+00	2.6602096942E-01	7.1266650812E-01
H7	-2.0626845601E-01	8.7084496498E-03	-8.0468945131E-02	-1.3878330030E-01	-1.9750536896E-01	3.4505175630E-01
H8	3.9371865373E-01	-2.7277566634E-02	-1.6884821073E-01	-1.7936792228E-01	1.1620907733E-02	-2.1435073145E-01
H9	1.6445850314E-02	1.8593660469E-01	2.3061439598E-01	-3.8632705588E-03	2.3041880269E-01	-1.2582579755E-02

C10 -2.4493885430E+00 9.9685240989E-01 -2.5824749547E-01 1.7365909065E+00
9.9775105300E-02 7.1279763650E-01

H11 -1.6729855946E-01 -3.9806044285E-02 1.1553892554E-01 -1.4662395671E-01 -2.1904009754E-
01 3.1392251618E-01

H12 -1.5667338526E-01 -7.9789826933E-02 -9.4639377952E-02 1.1351428706E-01 3.2485362532E-
01 4.3159098202E-02

H13 -7.5747871953E-03 2.7150205588E-01 -6.5496596963E-02 2.4795193345E-01 -9.1320938230E-
02 -2.4037714626E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)

B1	1	-3.4927099431E-01	-5.2436971920E-03	2.8069584028E-02	9.9959221790E-01
B1	2	1.6950586332E-01	4.9498118232E-01	8.6863029398E-01	-2.1795447383E-02
B1	3	1.7976513099E-01	8.6888787124E-01	-4.9466504913E-01	1.8448750123E-02
C2	1	-2.6927838944E+00	6.8801786651E-01	7.2314097032E-01	-6.0815724993E-02
C2	2	7.3154347303E-01	7.0438561382E-02	1.6861180195E-02	9.9737360586E-01
C2	3	1.9612404214E+00	-7.2226714202E-01	6.9049463260E-01	3.9336216401E-02
H3	1	-2.3709773959E-01	8.6866481644E-01	-2.6398059902E-01	4.1920839688E-01
H3	2	-1.8854035013E-01	2.4337218323E-01	9.6444653530E-01	1.0301874095E-01
H3	3	4.2563808973E-01	-4.3149903489E-01	1.2534907082E-02	9.0202630726E-01
H4	1	-2.4784913750E-01	-6.5788077549E-01	1.2856792071E-01	7.4206682651E-01
H4	2	-1.8157759676E-01	2.2852092287E-01	9.7294417569E-01	3.4026736434E-02
H4	3	4.2942673426E-01	7.1761485008E-01	-1.9196333178E-01	6.6946172870E-01
H5	1	-2.6136280964E-01	1.1917581257E-01	-1.2947485508E-01	9.8439493477E-01
H5	2	-1.7971348553E-01	8.8604144473E-01	4.6125799952E-01	-4.6600601935E-02
H5	3	4.4107629517E-01	-4.4802643216E-01	8.7776837479E-01	1.6969088455E-01

C6	1	-2.7062422458E+00 -3.0413882338E-01 9.4907425985E-01 -8.2204777238E-02
C6	2	7.3587126796E-01 -1.8664492648E-02 8.0339437717E-02 9.9659280123E-01
C6	3	1.9703709778E+00 9.5244486078E-01 3.0463687241E-01 -6.7203525125E-03
H7	1	-2.3161041514E-01 7.6311039655E-01 5.7128594658E-01 3.0215044253E-01
H7	2	-1.9364756452E-01 -6.3429881222E-01 7.5164231738E-01 1.8082821556E-01
H7	3	4.2525797965E-01 -1.2380444053E-01 -3.2964555809E-01 9.3595206423E-01
H8	1	-2.5834021364E-01 2.4805521897E-01 -5.6628889231E-02 9.6708933261E-01
H8	2	-1.8050845696E-01 6.0017877781E-02 9.9727062512E-01 4.3001797813E-02
H8	3	4.3884867061E-01 9.6688492733E-01 -4.7375828995E-02 -2.5077692904E-01
H9	1	-2.5236176575E-01 -3.6037020655E-01 -4.7484499796E-01 8.0290444148E-01
H9	2	-1.7927820719E-01 -7.3090396872E-01 6.7853906614E-01 7.3240181846E-02
H9	3	4.3163997294E-01 5.7957976391E-01 5.6045246332E-01 5.9159135695E-01
C10	1	-2.6966611848E+00 9.7211863684E-01 -2.2039103330E-01 8.0082135062E-02
C10	2	7.3347959476E-01 -8.5314533934E-02 -1.4310554294E-02 9.9625129276E-01
C10	3	1.9631815900E+00 2.1841883210E-01 9.7530661870E-01 3.2714114822E-02
H11	1	-2.3495297775E-01 -1.3244405371E-01 9.1068032192E-01 3.9130541002E-01
H11	2	-1.9159878014E-01 -9.7052415169E-01 -1.9934475549E-01 1.3544201503E-01
H11	3	4.2655175789E-01 2.0134905913E-01 -3.6183286159E-01 9.1023927440E-01
H12	1	-2.5244241644E-01 2.2855596710E-01 -6.1794376036E-01 7.5226835566E-01
H12	2	-1.7825358778E-01 9.5181909351E-01 3.0412302398E-01 -3.9364952873E-02
H12	3	4.3069600422E-01 -2.0445680016E-01 7.2502047924E-01 6.5767980169E-01
H13	1	-2.5940932215E-01 1.5350432009E-01 9.4892567962E-02 9.8358112236E-01
H13	2	-1.7937808284E-01 8.3394322985E-01 -5.4639016099E-01 -7.7436950824E-02
H13	3	4.3878740498E-01 5.3007085668E-01 8.3213772449E-01 -1.6300826478E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho}*r \rangle (A)$$

$$R+2(A) = \langle \text{Rho}*r*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
B1	9.2149610705E+01 1.8340060440E+00		1.0431254822E+01	2.9460296488E+00	1.7579306417E+00
C2	1.3776007933E+02 1.2919956347E+01		1.5315774887E+01	6.7016274120E+00	7.6491590816E+00
H3	2.8110428585E+00 1.7096436616E+00		1.2415990707E+00	9.8605809924E-01	1.1230213941E+00
H4	2.8346531169E+00 1.7109775343E+00		1.2496175933E+00	9.9066344838E-01	1.1263771488E+00
H5	2.8813367682E+00 1.7351082424E+00		1.2694757172E+00	1.0061311612E+00	1.1435960422E+00
C6	1.3776140107E+02 1.2922789037E+01		1.5316179722E+01	6.7021841230E+00	7.6502359387E+00
H7	2.8012308188E+00 1.7109700639E+00		1.2383448259E+00	9.8436075940E-01	1.1222213516E+00
H8	2.8763555304E+00 1.7331018851E+00		1.2673727228E+00	1.0045625974E+00	1.1420025572E+00
H9	2.8476402718E+00 1.7137720380E+00		1.2545780761E+00	9.9401108723E-01	1.1294230034E+00
C10	1.3776103630E+02 1.2927306651E+01		1.5316216328E+01	6.7024223338E+00	7.6512984266E+00
H11	2.8027054528E+00 1.7099268180E+00		1.2386275774E+00	9.8431125011E-01	1.1218850495E+00
H12	2.8444428159E+00 1.7113618058E+00		1.2531659445E+00	9.9280898323E-01	1.1279019148E+00
H13	2.8779630953E+00 1.7324965872E+00		1.2679600105E+00	1.0048627530E+00	1.1420347104E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(dRho/dx) + y^*(dRho/dy) + z^*(dRho/dz)$$

$$GR-2(A) = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$GR-1(A) = \langle \text{Dot}/r \rangle (A)$$

$$GR0(A) = \langle \text{Dot} \rangle (A)$$

$$GR+1(A) = \langle \text{Dot}*r \rangle (A)$$

$$GR+2(A) = \langle \text{Dot} * r * r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
B1	-9.0843228241E+01	-1.9242849879E+01	-6.7051222693E+00	-3.9805247684E+00	-4.3040792677E+00
C2	-1.3630507964E+02	-2.7961877721E+01	-1.4860238233E+01	-1.9485363965E+01	-3.9114486314E+01
H3	-2.1541402590E+00	-1.7684560472E+00	-2.0946574625E+00	-3.2879577307E+00	-6.5343426047E+00
H4	-2.1737883902E+00	-1.7817638730E+00	-2.1046776436E+00	-3.2906011397E+00	-6.5074333912E+00
H5	-2.2153572155E+00	-1.8161570972E+00	-2.1422419945E+00	-3.3383199062E+00	-6.5701862813E+00
C6	-1.3630607958E+02	-2.7961658121E+01	-1.4859222605E+01	-1.9483038888E+01	-3.9111695513E+01
H7	-2.1462585600E+00	-1.7634901146E+00	-2.0919523507E+00	-3.2912031268E+00	-6.5601486236E+00
H8	-2.2109527056E+00	-1.8124275700E+00	-2.1377713498E+00	-3.3310622361E+00	-6.5541812410E+00
H9	-2.1848822406E+00	-1.7900385994E+00	-2.1122525504E+00	-3.2969658694E+00	-6.5061880779E+00
C10	-1.3630670870E+02	-2.7964479858E+01	-1.4867576127E+01	-1.9509063032E+01	-3.9198925204E+01
H11	-2.1475515420E+00	-1.7642578117E+00	-2.0923958844E+00	-3.2908850459E+00	-6.5565845079E+00
H12	-2.1818894788E+00	-1.7874709206E+00	-2.1094020119E+00	-3.2937864082E+00	-6.5054193333E+00
H13	-2.2122071225E+00	-1.8132021854E+00	-2.1381343484E+00	-3.3305393323E+00	-6.5512447320E+00

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)

B1	1.4730148244E+00	1.4730148244E+00	2.9460296488E+00	0.0000000000E+00
C2	3.3508137060E+00	3.3508137060E+00	6.7016274120E+00	0.0000000000E+00
H3	4.9302904962E-01	4.9302904962E-01	9.8605809924E-01	0.0000000000E+00
H4	4.9533172419E-01	4.9533172419E-01	9.9066344838E-01	0.0000000000E+00
H5	5.0306558061E-01	5.0306558061E-01	1.0061311612E+00	0.0000000000E+00
C6	3.3510920615E+00	3.3510920615E+00	6.7021841230E+00	0.0000000000E+00
H7	4.9218037970E-01	4.9218037970E-01	9.8436075940E-01	0.0000000000E+00
H8	5.0228129868E-01	5.0228129868E-01	1.0045625974E+00	0.0000000000E+00
H9	4.9700554362E-01	4.9700554362E-01	9.9401108723E-01	0.0000000000E+00
C10	3.3512111669E+00	3.3512111669E+00	6.7024223338E+00	0.0000000000E+00
H11	4.9215562506E-01	4.9215562506E-01	9.8431125011E-01	0.0000000000E+00
H12	4.9640449161E-01	4.9640449161E-01	9.9280898323E-01	0.0000000000E+00
H13	5.0243137651E-01	5.0243137651E-01	1.0048627530E+00	0.0000000000E+00

Total	1.6000016828E+01	1.6000016828E+01	3.2000033657E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's

underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

Boradamantan

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\boradamantan\boradamantan.wfx

Sum File: D:\calc\ellipticity\boradamantan\boradamantan.sum

Wfx Title: boradamantan.wfn

Total memory allocated for AIMSum = 1.305 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted SCF

Restricted, closed-shell, single-determinant wavefunction.

Number of electrons (from MO Occs)	=	74.0000000000
Number of Alpha electrons (from MO Occs)	=	37.0000000000
Number of Beta electrons (from MO Occs)	=	37.0000000000
Number of electron pairs ($N*(N-1)/2$)	=	2701.0000000000
Number of electron pairs (from Muller 2EDM)	=	2701.0000000000

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	2.3863666000E+00	-2.3805795800E+00	8.5418019000E-02
H2	1.0	4.0735775500E+00	-2.4225137300E+00	-1.1182962700E+00
H3	1.0	2.4299429800E+00	-4.1022210400E+00	1.2355559600E+00
C4	6.0	1.2850182100E-04	-2.3681421100E+00	-1.5696768200E+00
H5	1.0	2.1423555200E-04	-4.0564001500E+00	-2.7649665100E+00
C6	6.0	2.4727728700E+00	1.8794325900E-06	1.7942226300E+00
H7	1.0	4.2166784200E+00	1.3299826800E-05	2.8996626700E+00
C8	6.0	2.3860964700E+00	2.3808340000E+00	8.5781476300E-02
H9	1.0	4.0733114800E+00	2.4231431800E+00	-1.1179149500E+00
H10	1.0	2.4294695500E+00	4.1023059300E+00	1.2361815800E+00
C11	6.0	4.1276866000E-06	2.3919153100E-04	-3.2422099100E+00
H12	1.0	-1.6676536500E+00	2.4307424100E-04	-4.4693197600E+00
H13	1.0	1.6676651500E+00	4.1274240800E-04	-4.4693149100E+00
C14	6.0	-1.2623873200E-04	2.3683785500E+00	-1.5693319200E+00
H15	1.0	-2.0770417300E-04	4.0568083100E+00	-2.7643794600E+00
C16	6.0	-2.3863623600E+00	2.3805783700E+00	8.5761127300E-02

H17	1.0	-2.4299344700E+00	4.1020530500E+00	1.2361498500E+00
H18	1.0	-4.0735748300E+00	2.4226933800E+00	-1.1179455600E+00
C19	6.0	-2.3860983500E+00	-2.3808352700E+00	8.5427138400E-02
H20	1.0	-2.4294806000E+00	-4.1024745800E+00	1.2355764500E+00
H21	1.0	-4.0733102300E+00	-2.4229668400E+00	-1.1182799900E+00
C22	6.0	-2.4727780300E+00	-2.4700880700E-04	1.7942178600E+00
H23	1.0	-4.2166889000E+00	-4.2449208900E-04	2.8996489000E+00
B24	5.0	-4.9346735800E-06	-2.9355498900E-04	3.4405813100E+00
H25	1.0	-5.9339885000E-06	-5.7255687500E-04	5.6970779300E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

C1	2.5564792700E-02	5.0918519085E-05	3.7861425935E+01	-3.8040594290E+01	3.8663376458E-02
H2	-1.7022894400E-02	7.7658109799E-05	6.2605251616E-01	-6.2901513040E-01	1.5703854871E-01
H3	-2.2681773100E-02	7.1275467352E-05	6.2930234617E-01	-6.3228033930E-01	1.5333633076E-01
C4	5.1064595500E-02	-3.3415426897E-04	3.7863841906E+01	-3.8043021694E+01	4.7127146553E-02
H5	-1.9927519500E-02	5.8645329711E-05	6.3354705014E-01	-6.3654513011E-01	1.5114049433E-01
C6		-6.1392244710E-01	-2.0965556803E-04	3.8173850679E+01	-3.8354497494E+01
		1.0889669161E+00			
H7	-2.2227675700E-02	5.7079910318E-05	6.3170901110E-01	-6.3469839307E-01	1.5256211806E-01

C8	2.5369631800E-02	-1.8311680270E-04	3.7861383434E+01	-3.8040551588E+01	3.8339087867E-02
H9	-1.7028959300E-02	7.4054701853E-05	6.2605287206E-01	-6.2901548798E-01	1.5703842991E-01
H10	-2.2683078800E-02	7.0031344273E-05	6.2930204899E-01	-6.3228004070E-01	1.5333786040E-01
C11	2.8476679600E-02	-1.5977566033E-06	3.7883067735E+01	-3.8062338504E+01	5.1627995461E-02
H12	-2.1250812600E-02	7.6142461337E-05	6.2812140430E-01	-6.3109380896E-01	1.5473773578E-01
H13	-2.1255638600E-02	7.2244093837E-05	6.2812078699E-01	-6.3109318872E-01	1.5474109085E-01
C14	5.0827934500E-02	-5.6153030517E-04	3.7863788902E+01	-3.8042968439E+01	4.7899662336E-02
H15	-1.9926191900E-02	6.0412355933E-05	6.3354763508E-01	-6.3654571782E-01	1.5114010023E-01
C16	2.5512772800E-02	-5.0723738142E-05	3.7861409723E+01	-3.8040578001E+01	3.8359043506E-02
H17	-2.2678730500E-02	7.2986183765E-05	6.2930191982E-01	-6.3227991093E-01	1.5333799074E-01
H18	-1.7027829600E-02	7.6399452483E-05	6.2605386830E-01	-6.2901648893E-01	1.5703728218E-01
C19	2.5615599400E-02	6.2414306492E-05	3.7861430982E+01	-3.8040599360E+01	3.8387626699E-02
H20	-2.2679838300E-02	7.1498243742E-05	6.2930127698E-01	-6.3227926505E-01	1.5333819026E-01
H21	-1.7023770100E-02	7.6833040945E-05	6.2605219759E-01	-6.2901481032E-01	1.5703986982E-01
C22	-6.1368250110E-01	-1.2004944726E-05	3.8173891561E+01	-3.8354538570E+01	1.0903984846E+00
H23	-2.2225318000E-02	6.0465185446E-05	6.3171031696E-01	-6.3469970512E-01	1.5256100688E-01
B24	1.9173071836E+00	7.3721777621E-05	2.3952751917E+01	-2.4066101456E+01	7.6301122059E-02
H25	-6.3629166740E-01	2.0119563427E-05	8.2932808263E-01	-8.3325264027E-01	3.0116667778E-01

Total	2.0254390000E-04	-1.6988333692E-04	3.7499434611E+02	-3.7676889945E+02	

Molecular charge q(Mol) from the wfx file: 0.0000000000E+00

Molecular energy E(Mol) from the wfx file: -3.7676893236E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0047322136E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0047304290E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	57	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C4	59	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H5	14	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C6	59	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H7	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C8	56	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H9	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H10	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C11	71	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00

H12	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H13	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C14	68	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H15	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C16	65	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H17	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H18	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C19	65	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H20	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H21	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C22	69	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H23	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
B24	56	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H25	31	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 883

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = $(-1/4)\text{DelSqRho}$

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 2.38636635022506E+00 -2.38057904937607E+00 8.54186387572412E-02

Type = (3,-3) NACP C1

Rho = 1.1963090346E+02 Rho at Nucleus = 1.1963090339E+02

GradRho = -1.0850931265E-10 2.1316637344E-10 2.0587920257E-10

HessRho_EigVals = -1.8159002181E+05 -1.8158966554E+05 -1.8158934462E+05

HessRho_EigVec1 = 1.3043882008E-01 6.3860010336E-01 7.5840333742E-01

HessRho_EigVec2 = -8.5139305435E-01 4.6412367603E-01 -2.4437487668E-01

HessRho_EigVec3 = 5.0805076638E-01 6.1382336330E-01 -6.0423943718E-01

DelSqRho = -5.4476903197E+05

Bond Ellipticity = NA

V = -1.3620759353E+05

G = 7.6677682761E+00

K = 1.3619992576E+05

L = 1.3619225799E+05

Vnuc = 7.0318902669E+06

Ven = -8.4123138564E+08

Vrep = 8.4109517804E+08

DelSqV = 4.6163328120E+09

DelSqVen = 3.8307565404E+12

DelSqVrep = -3.8261402076E+12

DelSqG = 2.0675375086E+08

DelSqK = -4.8230865629E+09

Stress_EigVals = -4.5402616194E+04 -4.5402541106E+04 -4.5402436229E+04

Stress_EigVec1 = 5.0337683364E-01 6.1796043550E-01 -6.0393432053E-01

Stress_EigVec2 = -8.5160859571E-01 4.7307418984E-01 -2.2575121399E-01

Stress_EigVec3 = 1.4620042089E-01 6.2795358990E-01 7.6439500644E-01

-DivStress = 3.7466325253E+02 -7.9671768913E+02 -9.3070350496E+02

CP# 2 Coords = 4.05252987718178E+00 -2.42192611408659E+00 -1.10344885829996E+00

Type = (3,-3) NACP H2

Rho = 4.4219859876E-01 Rho at Nucleus = 4.3934274804E-01

GradRho = -1.4860264234E-10 4.1805968409E-12 1.0488385854E-10

HessRho_EigVals = -9.0161901979E+00 -9.0150643089E+00 -8.3932499359E+00

HessRho_EigVec1 = 4.6742168895E-01 6.1580610414E-01 6.3427108306E-01

HessRho_EigVec2 = 3.4028295827E-01 -7.8752163104E-01 5.1382602986E-01

HessRho_EigVec3 = 8.1591940350E-01 -2.4341790211E-02 -5.7765301370E-01

DelSqRho = -2.6424504443E+01

Bond Ellipticity = NA

V = -6.6196318554E+00

G = 6.7528723543E-03

K = 6.6128789830E+00

L = 6.6061261107E+00
Vnuc = 5.3411870303E+01
Ven = -2.3618654205E+01
Vrep = 1.6999022350E+01
DelSqV = 1.7183001796E+03
DelSqVen = 1.4113822047E+03
DelSqVrep = 3.0691797489E+02
DelSqG = 1.3202500011E+02
DelSqK = -1.8503251797E+03
Stress_EigVals = -2.2593987771E+00 -2.2590354026E+00 -2.1011976758E+00
Stress_EigVec1 = 4.3437721848E-01 6.8449020784E-01 5.8548235450E-01
Stress_EigVec2 = 3.8091642660E-01 -7.2861900238E-01 5.6922493386E-01
Stress_EigVec3 = 8.1622246233E-01 -2.4238497150E-02 -5.7722905960E-01
-DivStress = 1.1707152067E+01 -3.2996310521E-01 -8.2564424644E+00

CP# 3 Coords = 2.42914540913215E+00 -4.08066382789341E+00 1.22138198572926E+00

Type = (3,-3) NACP H3

Rho = 4.4368278525E-01 Rho at Nucleus = 4.4080879911E-01

GradRho = -2.4107914233E-11 6.5756710233E-10 -4.3258776465E-10

HessRho_EigVals = -9.0399557248E+00 -9.0388458956E+00 -8.4146542685E+00

HessRho_EigVec1 = -5.1905740556E-01 -4.8329749352E-01 -7.0498435620E-01

HessRho_EigVec2 = 8.5424345740E-01 -2.6522931336E-01 -4.4712585122E-01

HessRho_EigVec3 = -2.9112286462E-02 8.3431225814E-01 -5.5052296109E-01

DelSqRho = -2.6493455889E+01

Bond Ellipticity = NA

V = -6.6369170863E+00

G = 6.7765570423E-03

K = 6.6301405293E+00

L = 6.6233639722E+00

Vnuc = 5.3217712187E+01

Ven = -2.3611782768E+01

Vrep = 1.6974865682E+01

DelSqV = 1.7224848297E+03

DelSqVen = 1.4099211127E+03

DelSqVrep = 3.1256371696E+02

DelSqG = 1.3227097701E+02

DelSqK = -1.8547558067E+03

Stress_EigVals = -2.2653851481E+00 -2.2651268724E+00 -2.1064050658E+00

Stress_EigVec1 = 4.5454732130E-01 5.0103346350E-01 7.3644565390E-01

Stress_EigVec2 = 8.9024262881E-01 -2.2840756820E-01 -3.9407872898E-01

Stress_EigVec3 = -2.9236869550E-02 8.3474274555E-01 -5.4986339596E-01

-DivStress = 4.4711730565E-01 -1.2020709520E+01 7.9023081620E+00

CP# 4 Coords = 1.28501801426933E-04 -2.36814157138588E+00 -1.56967637304119E+00

Type = (3,-3) NACP C4

Rho = 1.1960176815E+02 Rho at Nucleus = 1.1960176811E+02

GradRho = -3.5084274082E-15 1.0802136963E-10 1.1078532536E-10

HessRho_EigVals = -1.8154795456E+05 -1.8154788299E+05 -1.8154748697E+05

HessRho_EigVec1 = 9.9999999864E-01 5.2176887464E-05 -1.2959706165E-06

HessRho_EigVec2 = 3.0345460569E-05 -5.6102732447E-01 8.2779728211E-01

HessRho_EigVec3 = -4.2464810704E-05 8.2779728102E-01 5.6102732529E-01

DelSqRho = -5.4464332452E+05

Bond Ellipticity = NA

V = -1.3617610839E+05

G = 7.6386292648E+00

K = 1.3616846976E+05

L = 1.3616083113E+05

Vnuc = 8.5725177123E+06

Ven = -1.0252882759E+09

Vrep = 1.0251520998E+09

DelSqV = 4.6152755197E+09

DelSqVen = 4.6689630945E+12

DelSqVrep = -4.6643478190E+12

DelSqG = 2.0670860061E+08

DelSqK = -4.8219841204E+09

Stress_EigVals = -4.5392115365E+04 -4.5392004443E+04 -4.5391988582E+04

Stress_EigVec1 = -4.2598597443E-05 8.3243563581E-01 5.5412174694E-01

Stress_EigVec2 = 4.6354113234E-06 -5.5412174727E-01 8.3243563666E-01

Stress_EigVec3 = 9.9999999908E-01 3.8029172804E-05 1.9746127674E-05

-DivStress = 2.9336142461E-02 -8.0752745444E+02 -6.7024377024E+02

CP# 5 Coords = 2.13162989735783E-04 -4.03532003842826E+00 -2.75000569092603E+00

Type = (3,-3) NACP H5

Rho = 4.4642873940E-01 Rho at Nucleus = 4.4352707465E-01

GradRho = -8.7349268952E-15 1.7169186732E-10 1.2182824541E-10

HessRho_EigVals = -9.1016660452E+00 -9.1015274449E+00 -8.4702697751E+00

HessRho_EigVec1 = -6.8369433344E-06 -5.7833823308E-01 8.1579708759E-01

HessRho_EigVec2 = 9.9999999912E-01 2.9880928215E-05 2.9564001787E-05

HessRho_EigVec3 = -4.1474766768E-05 8.1579708707E-01 5.7833823236E-01

DelSqRho = -2.6673463265E+01

Bond Ellipticity = NA

V = -6.6818370122E+00

G = 6.7355979267E-03

K = 6.6751014142E+00

L = 6.6683658163E+00

Vnuc = 5.3330251496E+01

Ven = -2.3808156947E+01

Vrep = 1.7126319935E+01

DelSqV = 1.7340995555E+03

DelSqVen = 1.4225025048E+03

DelSqVrep = 3.1159705065E+02

DelSqG = 1.3324794735E+02

DelSqK = -1.8673475028E+03

Stress_EigVals = -2.2807562682E+00 -2.2806964518E+00 -2.1203842922E+00

Stress_EigVec1 = 4.4947775084E-05 -5.7837788153E-01 8.1576897718E-01

Stress_EigVec2 = 9.9999999813E-01 5.9805750029E-05 -1.2696550475E-05

Stress_EigVec3 = -4.1444271564E-05 8.1576897623E-01 5.7837788314E-01

-DivStress = 6.0199978614E-04 -1.1833106483E+01 -8.3979313694E+00

CP# 6 Coords = 2.47277447094297E+00 1.87970960075252E-06 1.79421982294395E+00

Type = (3,-3) NACP C6

Rho = 1.1960058523E+02 Rho at Nucleus = 1.1960058428E+02

GradRho = -5.1847415250E-14 7.1394713058E-17 -6.4638294717E-12

HessRho_EigVals = -1.8154508692E+05 -1.8154437025E+05 -1.8154296775E+05

HessRho_EigVec1 = -5.0232086634E-05 9.9999999394E-01 9.8009094113E-05

HessRho_EigVec2 = 4.9691411254E-01 -6.0091232444E-05 8.6779972410E-01

HessRho_EigVec3 = 8.6779972473E-01 9.2293492944E-05 -4.9691410651E-01

DelSqRho = -5.4463242493E+05

Bond Ellipticity = NA

V = -1.3617359958E+05

G = 7.7466764076E+00

K = 1.3616585291E+05

L = 1.3615810623E+05

Vnuc = 1.8567394426E+06

Ven = -2.2206712395E+08

Vrep = 2.2193095035E+08

DelSqV = 4.6151839845E+09

DelSqVen = 1.0112404890E+12

DelSqVrep = -1.0066253050E+12

DelSqG = 2.0670262292E+08

DelSqK = -4.8218866074E+09

Stress_EigVals = -4.5391492753E+04 -4.5391147858E+04 -4.5390958974E+04

Stress_EigVec1 = 8.9234625861E-01 9.1922915149E-05 -4.5135146647E-01

Stress_EigVec2 = 4.5135147281E-01 -6.6020481264E-05 8.9234625770E-01

Stress_EigVec3 = -5.2228628295E-05 9.9999999360E-01 1.0040267259E-04

-DivStress = -2.4045901882E+03 -4.1592816683E-01 4.2138268219E+03

CP# 7 Coords = 4.19500612452539E+00 1.31783941290453E-05 2.88563721207009E+00

Type = (3,-3) NACP H7

Rho = 4.4451006923E-01 Rho at Nucleus = 4.4162858920E-01

GradRho = -8.5624056803E-10 -4.8343600783E-15 -5.5380848518E-10

HessRho_EigVals = -9.0605885063E+00 -9.0576760799E+00 -8.4346112730E+00

HessRho_EigVec1 = -2.9077779811E-05 9.9999999893E-01 3.5866582677E-05

HessRho_EigVec2 = -5.4175162009E-01 -4.5900182455E-05 8.4053862494E-01

HessRho_EigVec3 = 8.4053862569E-01 5.0102177869E-06 5.4175162085E-01

DelSqRho = -2.6552875859E+01

Bond Ellipticity = NA

V = -6.6526998519E+00

G = 7.2404435508E-03

K = 6.6454594083E+00

L = 6.6382189648E+00

Vnuc = 5.3014998697E+01

Ven = -2.3565700741E+01

Vrep = 1.6913000889E+01

DelSqV = 1.7265440027E+03

DelSqVen = 1.4077006821E+03

DelSqVrep = 3.1884332057E+02

DelSqG = 1.3263386814E+02

DelSqK = -1.8591778708E+03

Stress_EigVals = -2.2709633696E+00 -2.2703326977E+00 -2.1114037846E+00

Stress_EigVec1 = -5.4275201709E-01 -1.2786951556E-04 8.3989298818E-01

Stress_EigVec2 = -7.3530338843E-05 9.9999999181E-01 1.0472854998E-04

Stress_EigVec3 = 8.3989299470E-01 4.9159842656E-06 5.4275202205E-01

-DivStress = 1.2112263593E+01 6.7877535375E-05 7.8389441789E+00

CP# 8 Coords = 2.38609622031306E+00 2.38083346929264E+00 8.57820959240760E-02

Type = (3,-3) NACP C8

Rho = 1.1963090310E+02 Rho at Nucleus = 1.1963090303E+02

GradRho = -6.4249494613E-11 -1.9503787474E-10 2.0632201503E-10

HessRho_EigVals = -1.8159002124E+05 -1.8158966499E+05 -1.8158934408E+05

HessRho_EigVec1 = 1.3051388338E-01 -6.3870454178E-01 7.5830246904E-01
HessRho_EigVec2 = 8.5132596975E-01 4.6420027126E-01 2.4446308799E-01
HessRho_EigVec3 = 5.0814389643E-01 -6.1365675786E-01 -6.0433034348E-01
DelSqRho = -5.4476903032E+05
Bond Ellipticity = NA
V = -1.3620759312E+05
G = 7.6677701539E+00
K = 1.3619992535E+05
L = 1.3619225758E+05
Vnuc = 7.0324720159E+06
Ven = -8.4130097827E+08
Vrep = 8.4116477068E+08
DelSqV = 4.6163327982E+09
DelSqVen = 3.8310726861E+12
DelSqVrep = -3.8264563533E+12
DelSqG = 2.0675375022E+08
DelSqK = -4.8230865484E+09
Stress_EigVals = -4.5402616054E+04 -4.5402540968E+04 -4.5402436098E+04
Stress_EigVec1 = 5.0346519725E-01 -6.1780031598E-01 -6.0402447363E-01
Stress_EigVec2 = 8.5154464565E-01 4.7314709723E-01 2.2583963526E-01
Stress_EigVec3 = 1.4626862833E-01 -6.2805620287E-01 7.6429764778E-01
-DivStress = 3.7453110072E+02 7.9684290857E+02 -9.3050356713E+02

CP# 9 Coords = 4.05226380331587E+00 2.42255090615486E+00 -1.10306780922760E+00

Type = (3,-3) NACP H9

Rho = 4.4219870474E-01 Rho at Nucleus = 4.3934286338E-01

GradRho = -1.4860166916E-10 -4.2124619765E-12 1.0488148544E-10

HessRho_EigVals = -9.0161923770E+00 -9.0150664522E+00 -8.3932533253E+00

HessRho_EigVec1 = -4.6748326946E-01 6.1585828032E-01 -6.3417503210E-01

HessRho_EigVec2 = 3.4019487126E-01 7.8747522252E-01 5.1395546839E-01

HessRho_EigVec3 = 8.1592085544E-01 2.4522489317E-02 -5.7764332003E-01

DelSqRho = -2.6424512155E+01

Bond Ellipticity = NA

V = -6.6196338026E+00

G = 6.7528819877E-03

K = 6.6128809206E+00

L = 6.6061280386E+00

Vnuc = 5.3411934381E+01

Ven = -2.3618688201E+01

Vrep = 1.6999054398E+01

DelSqV = 1.7183008168E+03

DelSqVen = 1.4113843098E+03

DelSqVrep = 3.0691650703E+02

DelSqG = 1.3202504517E+02

DelSqK = -1.8503258620E+03

Stress_EigVals = -2.2593993386E+00 -2.2590359362E+00 -2.1011985278E+00

Stress_EigVec1 = -4.3444840133E-01 6.8453428248E-01 -5.8537799983E-01

Stress_EigVec2 = 3.8083204211E-01 7.2857156495E-01 5.6934210317E-01

Stress_EigVec3 = 8.1622395351E-01 2.4419067452E-02 -5.7721934034E-01

-DivStress = 1.1707157452E+01 3.3255348359E-01 -8.2562937217E+00

CP# 10 Coords = 2.42867453659910E+00 4.08075079804349E+00 1.22200432494437E+00

Type = (3,-3) NACP H10

Rho = 4.4368270742E-01 Rho at Nucleus = 4.4080872510E-01

GradRho = -2.3912825713E-11 -6.5434509981E-10 -4.3061517633E-10

HessRho_EigVals = -9.0399533985E+00 -9.0388436076E+00 -8.4146526551E+00

HessRho_EigVec1 = -5.1911897590E-01 4.8334213193E-01 -7.0490841416E-01

HessRho_EigVec2 = 8.5420940411E-01 2.6540107558E-01 -4.4708898780E-01

HessRho_EigVec3 = 2.9013493222E-02 8.3423177390E-01 5.5065012906E-01

DelSqRho = -2.6493449661E+01

Bond Ellipticity = NA

V = -6.6369154990E+00

G = 6.7765418710E-03

K = 6.6301389572E+00

L = 6.6233624153E+00
Vnuc = 5.3217734901E+01
Ven = -2.3611788704E+01
Vrep = 1.6974873205E+01
DelSqV = 1.7224844422E+03
DelSqVen = 1.4099213830E+03
DelSqVrep = 3.1256305914E+02
DelSqG = 1.3227093709E+02
DelSqK = -1.8547553793E+03
Stress_EigVals = -2.2653845552E+00 -2.2651262875E+00 -2.1064046563E+00
Stress_EigVec1 = 4.5460266310E-01 -5.0109292699E-01 7.3637103231E-01
Stress_EigVec2 = 8.9021761053E-01 2.2857081500E-01 -3.9404059237E-01
Stress_EigVec3 = 2.9138026785E-02 8.3466236351E-01 5.4999064932E-01
-DivStress = 4.4569109708E-01 1.2019547094E+01 7.9041356413E+00

CP# 11 Coords = 4.12768231352039E-06 2.39191502990518E-04 -3.24220958393942E+00

Type = (3,-3) NACP C11
Rho = 1.1962846547E+02 Rho at Nucleus = 1.1962846546E+02
GradRho = -2.6910575547E-16 7.8253647052E-16 -5.7821525346E-12
HessRho_EigVals = -1.8158540286E+05 -1.8158537548E+05 -1.8158500519E+05
HessRho_EigVec1 = -4.7046342803E-05 9.9999999878E-01 -1.5376201767E-05
HessRho_EigVec2 = -9.9470430918E-07 1.5376154987E-05 9.9999999888E-01
HessRho_EigVec3 = 9.9999999889E-01 4.7046358093E-05 9.9398091611E-07
DelSqRho = -5.4475578353E+05
Bond Ellipticity = NA
V = -1.3620438930E+05
G = 7.7217083106E+00
K = 1.3619666759E+05
L = 1.3618894588E+05
Vnuc = 1.8401503683E+07
Ven = -2.2013436478E+09
Vrep = 2.2012074435E+09

DelSqV = 4.6162220665E+09
DelSqVen = 1.0024327840E+13
DelSqVrep = -1.0019711618E+13
DelSqG = 2.0674804364E+08
DelSqK = -4.8229701101E+09
Stress_EigVals = -4.5401526014E+04 -4.5401442608E+04 -4.5401420678E+04
Stress_EigVec1 = 9.9999999906E-01 4.3391422926E-05 -1.7616846766E-07
Stress_EigVec2 = 1.7812362019E-07 -4.5058502490E-05 9.9999999898E-01
Stress_EigVec3 = -4.3391414944E-05 9.9999999804E-01 4.5058510177E-05
-DivStress = 6.4405877400E-03 4.2038265047E-02 -4.8908585561E+02

CP# 12 Coords = -1.64697005433208E+00 2.42999805069383E-04 -4.45388174545609E+00

Type = (3,-3) NACP H12
Rho = 4.4332077356E-01 Rho at Nucleus = 4.4044855775E-01
GradRho = 2.9590033548E-11 -1.0691503970E-16 2.2082825152E-11
HessRho_EigVals = -9.0355769106E+00 -9.0348347254E+00 -8.4108675322E+00
HessRho_EigVec1 = -6.9158432061E-05 9.9999999288E-01 9.7279209757E-05
HessRho_EigVec2 = -5.9809887426E-01 -1.1932531042E-04 8.0142231212E-01
HessRho_EigVec3 = 8.0142231802E-01 -2.7574753189E-06 5.9809887825E-01
DelSqRho = -2.6481279168E+01
Bond Ellipticity = NA
V = -6.6337674642E+00
G = 6.7238360526E-03
K = 6.6270436281E+00
L = 6.6203197920E+00
Vnuc = 5.3443221685E+01
Ven = -2.3692490379E+01
Vrep = 1.7058722915E+01
DelSqV = 1.7218044336E+03
DelSqVen = 1.4152448732E+03
DelSqVrep = 3.0655956037E+02
DelSqG = 1.3225622914E+02

DelSqK = -1.8540606627E+03

Stress_EigVals = -2.2643005784E+00 -2.2639805891E+00 -2.1054862966E+00

Stress_EigVec1 = -6.8061848406E-05 9.9999999309E-01 9.5890853002E-05

Stress_EigVec2 = -5.9840679079E-01 -1.1755569797E-04 8.0119242315E-01

Stress_EigVec3 = 8.0119242889E-01 -2.8511003626E-06 5.9840679465E-01

-DivStress = -1.1526452330E+01 4.1865163315E-05 -8.6077103666E+00

CP# 13 Coords = 1.64698150617404E+00 4.10570538375241E-04 -4.45387694777461E+00

Type = (3,-3) NACP H13

Rho = 4.4332083680E-01 Rho at Nucleus = 4.4044861901E-01

GradRho = -2.9596563048E-11 -3.1054134729E-15 2.2086891344E-11

HessRho_EigVals = -9.0355780910E+00 -9.0348359059E+00 -8.4108683792E+00

HessRho_EigVec1 = -6.8634996326E-05 9.9999999647E-01 4.8563074295E-05

HessRho_EigVec2 = 5.9809666557E-01 2.1307506870E-06 8.0142396934E-01

HessRho_EigVec3 = 8.0142396640E-01 8.4051143997E-05 -5.9809666361E-01

DelSqRho = -2.6481282376E+01

Bond Ellipticity = NA

V = -6.6337682687E+00

G = 6.7238373489E-03

K = 6.6270444314E+00

L = 6.6203205940E+00

Vnuc = 5.3443211854E+01

Ven = -2.3692489400E+01

Vrep = 1.7058721132E+01

DelSqV = 1.7218046181E+03

DelSqVen = 1.4152447843E+03

DelSqVrep = 3.0655983382E+02

DelSqG = 1.3225624247E+02

DelSqK = -1.8540608606E+03

Stress_EigVals = -2.2643008741E+00 -2.2639808881E+00 -2.1054865065E+00

Stress_EigVec1 = -6.2424559672E-05 9.9999999644E-01 5.6769265227E-05

Stress_EigVec2 = 5.9840459271E-01 -8.1280556786E-06 8.0119407347E-01

Stress_EigVec3 = 8.0119407107E-01 8.3985176285E-05 -5.9840459007E-01

-DivStress = 1.1526480551E+01 1.2104754966E-03 -8.6076822428E+00

CP# 14 Coords = -1.26238690943241E-04 2.36837801130405E+00 -1.56933147316221E+00

Type = (3,-3) NACP C14

Rho = 1.1960176780E+02 Rho at Nucleus = 1.1960176775E+02

GradRho = 1.1191243245E-14 -1.0408141016E-10 1.1897549612E-10

HessRho_EigVals = -1.8154795384E+05 -1.8154788230E+05 -1.8154748627E+05

HessRho_EigVec1 = 9.9999999573E-01 7.7727435136E-05 4.9959272764E-05

HessRho_EigVec2 = -8.4958761651E-05 5.6092239171E-01 8.2786838523E-01

HessRho_EigVec3 = -3.6324811447E-05 8.2786838594E-01 -5.6092239592E-01

DelSqRho = -5.4464332241E+05

Bond Ellipticity = NA

V = -1.3617610786E+05

G = 7.6386297642E+00

K = 1.3616846923E+05

L = 1.3616083060E+05

Vnuc = 8.5726927650E+06

Ven = -1.0253092095E+09

Vrep = 1.0251730334E+09

DelSqV = 4.6152755017E+09

DelSqVen = 4.6690595635E+12

DelSqVrep = -4.6644442880E+12

DelSqG = 2.0670859962E+08

DelSqK = -4.8219841013E+09

Stress_EigVals = -4.5392115188E+04 -4.5392004264E+04 -4.5391988410E+04

Stress_EigVec1 = -3.4335655144E-05 8.3250486455E-01 -5.5401773376E-01

Stress_EigVec2 = -9.5134056782E-05 5.5401772886E-01 8.3250486308E-01

Stress_EigVec3 = 9.9999999489E-01 8.1290554426E-05 6.0177003373E-05

-DivStress = -6.1612784081E-02 8.0765023593E+02 -6.7006225441E+02

CP# 15 Coords = -2.06691888805488E-04 4.03572605703862E+00 -2.74942168432582E+00

Type = (3,-3) NACP H15

Rho = 4.4642881117E-01 Rho at Nucleus = 4.4352714915E-01

GradRho = 8.3057651587E-15 -1.7296803226E-10 1.2270306472E-10

HessRho_EigVals = -9.1016676787E+00 -9.1015291077E+00 -8.4702718047E+00

HessRho_EigVec1 = -8.9977108731E-05 5.7822094522E-01 8.1588021818E-01

HessRho_EigVec2 = 9.9999999518E-01 8.4017326783E-05 5.0738489877E-05

HessRho_EigVec3 = -3.9210017331E-05 8.1588021881E-01 -5.7822094999E-01

DelSqRho = -2.6673468591E+01

Bond Ellipticity = NA

V = -6.6818383325E+00

G = 6.7355923980E-03

K = 6.6751027401E+00

L = 6.6683671478E+00

Vnuc = 5.3330269869E+01

Ven = -2.3808168977E+01

Vrep = 1.7126330644E+01

DelSqV = 1.7340999420E+03

DelSqVen = 1.4225032789E+03

DelSqVrep = 3.1159666309E+02

DelSqG = 1.3324797862E+02

DelSqK = -1.8673479206E+03

Stress_EigVals = -2.2807566685E+00 -2.2806968641E+00 -2.1203847999E+00

Stress_EigVec1 = -1.8544761327E-05 5.7826062176E-01 8.1585210239E-01

Stress_EigVec2 = 9.999999906E-01 4.2666663802E-05 -7.5107856080E-06

Stress_EigVec3 = -3.9152878921E-05 8.1585210149E-01 -5.7826062201E-01

-DivStress = -5.6815273343E-04 1.1834310763E+01 -8.3962247423E+00

CP# 16 Coords = -2.38636211026447E+00 2.38057783932448E+00 8.57617469213465E-02

Type = (3,-3) NACP C16

Rho = 1.1963090258E+02 Rho at Nucleus = 1.1963090252E+02

GradRho = 1.1369716280E-10 -1.3648288055E-10 2.0484647312E-10

HessRho_EigVals = -1.8159002040E+05 -1.8158966416E+05 -1.8158934324E+05

HessRho_EigVec1 = -1.3044249622E-01 -6.3871724164E-01 7.5830405539E-01

HessRho_EigVec2 = -8.5138692650E-01 4.6409475733E-01 2.4445113540E-01

HessRho_EigVec3 = 5.0806009149E-01 6.1372334277E-01 6.0433318789E-01

DelSqRho = -5.4476902779E+05

Bond Ellipticity = NA

V = -1.3620759249E+05

G = 7.6677730873E+00

K = 1.3619992472E+05

L = 1.3619225695E+05

Vnuc = 7.0325343864E+06

Ven = -8.4130843607E+08

Vrep = 8.4117222848E+08

DelSqV = 4.6163327769E+09

DelSqVen = 3.8311070269E+12

DelSqVrep = -3.8264906942E+12

DelSqG = 2.0675374921E+08

DelSqK = -4.8230865261E+09

Stress_EigVals = -4.5402615845E+04 -4.5402540758E+04 -4.5402435891E+04

Stress_EigVec1 = 5.0338377191E-01 6.1786474491E-01 6.0402643583E-01

Stress_EigVec2 = -8.5160417949E-01 4.7304624579E-01 2.2582641746E-01

Stress_EigVec3 = -1.4620225601E-01 -6.2806879109E-01 7.6430000261E-01

-DivStress = -3.7460406937E+02 7.9679510190E+02 -9.3049946824E+02

CP# 17 Coords = -2.42913696703105E+00 4.08049792655797E+00 1.22197273996986E+00

Type = (3,-3) NACP H17

Rho = 4.4368272261E-01 Rho at Nucleus = 4.4080874238E-01

GradRho = 2.3988385280E-11 -6.5433508091E-10 -4.3060118318E-10

HessRho_EigVals = -9.0399536930E+00 -9.0388439526E+00 -8.4146531822E+00

HessRho_EigVec1 = -5.1904621234E-01 -4.8340270963E-01 7.0492045634E-01

HessRho_EigVec2 = -8.5425033933E-01 2.6528982192E-01 -4.4707680339E-01

HessRho_EigVec3 = -2.9109915842E-02 8.3423206046E-01 5.5064460598E-01

DelSqRho = -2.6493450828E+01

Bond Ellipticity = NA

V = -6.6369157902E+00

G = 6.7765416410E-03

K = 6.6301392486E+00

L = 6.6233627069E+00

Vnuc = 5.3217738784E+01

Ven = -2.3611791235E+01

Vrep = 1.6974875445E+01

DelSqV = 1.7224845432E+03

DelSqVen = 1.4099215480E+03

DelSqVrep = 3.1256299518E+02

DelSqG = 1.3227094412E+02

DelSqK = -1.8547554873E+03

Stress_EigVals = -2.2653846292E+00 -2.2651263672E+00 -2.1064047938E+00

Stress_EigVec1 = -4.5453526148E-01 -5.0114300970E-01 7.3637855746E-01

Stress_EigVec2 = 8.9024886504E-01 -2.2845999066E-01 3.9403425100E-01

Stress_EigVec3 = -2.9234472109E-02 8.3466263633E-01 5.4998511721E-01

-DivStress = -4.4707929119E-01 1.2019542630E+01 7.9040550583E+00

CP# 18 Coords = -4.05252717251122E+00 2.42210351950576E+00 -1.10309829145543E+00

Type = (3,-3) NACP H18

Rho = 4.4219879020E-01 Rho at Nucleus = 4.3934294779E-01

GradRho = 1.4858929712E-10 -4.1970272743E-12 1.0487465237E-10

HessRho_EigVals = -9.0161939297E+00 -9.0150679907E+00 -8.3932547272E+00

HessRho_EigVec1 = 4.6741637104E-01 6.1591196277E-01 -6.3417220863E-01

HessRho_EigVec2 = -3.4028835209E-01 7.8743614712E-01 5.1395345279E-01

HessRho_EigVec3 = 8.1592020046E-01 -2.4428841971E-02 5.7764821316E-01

DelSqRho = -2.6424516648E+01

Bond Ellipticity = NA

V = -6.6196349034E+00

G = 6.7528707447E-03

K = 6.6128820326E+00

L = 6.6061291619E+00
Vnuc = 5.3411928707E+01
Ven = -2.3618690257E+01
Vrep = 1.6999055353E+01
DelSqV = 1.7183010917E+03
DelSqVen = 1.4113843998E+03
DelSqVrep = 3.0691669182E+02
DelSqG = 1.3202506403E+02
DelSqK = -1.8503261557E+03
Stress_EigVals = -2.2593997065E+00 -2.2590363213E+00 -2.1011988756E+00
Stress_EigVec1 = 4.3437546994E-01 6.8458017535E-01 -5.8537845418E-01
Stress_EigVec2 = -3.8091664291E-01 7.2853157371E-01 5.6933668181E-01
Stress_EigVec3 = 8.1622329192E-01 -2.4325493121E-02 5.7722422690E-01
-DivStress = -1.1707149053E+01 3.3121129108E-01 -8.2563661354E+00

CP# 19 Coords = -2.38609810030821E+00 -2.38083473934545E+00 8.54277581818776E-02

Type = (3,-3) NACP C19
Rho = 1.1963090368E+02 Rho at Nucleus = 1.1963090361E+02
GradRho = 1.2126910587E-10 1.8808382629E-10 2.0584378646E-10
HessRho_EigVals = -1.8159002222E+05 -1.8158966593E+05 -1.8158934502E+05
HessRho_EigVec1 = -1.3049865632E-01 6.3859515835E-01 7.5839720756E-01
HessRho_EigVec2 = 8.5133295319E-01 4.6422116584E-01 -2.4439908347E-01
HessRho_EigVec3 = 5.0813610727E-01 -6.1375478240E-01 6.0423734043E-01
DelSqRho = -5.4476903317E+05
Bond Ellipticity = NA
V = -1.3620759383E+05
G = 7.6677667109E+00
K = 1.3619992606E+05
L = 1.3619225829E+05
Vnuc = 7.0317864246E+06
Ven = -8.4121896446E+08
Vrep = 8.4108275686E+08

DelSqV = 4.6163328222E+09

DelSqVen = 3.8306988687E+12

DelSqVrep = -3.8260825359E+12

DelSqG = 2.0675375138E+08

DelSqK = -4.8230865736E+09

Stress_EigVals = -4.5402616293E+04 -4.5402541208E+04 -4.5402436326E+04

Stress_EigVec1 = 5.0346183589E-01 -6.1789356357E-01 6.0393188681E-01

Stress_EigVec2 = 8.5154959431E-01 4.7316610759E-01 -2.2578113973E-01

Stress_EigVec3 = -1.4625138712E-01 6.2795014032E-01 7.6438809059E-01

-DivStress = -3.7453833219E+02 -7.9676365599E+02 -9.3074051684E+02

CP# 20 Coords = -2.42868545088418E+00 -4.08091736991926E+00 1.22140234770447E+00

Type = (3,-3) NACP H2O

Rho = 4.4368263184E-01 Rho at Nucleus = 4.4080864793E-01

GradRho = 2.4034915985E-11 6.5756163015E-10 -4.3258948073E-10

HessRho_EigVals = -9.0399527865E+00 -9.0388428691E+00 -8.4146518197E+00

HessRho_EigVec1 = -5.1914604876E-01 4.8323287879E-01 7.0496337842E-01

HessRho_EigVec2 = -8.5419278245E-01 -2.6534758954E-01 -4.4715248757E-01

HessRho_EigVec3 = 2.9018450650E-02 8.3431207685E-01 -5.5052818996E-01

DelSqRho = -2.6493447475E+01

Bond Ellipticity = NA

V = -6.6369149765E+00

G = 6.7765538324E-03

K = 6.6301384226E+00

L = 6.6233618688E+00

Vnuc = 5.3217733783E+01

Ven = -2.3611784186E+01

Vrep = 1.6974869209E+01

DelSqV = 1.7224843064E+03

DelSqVen = 1.4099212371E+03

DelSqVrep = 3.1256306930E+02

DelSqG = 1.3227093851E+02

DelSqK = -1.8547552449E+03

Stress_EigVals = -2.2653844008E+00 -2.2651261244E+00 -2.1064044513E+00

Stress_EigVec1 = -4.5461954195E-01 5.0098289572E-01 7.3643547598E-01

Stress_EigVec2 = 8.9020882648E-01 2.2851904418E-01 3.9409046131E-01

Stress_EigVec3 = 2.9143049411E-02 8.3474258586E-01 -5.4986861888E-01

-DivStress = -4.4576682227E-01 -1.2020704852E+01 7.9023770787E+00

CP# 21 Coords = -4.05226256829535E+00 -2.42237676533380E+00 -1.10343268829094E+00

Type = (3,-3) NACP H21

Rho = 4.4219836140E-01 Rho at Nucleus = 4.3934251560E-01

GradRho = 1.4859494191E-10 4.1974670267E-12 1.0487808018E-10

HessRho_EigVals = -9.0161857785E+00 -9.0150598679E+00 -8.3932463358E+00

HessRho_EigVec1 = -4.6749480472E-01 6.1574196890E-01 6.3427946151E-01

HessRho_EigVec2 = -3.4018284400E-01 -7.8756882351E-01 5.1381998880E-01

HessRho_EigVec3 = 8.1591926084E-01 2.4437184217E-02 5.7764918750E-01

DelSqRho = -2.6424491982E+01

Bond Ellipticity = NA

V = -6.6196287558E+00

G = 6.7528801422E-03

K = 6.6128758757E+00

L = 6.6061229956E+00

Vnuc = 5.3411893497E+01

Ven = -2.3618651784E+01

Vrep = 1.6999023028E+01

DelSqV = 1.7182994309E+03

DelSqVen = 1.4113821520E+03

DelSqVrep = 3.0691727884E+02

DelSqG = 1.3202494671E+02

DelSqK = -1.8503243776E+03

Stress_EigVals = -2.2593976837E+00 -2.2590342922E+00 -2.1011967799E+00

Stress_EigVec1 = -4.3444877336E-01 6.8445022166E-01 5.8547600924E-01

Stress_EigVec2 = -3.8083502679E-01 -7.2865338683E-01 5.6923538561E-01

Stress_EigVec3 = 8.1622236290E-01 2.4333843362E-02 5.7722518862E-01

-DivStress = -1.1707140140E+01 -3.3133048019E-01 -8.2563774313E+00

CP# 22 Coords = -2.47277963093575E+00 -2.47008818605387E-04 1.79421505292014E+00

Type = (3,-3) NACP C22

Rho = 1.1960058552E+02 Rho at Nucleus = 1.1960058457E+02

GradRho = 3.9324932199E-12 -3.5246328425E-15 7.5739414740E-12

HessRho_EigVals = -1.8154508740E+05 -1.8154437073E+05 -1.8154296823E+05

HessRho_EigVec1 = -7.1311237737E-05 9.9999999083E-01 1.1515941509E-04

HessRho_EigVec2 = -4.9691741856E-01 -1.3537088707E-04 8.6779782254E-01

HessRho_EigVec3 = 8.6779783017E-01 4.6590175637E-06 4.9691742366E-01

DelSqRho = -5.4463242636E+05

Bond Ellipticity = NA

V = -1.3617359994E+05

G = 7.7466763848E+00

K = 1.3616585327E+05

L = 1.3615810659E+05

Vnuc = 1.8567296222E+06

Ven = -2.2206594997E+08

Vrep = 2.2192977637E+08

DelSqV = 4.6151839966E+09

DelSqVen = 1.0112351396E+12

DelSqVrep = -1.0066199556E+12

DelSqG = 2.0670262351E+08

DelSqK = -4.8218866201E+09

Stress_EigVals = -4.5391492874E+04 -4.5391147977E+04 -4.5390959092E+04

Stress_EigVec1 = 8.9234489442E-01 3.9576316579E-06 4.5135417289E-01

Stress_EigVec2 = -4.5135416785E-01 -1.4189260996E-04 8.9234488570E-01

Stress_EigVec3 = -6.7575393978E-05 9.9999998993E-01 1.2483085251E-04

-DivStress = 2.4045793449E+03 1.7526612683E-02 4.2138625939E+03

CP# 23 Coords = -4.19501652080345E+00 -4.22266835935786E-04 2.88562355318863E+00

Type = (3,-3) NACP H23

Rho = 4.4451014122E-01 Rho at Nucleus = 4.4162865859E-01

GradRho = 8.5640186609E-10 8.7893445480E-14 -5.5390376660E-10

HessRho_EigVals = -9.0605898476E+00 -9.0576774459E+00 -8.4346121872E+00

HessRho_EigVec1 = -8.7462213328E-05 9.9999999591E-01 2.2951141489E-05

HessRho_EigVec2 = 5.4174716313E-01 2.8091019210E-05 8.4054149835E-01

HessRho_EigVec3 = 8.4054149427E-01 8.5949335632E-05 -5.4174716337E-01

DelSqRho = -2.6552879481E+01

Bond Ellipticity = NA

V = -6.6527007576E+00

G = 7.2404437240E-03

K = 6.6454603139E+00

L = 6.6382198702E+00

Vnuc = 5.3014983228E+01

Ven = -2.3565697682E+01

Vrep = 1.6912996924E+01

DelSqV = 1.7265442063E+03

DelSqVen = 1.4077004634E+03

DelSqVrep = 3.1884374288E+02

DelSqG = 1.3263388297E+02

DelSqK = -1.8591780892E+03

Stress_EigVals = -2.2709637082E+00 -2.2703330384E+00 -2.1114040110E+00

Stress_EigVec1 = 5.4274753475E-01 -6.1837998506E-05 8.3989589218E-01

Stress_EigVec2 = -3.8590757204E-05 9.9999999440E-01 9.8563449670E-05

Stress_EigVec3 = 8.3989589357E-01 8.5907287776E-05 -5.4274752933E-01

-DivStress = -1.2112312029E+01 -1.2434932985E-03 7.8388831004E+00

CP# 24 Coords = -4.93466317066841E-06 -2.93555227927823E-04 3.44058285656941E+00

Type = (3,-3) NACP B24

Rho = 6.7312062646E+01 Rho at Nucleus = 6.7312062566E+01

GradRho = 2.6628437343E-15 -5.8835694563E-14 3.8609149211E-10

HessRho_EigVals = -6.7280946712E+04 -6.7278268462E+04 -6.7278216252E+04

HessRho_EigVec1 = -4.6586948877E-05 9.9999999129E-01 1.2348008122E-04

HessRho_EigVec2 = -1.4472101246E-05 -1.2348075555E-04 9.9999999227E-01

HessRho_EigVec3 = 9.9999999881E-01 4.6585161501E-05 1.4477853712E-05

DelSqRho = -2.0183743143E+05

Bond Ellipticity = NA

V = -5.0462684916E+04

G = 1.6635300969E+00

K = 5.0461021386E+04

L = 5.0459357856E+04

Vnuc = 3.2329768170E+06

Ven = -2.1761833804E+08

Vrep = 2.1756787536E+08

DelSqV = 1.0754007170E+09

DelSqVen = 6.5253572608E+11

DelSqVrep = -6.5146032536E+11

DelSqG = 5.0438980018E+07

DelSqK = -1.1258396970E+09

Stress_EigVals = -1.6821161898E+04 -1.6821158564E+04 -1.6820364454E+04

Stress_EigVec1 = 9.9999999544E-01 4.6906317967E-05 8.3224865093E-05

Stress_EigVec2 = -8.3219139231E-05 -1.2205890895E-04 9.9999998909E-01

Stress_EigVec3 = -4.6916475791E-05 9.9999999145E-01 1.2205500489E-04

-DivStress = -3.6416193432E-03 8.3501599821E-02 -5.4086826159E+02

CP# 25 Coords = -5.92659211395078E-06 -5.70093220713090E-04 5.67715860284328E+00

Type = (3,-3) NACP H25

Rho = 4.2667265311E-01 Rho at Nucleus = 4.2499533625E-01

GradRho = -2.1016475608E-18 -7.4433020240E-20 9.5409791179E-18

HessRho_EigVals = -8.6894674088E+00 -8.6884200570E+00 -8.3331910837E+00

HessRho_EigVec1 = 9.9999999818E-01 6.0267820482E-05 3.9967330256E-07

HessRho_EigVec2 = -6.0267869575E-05 9.9999999050E-01 1.2399087047E-04

HessRho_EigVec3 = -3.9220063924E-07 -1.2399089433E-04 9.9999999231E-01

DelSqRho = -2.5711078549E+01

Bond Ellipticity = NA

V = -6.4311824174E+00

G = 1.7063899988E-03

K = 6.4294760274E+00

L = 6.4277696374E+00

Vnuc = 6.2868256267E+01

Ven = -2.6824165698E+01

Vrep = 2.0392983280E+01

DelSqV = 1.6841590274E+03

DelSqVen = 1.6164106752E+03

DelSqVrep = 6.7748352283E+01

DelSqG = 1.2923324725E+02

DelSqK = -1.8133922747E+03

Stress_EigVals = -2.1747455757E+00 -2.1723154133E+00 -2.0841214284E+00

Stress_EigVec1 = 9.9999999891E-01 4.6623079943E-05 3.8681354656E-07

Stress_EigVec2 = -4.6623127519E-05 9.9999999124E-01 1.2392009935E-04

Stress_EigVec3 = -3.8103600647E-07 -1.2392011725E-04 9.9999999232E-01

-DivStress = -3.9956718327E-06 -1.3309578383E-03 1.0762074894E+01

CP# 26 Coords = 1.21313181827239E+00 1.22084548623423E-04 -7.24655369727646E-01

Type = (3,+1) RCP C1 C4 C11 C14 C8 C6

Rho = 1.9767818547E-02

GradRho = -1.0718422677E-13 -2.1685670071E-14 -1.6610844644E-14

HessRho_EigVals = -1.6036675083E-02 6.5364873473E-02 6.8546821686E-02

HessRho_EigVec1 = 8.0489089362E-01 8.8659408177E-05 -5.9342281849E-01

HessRho_EigVec2 = 5.9342282198E-01 -1.7506425757E-05 8.0489089574E-01

HessRho_EigVec3 = -6.0972437949E-05 9.9999999592E-01 6.6703278867E-05

DelSqRho = 1.1787502008E-01

Bond Ellipticity = NA

V = -1.9128259462E-02

G = 2.4298507241E-02

K = -5.1702477784E-03

L = -2.9468755019E-02
Vnuc = 2.1192523049E+01
Ven = -4.1892995018E-01
Vrep = 3.9980169072E-01
DelSqV = -1.2020797788E-01
DelSqVen = -2.4980690799E+00
DelSqVrep = 2.3778611020E+00
DelSqG = 9.3204607910E-02
DelSqK = 2.7003369967E-02
Stress_EigVals = -7.0085952035E-03 -6.0838144158E-03 -6.0358498428E-03
Stress_EigVec1 = 7.8662449289E-01 9.2592365054E-05 -6.1743169550E-01
Stress_EigVec2 = 6.1743170057E-01 -4.0218040546E-05 7.8662449333E-01
Stress_EigVec3 = -4.8003529283E-05 9.9999999490E-01 8.8805957166E-05
-DivStress = -2.1457030198E-04 -3.5338653268E-08 1.0058183672E-04

CP# 27 Coords = 3.44988236340348E+00 -2.40257591010200E+00 -6.75839210074817E-01

Type = (3,-1) BCP H2 C1
Rho = 2.7103076129E-01
GradRho = -1.0408340856E-17 2.4286128664E-17 3.4694469520E-18
HessRho_EigVals = -6.8396668289E-01 -6.8248839695E-01 4.7725927975E-01
HessRho_EigVec1 = 5.2151364383E-01 4.7240286491E-01 7.1053434296E-01
HessRho_EigVec2 = 2.5339498977E-01 -8.8092491907E-01 3.9970272219E-01
HessRho_EigVec3 = 8.1474811964E-01 -2.8404580532E-02 -5.7911888361E-01
DelSqRho = -8.8919580009E-01
Bond Ellipticity = 2.1660235403E-03
V = -3.0936438404E-01
G = 4.3532717007E-02
K = 2.6583166703E-01
L = 2.2229895002E-01
Vnuc = 1.8637895870E+01
Ven = -5.0514431064E+00
Vrep = 4.7420787224E+00

DelSqV = -2.3257534175E+00

DelSqVen = 1.6572738730E+01

DelSqVrep = -1.8898492147E+01

DelSqG = 1.6482777867E+00

DelSqK = 6.7747563088E-01

Stress_EigVals = -2.1004732552E-01 -2.0974125736E-01 1.1042419884E-01

Stress_EigVec1 = 3.9544383184E-03 9.9917153349E-01 -4.0504432746E-02

Stress_EigVec2 = 5.7967409982E-01 3.0714678042E-02 8.1426933293E-01

Stress_EigVec3 = 8.1483881868E-01 -2.6699348442E-02 -5.7907239994E-01

-DivStress = -1.3998305510E-01 7.7997497314E-04 1.0078171258E-01

BPL = 2.0473887879E+00 = 7.3919504124E-01 + 1.3081937466E+00

GBL_I = 2.0472460536E+00

GBL_II = 2.0730092504E+00

GBL_III = 2.0472708018E+00 = 7.3919447203E-01 + 1.3080763298E+00

GBL_IV = 2.0730342216E+00 = 7.6495846444E-01 + 1.3080757571E+00

CP# 28 Coords = 6.71495396609746E-05 -1.22189146730887E+00 9.59626379239729E-01

Type = (3,+1) RCP C1 C4 C19 C22 B24 C6

Rho = 2.0223831359E-02

GradRho = -9.0396155518E-16 -3.0487426277E-15 -3.0887185171E-14

HessRho_EigVals = -1.6341458267E-02 6.2301229911E-02 6.3926032133E-02

HessRho_EigVec1 = -4.4886660816E-05 8.2056797934E-01 -5.7154893865E-01

HessRho_EigVec2 = 9.9999991894E-01 -1.9186466473E-04 -3.5399358435E-04

HessRho_EigVec3 = 4.0013584570E-04 5.7154890821E-01 8.2056790421E-01

DelSqRho = 1.0988580378E-01

Bond Ellipticity = NA

V = -1.8903974009E-02

G = 2.3187712476E-02

K = -4.2837384679E-03

L = -2.7471450944E-02

Vnuc = 2.0858220761E+01

Ven = -4.2183313912E-01

Vrep = 4.0292916511E-01
DelSqV = -1.0520348986E-01
DelSqVen = -2.2920223537E+00
DelSqVrep = 2.1868188638E+00
DelSqG = 7.9750098897E-02
DelSqK = 2.5453390959E-02
Stress_EigVals = -6.8724261540E-03 -6.2100452165E-03 -5.8215026381E-03
Stress_EigVec1 = -5.6950522755E-05 8.7341450469E-01 -4.8697751462E-01
Stress_EigVec2 = -5.8000530829E-05 4.8697751171E-01 8.7341450625E-01
Stress_EigVec3 = 9.999999670E-01 7.7986367063E-05 2.2924881044E-05
-DivStress = -2.5530729755E-08 1.4904495943E-04 2.8258081555E-04

CP# 29 Coords = 2.40823710438982E+00 -3.46325306371223E+00 8.12494907439081E-01

Type = (3,-1) BCP C1 H3
Rho = 2.7196396594E-01
GradRho = 9.3241386834E-18 -6.2450045135E-17 -1.4398204851E-16
HessRho_EigVals = -6.8612460847E-01 -6.8341594454E-01 4.7348875534E-01
HessRho_EigVec1 = 2.0091918162E-01 5.4672684659E-01 8.1284761036E-01
HessRho_EigVec2 = 9.7920921285E-01 -8.8420244262E-02 -1.8256828275E-01
HessRho_EigVec3 = -2.7942797258E-02 8.3262933867E-01 -5.5312528821E-01
DelSqRho = -8.9605179766E-01
Bond Ellipticity = 3.9634192770E-03
V = -3.1180990960E-01
G = 4.3898480091E-02
K = 2.6791142951E-01
L = 2.2401294942E-01
Vnuc = 1.8552441605E+01
Ven = -5.0455955966E+00
Vrep = 4.7337856870E+00
DelSqV = -2.2946149174E+00
DelSqVen = 1.6623948651E+01
DelSqVrep = -1.8918563568E+01

DelSqG = 1.6537834613E+00

DelSqK = 6.4083145613E-01

Stress_EigVals = -2.1101169346E-01 -2.1065981926E-01 1.0986160312E-01

Stress_EigVec1 = 9.9196777394E-01 -4.6185261625E-02 -1.1775762005E-01

Stress_EigVec2 = 1.2363578889E-01 5.5069856617E-01 8.2549699026E-01

Stress_EigVec3 = -2.6723158048E-02 8.3342546807E-01 -5.5198538205E-01

-DivStress = -1.4470295718E-03 1.4861169379E-01 -1.0068507966E-01

BPL = 2.0452417848E+00 = 1.3044163123E+00 + 7.4082547256E-01

GBL_I = 2.0451237193E+00

GBL_II = 2.0709334854E+00

GBL_III = 2.0451645082E+00 = 1.3043393928E+00 + 7.4082511539E-01

GBL_IV = 2.0709760225E+00 = 1.3043392937E+00 + 7.6663672880E-01

CP# 30 Coords = 1.18493242564711E+00 -2.36816747581178E+00 -7.39913942859085E-01

Type = (3,-1) BCP C1 C4

Rho = 2.3859921916E-01

GradRho = 1.7347234760E-17 1.0408340856E-16 -6.5919492087E-17

HessRho_EigVals = -4.3507731159E-01 -4.3367757207E-01 3.4491703010E-01

HessRho_EigVec1 = -5.0625309935E-01 4.5450207644E-01 7.3289539629E-01

HessRho_EigVec2 = -2.6179273408E-01 -8.9073771095E-01 3.7155200804E-01

HessRho_EigVec3 = 8.2168872682E-01 -3.7673339545E-03 5.6992406811E-01

DelSqRho = -5.2383785356E-01

Bond Ellipticity = 3.2276041353E-03

V = -2.4336435212E-01

G = 5.6202444363E-02

K = 1.8716190775E-01

L = 1.3095946339E-01

Vnuc = 2.1869012444E+01

Ven = -5.2179292927E+00

Vrep = 4.9745649406E+00

DelSqV = -1.6228960082E+00

DelSqVen = 1.1455816538E+01

DelSqVrep = -1.3078712546E+01

DelSqG = 1.0866276768E+00

DelSqK = 5.3626833140E-01

Stress_EigVals = -1.5793628164E-01 -1.5761943125E-01 7.2191360780E-02

Stress_EigVec1 = 4.1952322945E-01 6.8033209531E-01 -6.0095632124E-01

Stress_EigVec2 = -3.8519475691E-01 7.3289422276E-01 5.6079502271E-01

Stress_EigVec3 = 8.2196426881E-01 -3.7813149102E-03 5.6952650725E-01

-DivStress = -7.8674361047E-03 -2.4435777457E-04 -6.4786875521E-03

BPL = 2.9042048954E+00 = 1.4577056619E+00 + 1.4464992336E+00

GBL_I = 2.9040704637E+00

GBL_II = 2.9040705704E+00

GBL_III = 2.9041262996E+00 = 1.4576595599E+00 + 1.4464667397E+00

GBL_IV = 2.9041264155E+00 = 1.4576594194E+00 + 1.4464669961E+00

CP# 31 Coords = 1.82512204860323E-04 -3.43222666965680E+00 -2.32272055054377E+00

Type = (3,-1) BCP C4 H5

Rho = 2.7397554818E-01

GradRho = -2.2759775293E-18 -4.8572257327E-17 -5.7245874707E-17

HessRho_EigVals = -6.9365073523E-01 -6.9351134571E-01 4.7913616685E-01

HessRho_EigVec1 = 9.9999999884E-01 4.8093778651E-05 3.8386381870E-06

HessRho_EigVec2 = 2.4662419736E-05 -5.7793477050E-01 8.1608296174E-01

HessRho_EigVec3 = -4.1466995803E-05 8.1608296069E-01 5.7793477102E-01

DelSqRho = -9.0802591409E-01

Bond Ellipticity = 2.0099096597E-04

V = -3.1400265644E-01

G = 4.3498088961E-02

K = 2.7050456748E-01

L = 2.2700647852E-01

Vnuc = 1.8960117619E+01

Ven = -5.1946086181E+00

Vrep = 4.8806059617E+00

DelSqV = -2.3388142901E+00

DelSqVen = 1.7216278132E+01
DelSqVrep = -1.9555092422E+01
DelSqG = 1.6741980984E+00
DelSqK = 6.6461619167E-01
Stress_EigVals = -2.1265955623E-01 -2.1248159023E-01 1.1113849001E-01
Stress_EigVec1 = 5.2878207869E-05 -5.7785622291E-01 8.1613858066E-01
Stress_EigVec2 = 9.9999999775E-01 6.4342676828E-05 -1.9233732993E-05
Stress_EigVec3 = -4.1398208643E-05 8.1613857984E-01 5.7785622501E-01
-DivStress = -7.4770909868E-06 1.4630552406E-01 1.0360312175E-01
BPL = 2.0427094444E+00 = 1.3035922566E+00 + 7.3911718774E-01
GBL_I = 2.0427093153E+00
GBL_II = 2.0685581113E+00
GBL_III = 2.0427093818E+00 = 1.3035922033E+00 + 7.3911717850E-01
GBL_IV = 2.0685581866E+00 = 1.3035915055E+00 + 7.6496668112E-01

CP# 32 Coords = 2.42601541065275E+00 -1.17525215447336E+00 9.39470702935922E-01

Type = (3,-1) BCP C6 C1
Rho = 2.2575176465E-01
GradRho = 8.1098322502E-17 -8.3266726847E-17 -8.7603535537E-17
HessRho_EigVals = -4.0299679161E-01 -3.8791374092E-01 3.3441144663E-01
HessRho_EigVec1 = 6.3760228376E-01 -4.6421901352E-01 6.1478779692E-01
HessRho_EigVec2 = -7.6978144532E-01 -3.5284950309E-01 5.3191517614E-01
HessRho_EigVec3 = 2.9997569689E-02 8.1240256995E-01 5.8232483217E-01
DelSqRho = -4.5649908590E-01
Bond Ellipticity = 3.8882486215E-02
V = -2.2672799797E-01
G = 5.6301613250E-02
K = 1.7042638472E-01
L = 1.1412477147E-01
Vnuc = 2.1599792049E+01
Ven = -4.8761911713E+00
Vrep = 4.6494631733E+00

DelSqV = -1.5633870279E+00

DelSqVen = 9.8602853261E+00

DelSqVrep = -1.1423672354E+01

DelSqG = 1.0212872571E+00

DelSqK = 5.4209977085E-01

Stress_EigVals = -1.4899811799E-01 -1.4725264638E-01 6.9522766400E-02

Stress_EigVec1 = 9.1625442855E-01 2.0522170631E-01 -3.4403760467E-01

Stress_EigVec2 = 3.9911887464E-01 -5.4135989714E-01 7.4002269268E-01

Stress_EigVec3 = 3.4379442574E-02 8.1536097100E-01 5.7793125967E-01

-DivStress = -5.0117918862E-04 1.1705973158E-02 1.0314384312E-02

BPL = 2.9319309409E+00 = 1.4540909509E+00 + 1.4778399900E+00

GBL_I = 2.9316605210E+00

GBL_II = 2.9316628945E+00

GBL_III = 2.9317268321E+00 = 1.4539616614E+00 + 1.4777651708E+00

GBL_IV = 2.9317292149E+00 = 1.4539632599E+00 + 1.4777659550E+00

CP# 33 Coords = -5.85942010439085E-07 -2.73131786658799E-06 1.17862972312265E-01

Type = (3,+3) CCP C1 C4 C6 C8 C11 C14 C16 C19 C22 B24

Rho = 1.2161743438E-02

GradRho = -3.4674480700E-18 3.5456269776E-19 0.0000000000E+00

HessRho_EigVals = 2.2535865932E-02 2.5766540223E-02 2.7326579257E-02

HessRho_EigVec1 = 9.9999999996E-01 8.6559196658E-06 -1.6995324377E-06

HessRho_EigVec2 = -8.6556290368E-06 9.9999998535E-01 1.7093081976E-04

HessRho_EigVec3 = 1.7010119762E-06 -1.7093080504E-04 9.9999998539E-01

DelSqRho = 7.5628985411E-02

Bond Ellipticity = NA

V = -1.2328419347E-02

G = 1.5617832850E-02

K = -3.2894135029E-03

L = -1.8907246353E-02

Vnuc = 2.1574020168E+01

Ven = -2.6237769822E-01

Vrep = 2.5004927887E-01
DelSqV = -7.1451346508E-02
DelSqVen = -1.6316212566E+00
DelSqVrep = 1.5601699101E+00
DelSqG = 7.8135711733E-02
DelSqK = -6.6843652248E-03
Stress_EigVals = -4.1605278187E-03 -4.0871398625E-03 -4.0807516660E-03
Stress_EigVec1 = -7.4429960465E-06 -3.7023779721E-05 9.9999999929E-01
Stress_EigVec2 = 9.9999967355E-01 -8.0798887508E-04 7.4130788199E-06
Stress_EigVec3 = 8.0798860005E-04 9.9999967289E-01 3.7029781493E-05
-DivStress = -1.8697670865E-10 -2.7735868223E-08 3.2858581317E-04

CP# 34 Coords = 3.57118823103526E+00 9.38039972656264E-06 2.48469401443618E+00

Type = (3,-1) BCP H7 C6
Rho = 2.7238727543E-01
GradRho = 2.2898349883E-16 4.7501607682E-18 -5.5511151231E-17
HessRho_EigVals = -6.8953065252E-01 -6.7453921549E-01 4.7088159467E-01
HessRho_EigVec1 = -4.5877342767E-05 9.9999999703E-01 6.1882438892E-05
HessRho_EigVec2 = -5.4055356183E-01 -7.6861451099E-05 8.4130959872E-01
HessRho_EigVec3 = 8.4130960098E-01 5.1462760762E-06 5.4055356375E-01
DelSqRho = -8.9318827334E-01
Bond Ellipticity = 2.2224707902E-02
V = -3.1489727181E-01
G = 4.5800101738E-02
K = 2.6909717007E-01
L = 2.2329706834E-01
Vnuc = 1.8554644474E+01
Ven = -5.0540490549E+00
Vrep = 4.7391517830E+00
DelSqV = -2.2982513645E+00
DelSqVen = 1.6572790860E+01
DelSqVrep = -1.8871042225E+01

DelSqG = 1.6666442345E+00

DelSqK = 6.3160712998E-01

Stress_EigVals = -2.1412234513E-01 -2.1029022509E-01 1.0951529841E-01

Stress_EigVec1 = -5.3867499842E-01 -1.0511092689E-04 8.4251364086E-01

Stress_EigVec2 = -6.1113084514E-05 9.9999999446E-01 8.5685064431E-05

Stress_EigVec3 = 8.4251364520E-01 5.3322053910E-06 5.3867500186E-01

-DivStress = -1.5672695977E-01 -1.1040862667E-06 -9.8695221659E-02

BPL = 2.0390778406E+00 = 7.4155538144E-01 + 1.2975224591E+00

GBL_I = 2.0389393776E+00

GBL_II = 2.0647528301E+00

GBL_III = 2.0389632189E+00 = 7.4155526551E-01 + 1.2974079534E+00

GBL_IV = 2.0647777186E+00 = 7.6736990374E-01 + 1.2974078149E+00

CP# 35 Coords = 2.42588189763589E+00 1.17538096474575E+00 9.39649774427268E-01

Type = (3,-1) BCP C8 C6

Rho = 2.2575234277E-01

GradRho = 3.4260788651E-17 1.6306400674E-16 -8.5868812061E-17

HessRho_EigVals = -4.0299852813E-01 -3.8791611924E-01 3.3441236517E-01

HessRho_EigVec1 = 6.3755963879E-01 4.6419272731E-01 6.1485186744E-01

HessRho_EigVec2 = -7.6981315112E-01 3.5268638746E-01 5.3197746612E-01

HessRho_EigVec3 = -3.0090186919E-02 8.1248841469E-01 -5.8220027193E-01

DelSqRho = -4.5650228220E-01

Bond Ellipticity = 3.8880593379E-02

V = -2.2672822725E-01

G = 5.6301328352E-02

K = 1.7042689890E-01

L = 1.1412557055E-01

Vnuc = 2.1599787539E+01

Ven = -4.8762026403E+00

Vrep = 4.6494744131E+00

DelSqV = -1.5633902788E+00

DelSqVen = 9.8603523066E+00

DelSqVrep = -1.1423742585E+01

DelSqG = 1.0212899484E+00

DelSqK = 5.4210033045E-01

Stress_EigVals = -1.4899845262E-01 -1.4725286149E-01 6.9523086851E-02

Stress_EigVec1 = 9.1628146436E-01 -2.0506002690E-01 -3.4406200523E-01

Stress_EigVec2 = 3.9904882067E-01 5.4129395160E-01 7.4010870599E-01

Stress_EigVec3 = -3.4471971246E-02 8.1544542633E-01 -5.7780657652E-01

-DivStress = -4.9955847891E-04 -1.1707402048E-02 1.0312207130E-02

BPL = 2.9319306487E+00 = 1.4778395566E+00 + 1.4540910921E+00

GBL_I = 2.9316602198E+00

GBL_II = 2.9316625932E+00

GBL_III = 2.9317265348E+00 = 1.4777647489E+00 + 1.4539617859E+00

GBL_IV = 2.9317289175E+00 = 1.4777655332E+00 + 1.4539633843E+00

CP# 36 Coords = 3.44961485664239E+00 2.40306716225927E+00 -6.75465106510557E-01

Type = (3,-1) BCP H9 C8

Rho = 2.7103059429E-01

GradRho = -6.9388939039E-17 1.1622647289E-16 2.7755575616E-17

HessRho_EigVals = -6.8396561779E-01 -6.8248749645E-01 4.7725862167E-01

HessRho_EigVec1 = -5.2156547877E-01 4.7244008146E-01 -7.1047154819E-01

HessRho_EigVec2 = 2.5328524168E-01 8.8089912078E-01 3.9982912020E-01

HessRho_EigVec3 = 8.1474906426E-01 2.8585108716E-02 -5.7910867188E-01

DelSqRho = -8.8919449258E-01

Bond Ellipticity = 2.1657852303E-03

V = -3.0936424116E-01

G = 4.3532809009E-02

K = 2.6583143215E-01

L = 2.2229862314E-01

Vnuc = 1.8637892753E+01

Ven = -5.0514391491E+00

Vrep = 4.7420749079E+00

DelSqV = -2.3257436120E+00

DelSqVen = 1.6572711589E+01

DelSqVrep = -1.8898455201E+01

DelSqG = 1.6482760198E+00

DelSqK = 6.7746759220E-01

Stress_EigVals = -2.1004716159E-01 -2.0974110234E-01 1.1042402277E-01

Stress_EigVec1 = -4.1397579937E-03 9.9916870875E-01 4.0555565090E-02

Stress_EigVec2 = 5.7967113618E-01 -3.0649118804E-02 8.1427391300E-01

Stress_EigVec3 = 8.1484000655E-01 2.6879787434E-02 -5.7906238070E-01

-DivStress = -1.3998450596E-01 -8.1143197125E-04 1.0078135083E-01

BPL = 2.0473893803E+00 = 7.3919569937E-01 + 1.3081936809E+00

GBL_I = 2.0472466525E+00

GBL_II = 2.0730098030E+00

GBL_III = 2.0472714010E+00 = 7.3919513022E-01 + 1.3080762708E+00

GBL_IV = 2.0730347745E+00 = 7.6495907634E-01 + 1.3080756981E+00

CP# 37 Coords = -6.95737363635236E-05 1.22174417404327E+00 9.59803926191351E-01

Type = (3,+1) RCP C6 C8 C14 C16 C22 B24

Rho = 2.0223543452E-02

GradRho = -3.6750853757E-17 -2.0593065014E-17 1.6263032587E-17

HessRho_EigVals = -1.6341184154E-02 6.2301334560E-02 6.3925098312E-02

HessRho_EigVec1 = -4.5630583695E-05 8.2048071301E-01 5.7167420573E-01

HessRho_EigVec2 = 9.9999994955E-01 -1.4226700160E-04 2.8400426446E-04

HessRho_EigVec3 = -3.1435039654E-04 -5.7167418985E-01 8.2048066513E-01

DelSqRho = 1.0988524872E-01

Bond Ellipticity = NA

V = -1.8903762252E-02

G = 2.3187537216E-02

K = -4.2837749634E-03

L = -2.7471312179E-02

Vnuc = 2.0858211515E+01

Ven = -4.2182694690E-01

Vrep = 4.0292318465E-01

DelSqV = -1.0520281472E-01

DelSqVen = -2.2920097601E+00

DelSqVrep = 2.1868069454E+00

DelSqG = 7.9750068910E-02

DelSqK = 2.5452745814E-02

Stress_EigVals = -6.8723241346E-03 -6.2099891941E-03 -5.8214489237E-03

Stress_EigVec1 = -5.6672485777E-05 8.7331882991E-01 4.8714907176E-01

Stress_EigVec2 = 4.7223451084E-05 -4.8714906966E-01 8.7331883164E-01

Stress_EigVec3 = 9.9999999728E-01 7.2498009426E-05 -1.3633180323E-05

-DivStress = 1.6477683906E-08 -1.4912517948E-04 2.8250663464E-04

CP# 38 Coords = 2.40783921020521E+00 3.46339940647413E+00 8.13022953536647E-01

Type = (3,-1) BCP H10 C8

Rho = 2.7196380240E-01

GradRho = -2.3635607360E-17 8.1532003371E-17 1.0408340856E-16

HessRho_EigVals = -6.8612367301E-01 -6.8341520939E-01 4.7348786260E-01

HessRho_EigVec1 = 2.0097675964E-01 -5.4682739624E-01 8.1276573550E-01

HessRho_EigVec2 = 9.7920019672E-01 8.8559717078E-02 -1.8254903793E-01

HessRho_EigVec3 = 2.7844511507E-02 8.3254848221E-01 5.5325193894E-01

DelSqRho = -8.9605101981E-01

Bond Ellipticity = 3.9631304442E-03

V = -3.1180969720E-01

G = 4.3898471125E-02

K = 2.6791122608E-01

L = 2.2401275495E-01

Vnuc = 1.8552442938E+01

Ven = -5.0455929250E+00

Vrep = 4.7337832278E+00

DelSqV = -2.2946055142E+00

DelSqVen = 1.6623935414E+01

DelSqVrep = -1.8918540928E+01

DelSqG = 1.6537817720E+00

DelSqK = 6.4082374222E-01

Stress_EigVals = -2.1101147425E-01 -2.1065961422E-01 1.0986139127E-01

Stress_EigVec1 = 9.9196035464E-01 4.6329008749E-02 -1.1776365212E-01

Stress_EigVec2 = 1.2371651715E-01 -5.5080880098E-01 8.2541134481E-01

Stress_EigVec3 = 2.6624766609E-02 8.3334463921E-01 5.5211215717E-01

-DivStress = -1.4294462173E-03 -1.4859695866E-01 -1.0070808259E-01

BPL = 2.0452422163E+00 = 7.4082598673E-01 + 1.3044162296E+00

GBL_I = 2.0451241505E+00

GBL_II = 2.0709339025E+00

GBL_III = 2.0451649378E+00 = 7.4082562963E-01 + 1.3043393082E+00

GBL_IV = 2.0709764378E+00 = 7.6663722878E-01 + 1.3043392090E+00

CP# 39 Coords = 6.57802378078626E-05 -1.18308922393720E+00 -2.40167062833133E+00

Type = (3,-1) BCP C11 C4

Rho = 2.3955717704E-01

GradRho = -9.5206503271E-19 -2.4134340360E-16 -1.3530843113E-16

HessRho_EigVals = -4.3679153388E-01 -4.3642018393E-01 3.4453926963E-01

HessRho_EigVec1 = 9.999999892E-01 2.4545855356E-05 -3.9430739682E-05

HessRho_EigVec2 = 1.7992281106E-05 5.7794564256E-01 8.1607526241E-01

HessRho_EigVec3 = -4.2820089533E-05 8.1607526224E-01 -5.7794564150E-01

DelSqRho = -5.2867244818E-01

Bond Ellipticity = 8.5090003013E-04

V = -2.4562524692E-01

G = 5.6728567437E-02

K = 1.8889667948E-01

L = 1.3216811204E-01

Vnuc = 2.1980329308E+01

Ven = -5.2655456394E+00

Vrep = 5.0199203925E+00

DelSqV = -1.6332885763E+00

DelSqVen = 1.1620394507E+01

DelSqVrep = -1.3253683083E+01

DelSqG = 1.0972445081E+00

DelSqK = 5.3604406820E-01

Stress_EigVals = -1.5895760330E-01 -1.5879138530E-01 7.2123741680E-02

Stress_EigVec1 = 9.9999999717E-01 7.0726406099E-05 2.5687816413E-05

Stress_EigVec2 = -6.1845255478E-05 5.7806072808E-01 8.1599374436E-01

Stress_EigVec3 = -4.2863187079E-05 8.1599374364E-01 -5.7806073082E-01

-DivStress = 3.2854220557E-07 -3.2282784414E-03 3.6369131918E-03

BPL = 2.8994476267E+00 = 1.4514750059E+00 + 1.4479726208E+00

GBL_I = 2.8994128363E+00

GBL_II = 2.8994132065E+00

GBL_III = 2.8994238018E+00 = 1.4514723141E+00 + 1.4479514878E+00

GBL_IV = 2.8994241747E+00 = 1.4514725029E+00 + 1.4479516718E+00

CP# 40 Coords = 1.18467090151380E+00 2.36841111578838E+00 -7.39560731675852E-01

Type = (3,-1) BCP C8 C14

Rho = 2.3859964965E-01

GradRho = -6.9388939039E-18 0.0000000000E+00 -4.8572257327E-17

HessRho_EigVals = -4.3507836904E-01 -4.3367878807E-01 3.4491698328E-01

HessRho_EigVec1 = 5.0620322844E-01 4.5468425966E-01 -7.3281683628E-01

HessRho_EigVec2 = -2.6190404546E-01 8.9064470077E-01 3.7169649979E-01

HessRho_EigVec3 = 8.2168397970E-01 3.7737258120E-03 5.6993086993E-01

DelSqRho = -5.2384017383E-01

Bond Ellipticity = 3.2272294725E-03

V = -2.4336518444E-01

G = 5.6202570491E-02

K = 1.8716261395E-01

L = 1.3096004346E-01

Vnuc = 2.1869014168E+01

Ven = -5.2179391187E+00

Vrep = 4.9745739343E+00

DelSqV = -1.6228991531E+00

DelSqVen = 1.1455868183E+01

DelSqVrep = -1.3078767336E+01

DelSqG = 1.0866310737E+00

DelSqK = 5.3626807943E-01

Stress_EigVals = -1.5793670109E-01 -1.5761987933E-01 7.2191395983E-02

Stress_EigVec1 = -4.1963470165E-01 6.8013660814E-01 6.0109975165E-01

Stress_EigVec2 = -3.8508373009E-01 -7.3307560776E-01 5.6063417139E-01

Stress_EigVec3 = 8.2195938950E-01 3.7878187284E-03 5.6953350598E-01

-DivStress = -7.8672209238E-03 2.4463182856E-04 -6.4786212828E-03

BPL = 2.9042029070E+00 = 1.4577044612E+00 + 1.4464984458E+00

GBL_I = 2.9040684718E+00

GBL_II = 2.9040685785E+00

GBL_III = 2.9041243112E+00 = 1.4576583600E+00 + 1.4464659512E+00

GBL_IV = 2.9041244271E+00 = 1.4576582195E+00 + 1.4464662075E+00

CP# 41 Coords = -1.21313039033698E+00 -7.01436946770473E-06 -7.24658144993906E-01

Type = (3,+1) RCP C4 C11 C14 C16 C22 C19

Rho = 1.9767821176E-02

GradRho = 1.7780915629E-17 1.9489960110E-17 -1.4311468677E-17

HessRho_EigVals = -1.6036691003E-02 6.5364821169E-02 6.8546924731E-02

HessRho_EigVec1 = 8.0488944302E-01 1.3117466163E-06 5.9342479264E-01

HessRho_EigVec2 = -5.9342479103E-01 -7.1812221385E-05 8.0488944100E-01

HessRho_EigVec3 = -4.3670963585E-05 9.9999999742E-01 5.7022475911E-05

DelSqRho = 1.1787505490E-01

Bond Ellipticity = NA

V = -1.9128263699E-02

G = 2.4298513711E-02

K = -5.1702500129E-03

L = -2.9468763724E-02

Vnuc = 2.1192523123E+01

Ven = -4.1893000736E-01

Vrep = 3.9980174366E-01

DelSqV = -1.2020801862E-01

DelSqVen = -2.4980698266E+00

DelSqVrep = 2.3778618080E+00

DelSqG = 9.3204634351E-02

DelSqK = 2.7003384272E-02

Stress_EigVals = -7.0085976569E-03 -6.0838178387E-03 -6.0358482029E-03

Stress_EigVec1 = 7.8662302052E-01 -3.8569003633E-06 6.1743357827E-01

Stress_EigVec2 = -6.1743357333E-01 -1.3156826462E-04 7.8662301341E-01

Stress_EigVec3 = -7.8200737823E-05 9.9999999134E-01 1.0587600549E-04

-DivStress = 2.1457076866E-04 4.0857423757E-09 1.0058106391E-04

CP# 42 Coords = -6.05506750814247E-05 1.18344668587502E+00 -2.40149743440278E+00

Type = (3,-1) BCP C14 C11

Rho = 2.3955684072E-01

GradRho = -3.5826317295E-18 -1.1579279202E-16 -1.0755285551E-16

HessRho_EigVals = -4.3679063070E-01 -4.3641936067E-01 3.4453917042E-01

HessRho_EigVec1 = 9.9999999687E-01 7.4296311213E-05 -2.7145778062E-05

HessRho_EigVec2 = 6.5098758900E-05 -5.7806424870E-01 8.1599125003E-01

HessRho_EigVec3 = -4.4933136059E-05 8.1599124925E-01 5.7806425173E-01

DelSqRho = -5.2867082095E-01

Bond Ellipticity = 8.5071852539E-04

V = -2.4562459645E-01

G = 5.6728445604E-02

K = 1.8889615084E-01

L = 1.3216770524E-01

Vnuc = 2.1980325015E+01

Ven = -5.2655372186E+00

Vrep = 5.0199126222E+00

DelSqV = -1.6332859287E+00

DelSqVen = 1.1620356471E+01

DelSqVrep = -1.3253642399E+01

DelSqG = 1.0972419430E+00

DelSqK = 5.3604398566E-01

Stress_EigVals = -1.5895726159E-01 -1.5879104958E-01 7.2123714726E-02
Stress_EigVec1 = 9.9999999885E-01 4.6167262995E-05 1.2758756418E-05
Stress_EigVec2 = 1.6282969779E-05 -5.7817943650E-01 8.1590963896E-01
Stress_EigVec3 = -4.5045165479E-05 8.1590963782E-01 5.7817943658E-01
-DivStress = -3.4760967561E-07 3.2290344911E-03 3.6381876605E-03
BPL = 2.8994489865E+00 = 1.4479722514E+00 + 1.4514767351E+00
GBL_I = 2.8994141926E+00
GBL_II = 2.8994145629E+00
GBL_III = 2.8994251600E+00 = 1.4479511170E+00 + 1.4514740429E+00
GBL_IV = 2.8994255328E+00 = 1.4479513011E+00 + 1.4514742318E+00

CP# 43 Coords = -1.05367127282525E+00 2.41037764876051E-04 -4.01083409290742E+00

Type = (3,-1) BCP C11 H12
Rho = 2.7175077658E-01
GradRho = -4.1633363423E-17 5.0821976835E-20 1.2490009027E-16
HessRho_EigVals = -6.8408919409E-01 -6.8394328579E-01 4.7378713305E-01
HessRho_EigVec1 = -5.9904765861E-01 -1.9646619549E-04 8.0071334703E-01
HessRho_EigVec2 = -1.1560057635E-04 9.9999998070E-01 1.5887825222E-04
HessRho_EigVec3 = 8.0071336279E-01 -2.6127205844E-06 5.9904766976E-01
DelSqRho = -8.9424534683E-01
Bond Ellipticity = 2.1333391845E-04
V = -3.1143968554E-01
G = 4.3939174416E-02
K = 2.6750051112E-01
L = 2.2356133671E-01
Vnuc = 1.8771919476E+01
Ven = -5.1012836954E+00
Vrep = 4.7898440099E+00
DelSqV = -2.3064592055E+00
DelSqVen = 1.6786701643E+01
DelSqVrep = -1.9093160848E+01
DelSqG = 1.6589332872E+00

DelSqK = 6.4752591828E-01

Stress_EigVals = -2.1077975750E-01 -2.1055080604E-01 1.0989087800E-01

Stress_EigVec1 = -9.9618054340E-05 9.9999998553E-01 1.3789540503E-04

Stress_EigVec2 = -5.9790701760E-01 -1.7009452851E-04 8.0156544921E-01

Stress_EigVec3 = 8.0156546107E-01 -2.5982398860E-06 5.9790702590E-01

-DivStress = 1.4528279377E-01 -5.2605016089E-08 1.0371752748E-01

BPL = 2.0447962705E+00 = 1.3043270140E+00 + 7.4046925645E-01

GBL_I = 2.0446695046E+00

GBL_II = 2.0704784586E+00

GBL_III = 2.0446990643E+00 = 1.3042298438E+00 + 7.4046922054E-01

GBL_IV = 2.0705086259E+00 = 1.3042296516E+00 + 7.6627897427E-01

CP# 44 Coords = 1.05368157041197E+00 3.48331805516285E-04 -4.01083099892901E+00

Type = (3,-1) BCP H13 C11

Rho = 2.7175085709E-01

GradRho = -4.1633363423E-17 -2.6202964223E-18 6.9388939039E-18

HessRho_EigVals = -6.8408949066E-01 -6.8394359696E-01 4.7378720250E-01

HessRho_EigVec1 = 5.9904542031E-01 1.5976150504E-04 8.0071502976E-01

HessRho_EigVec2 = -1.6302719170E-04 9.9999998370E-01 -7.7556693139E-05

HessRho_EigVec3 = 8.0071502910E-01 8.4078340818E-05 -5.9904543659E-01

DelSqRho = -8.9424588512E-01

Bond Ellipticity = 2.1331248122E-04

V = -3.1143984163E-01

G = 4.3939185173E-02

K = 2.6750065645E-01

L = 2.2356147128E-01

Vnuc = 1.8771920803E+01

Ven = -5.1012855674E+00

Vrep = 4.7898457258E+00

DelSqV = -2.3064607418E+00

DelSqVen = 1.6786712934E+01

DelSqVrep = -1.9093173676E+01

DelSqG = 1.6589342014E+00

DelSqK = 6.4752654042E-01

Stress_EigVals = -2.1077984365E-01 -2.1055089886E-01 1.0989090089E-01

Stress_EigVec1 = -6.8923505505E-05 9.9999999648E-01 4.7838829881E-05

Stress_EigVec2 = 5.9790480624E-01 2.8636622784E-06 8.0156711676E-01

Stress_EigVec3 = 8.0156711380E-01 8.3849881895E-05 -5.9790480434E-01

-DivStress = -1.4528315605E-01 -1.4994825049E-05 1.0371714198E-01

BPL = 2.0447960103E+00 = 7.4046916452E-01 + 1.3043268457E+00

GBL_I = 2.0446692435E+00

GBL_II = 2.0704782048E+00

GBL_III = 2.0446988035E+00 = 7.4046912862E-01 + 1.3042296749E+00

GBL_IV = 2.0705083725E+00 = 7.6627888974E-01 + 1.3042294827E+00

CP# 45 Coords = -1.77663140032330E-04 3.43257107425893E+00 -2.32222300224003E+00

Type = (3,-1) BCP H15 C14

Rho = 2.7397549539E-01

GradRho = -2.8375603733E-19 4.1633363423E-17 -3.2959746044E-17

HessRho_EigVals = -6.9365040819E-01 -6.9351104279E-01 4.7913587540E-01

HessRho_EigVec1 = 9.9999998327E-01 -7.1140384489E-05 -1.6854952785E-04

HessRho_EigVec2 = 1.7867054702E-04 5.7781761304E-01 8.1616589866E-01

HessRho_EigVec3 = -3.9328530026E-05 8.1616591512E-01 -5.7781761608E-01

DelSqRho = -9.0802557557E-01

Bond Ellipticity = 2.0095628209E-04

V = -3.1400259034E-01

G = 4.3498098225E-02

K = 2.7050449212E-01

L = 2.2700639389E-01

Vnuc = 1.8960114066E+01

Ven = -5.1946066439E+00

Vrep = 4.8806040536E+00

DelSqV = -2.3388095820E+00

DelSqVen = 1.7216268488E+01

DelSqVrep = -1.9555078070E+01

DelSqG = 1.6741974419E+00

DelSqK = 6.6461214011E-01

Stress_EigVals = -2.1265945988E-01 -2.1248153584E-01 1.1113840538E-01

Stress_EigVec1 = -3.0968564823E-05 5.7773912161E-01 8.1622148122E-01

Stress_EigVec2 = 9.9999999875E-01 4.9905652217E-05 2.6170802392E-06

Stress_EigVec3 = -3.9222075735E-05 8.1622148028E-01 -5.7773912244E-01

-DivStress = 7.1438222804E-06 -1.4632079132E-01 1.0358232827E-01

BPL = 2.0427097066E+00 = 7.3911748841E-01 + 1.3035922182E+00

GBL_I = 2.0427095776E+00

GBL_II = 2.0685583588E+00

GBL_III = 2.0427096441E+00 = 7.3911747919E-01 + 1.3035921649E+00

GBL_IV = 2.0685584340E+00 = 7.6496696695E-01 + 1.3035914671E+00

CP# 46 Coords = -1.18493014552174E+00 2.36828461827350E+00 -7.39571102015328E-01

Type = (3,-1) BCP C14 C16

Rho = 2.3860006937E-01

GradRho = 1.2836953722E-16 6.5919492087E-17 -1.3530843113E-16

HessRho_EigVals = -4.3507951366E-01 -4.3367985084E-01 3.4491704911E-01

HessRho_EigVec1 = -5.0624630952E-01 4.5462850630E-01 -7.3282166681E-01

HessRho_EigVec2 = 2.6180469893E-01 8.9067352984E-01 3.7169740765E-01

HessRho_EigVec3 = 8.2168909796E-01 -3.6857149642E-03 -5.6992406669E-01

DelSqRho = -5.2384231539E-01

Bond Ellipticity = 3.2274103089E-03

V = -2.4336597456E-01

G = 5.6202697857E-02

K = 1.8716327670E-01

L = 1.3096057885E-01

Vnuc = 2.1869014447E+01

Ven = -5.2179483641E+00

Vrep = 4.9745823896E+00

DelSqV = -1.6229021338E+00

DelSqVen = 1.1455915163E+01
DelSqVrep = -1.3078817297E+01
DelSqG = 1.0866342041E+00
DelSqK = 5.3626792974E-01
Stress_EigVals = -1.5793712488E-01 -1.5762027295E-01 7.2191423271E-02
Stress_EigVec1 = 4.1954833638E-01 6.8019755079E-01 6.0109107907E-01
Stress_EigVec2 = 3.8516680820E-01 -7.3301951177E-01 5.6065044834E-01
Stress_EigVec3 = 8.2196455112E-01 -3.6996305308E-03 -5.6952663628E-01
-DivStress = 7.8668347297E-03 2.4532941182E-04 -6.4780512799E-03
BPL = 2.9042012287E+00 = 1.4464980402E+00 + 1.4577031885E+00
GBL_I = 2.9040668101E+00
GBL_II = 2.9040669168E+00
GBL_III = 2.9041226404E+00 = 1.4464655474E+00 + 1.4576570930E+00
GBL_IV = 2.9041227562E+00 = 1.4464658038E+00 + 1.4576569525E+00

CP# 47 Coords = -2.40823028415854E+00 3.46314621985840E+00 8.12995496579383E-01

Type = (3,-1) BCP H17 C16
Rho = 2.7196378105E-01
GradRho = 8.5435131192E-17 -1.2143064332E-17 -3.6429192996E-17
HessRho_EigVals = -6.8612361951E-01 -6.8341520875E-01 4.7348809792E-01
HessRho_EigVec1 = -2.0089193732E-01 -5.4684709293E-01 8.1277345336E-01
HessRho_EigVec2 = 9.7921486128E-01 -8.8433233866E-02 1.8253169202E-01
HessRho_EigVec3 = -2.7940740270E-02 8.3254898961E-01 5.5324632392E-01
DelSqRho = -8.9605073034E-01
Bond Ellipticity = 3.9630531052E-03
V = -3.1180962963E-01
G = 4.3898473522E-02
K = 2.6791115611E-01
L = 2.2401268259E-01
Vnuc = 1.8552433146E+01
Ven = -5.0455898660E+00
Vrep = 4.7337802364E+00

DelSqV = -2.2946066046E+00

DelSqVen = 1.6623921270E+01

DelSqVrep = -1.8918527874E+01

DelSqG = 1.6537819372E+00

DelSqK = 6.4082466744E-01

Stress_EigVals = -2.1101145644E-01 -2.1065960594E-01 1.0986143276E-01

Stress_EigVec1 = 9.9196385766E-01 -4.6221781634E-02 1.1777627942E-01

Stress_EigVec2 = -1.2366765439E-01 -5.5081683812E-01 8.2541330381E-01

Stress_EigVec3 = -2.6721084347E-02 8.3334528123E-01 5.5210653492E-01

-DivStress = 1.4466730475E-03 -1.4859736264E-01 -1.0070705178E-01

BPL = 2.0452423677E+00 = 7.4082598070E-01 + 1.3044163870E+00

GBL_I = 2.0451243023E+00

GBL_II = 2.0709340443E+00

GBL_III = 2.0451650895E+00 = 7.4082562363E-01 + 1.3043394659E+00

GBL_IV = 2.0709765795E+00 = 7.6663721284E-01 + 1.3043393667E+00

CP# 48 Coords = -3.44987844189143E+00 2.40268901206001E+00 -6.75491881823001E-01

Type = (3,-1) BCP C16 H18

Rho = 2.7103063500E-01

GradRho = -9.0205620751E-17 -6.7654215563E-17 -6.9388939039E-18

HessRho_EigVals = -6.8396573189E-01 -6.8248750401E-01 4.7725833945E-01

HessRho_EigVec1 = 5.2150669053E-01 4.7253041243E-01 -7.1045462984E-01

HessRho_EigVec2 = -2.5340691116E-01 8.8085370414E-01 3.9985208426E-01

HessRho_EigVec3 = 8.1474886260E-01 -2.8491423893E-02 5.7911357233E-01

DelSqRho = -8.8919489645E-01

Bond Ellipticity = 2.1659413107E-03

V = -3.0936433320E-01

G = 4.3532804542E-02

K = 2.6583152865E-01

L = 2.2229872411E-01

Vnuc = 1.8637890844E+01

Ven = -5.0514393905E+00

Vrep = 4.7420750573E+00
DelSqV = -2.3257409278E+00
DelSqVen = 1.6572717419E+01
DelSqVrep = -1.8898458347E+01
DelSqG = 1.6482763854E+00
DelSqK = 6.7746454238E-01
Stress_EigVals = -2.1004717102E-01 -2.0974110936E-01 1.1042394718E-01
Stress_EigVec1 = 3.9958548126E-03 9.9916764120E-01 4.0596279776E-02
Stress_EigVec2 = -5.7967269883E-01 -3.0765588183E-02 8.1426840834E-01
Stress_EigVec3 = 8.1483961328E-01 -2.6786253399E-02 5.7906726833E-01
-DivStress = 1.3998427873E-01 -7.9521942924E-04 1.0078247901E-01
BPL = 2.0473893180E+00 = 1.3081934722E+00 + 7.3919584585E-01
GBL_I = 2.0472465869E+00
GBL_II = 2.0730097400E+00
GBL_III = 2.0472713368E+00 = 1.3080760600E+00 + 7.3919527674E-01
GBL_IV = 2.0730347129E+00 = 1.3080754874E+00 + 7.6495922545E-01

CP# 49 Coords = -1.18466975004686E+00 -2.36829383838785E+00 -7.39909335339875E-01

Type = (3,-1) BCP C4 C19
Rho = 2.3859988519E-01
GradRho = 3.2959746044E-17 1.0408340856E-17 8.6736173799E-18
HessRho_EigVals = -4.3507888989E-01 -4.3367925574E-01 3.4491696059E-01
HessRho_EigVec1 = 5.0619948251E-01 4.5458489268E-01 7.3288106760E-01
HessRho_EigVec2 = 2.6190611809E-01 -8.9069507237E-01 3.7157431741E-01
HessRho_EigVec3 = 8.2168562675E-01 3.8553082476E-03 -5.6992794930E-01
DelSqRho = -5.2384118505E-01
Bond Ellipticity = 3.2273486134E-03
V = -2.4336562997E-01
G = 5.6202666856E-02
K = 1.8716296312E-01
L = 1.3096029626E-01
Vnuc = 2.1869023709E+01

Ven = -5.2179465462E+00
Vrep = 4.9745809163E+00
DelSqV = -1.6229002930E+00
DelSqVen = 1.1455895296E+01
DelSqVrep = -1.3078795589E+01
DelSqG = 1.0866321234E+00
DelSqK = 5.3626816963E-01
Stress_EigVals = -1.5793693066E-01 -1.5762009965E-01 7.2191400346E-02
Stress_EigVec1 = -4.1961279734E-01 6.8026095604E-01 -6.0097431891E-01
Stress_EigVec2 = 3.8510392915E-01 7.3295979380E-01 5.6077170437E-01
Stress_EigVec3 = 8.2196110860E-01 3.8694120070E-03 -5.6953047644E-01
-DivStress = 7.8680339446E-03 -2.4374097328E-04 -6.4793425778E-03
BPL = 2.9042019760E+00 = 1.4464972399E+00 + 1.4577047362E+00
GBL_I = 2.9040675265E+00
GBL_II = 2.9040676331E+00
GBL_III = 2.9041233717E+00 = 1.4464647447E+00 + 1.4576586270E+00
GBL_IV = 2.9041234875E+00 = 1.4464650010E+00 + 1.4576584865E+00

CP# 50 Coords = -2.42601580277653E+00 1.17512943709038E+00 9.39636814059142E-01

Type = (3,-1) BCP C16 C22
Rho = 2.2575332906E-01
GradRho = -2.2551405188E-17 -8.3266726847E-17 9.5409791179E-18
HessRho_EigVals = -4.0300094117E-01 -3.8791883383E-01 3.3441260728E-01
HessRho_EigVec1 = 6.3761654362E-01 -4.6412470849E-01 -6.1484420650E-01
HessRho_EigVec2 = 7.6976949356E-01 3.5277836482E-01 5.3197965384E-01
HessRho_EigVec3 = 3.0001167974E-02 8.1248734161E-01 -5.8220636345E-01
DelSqRho = -4.5650716772E-01
Bond Ellipticity = 3.8879543940E-02
V = -2.2672988272E-01
G = 5.6301545394E-02
K = 1.7042833732E-01
L = 1.1412679193E-01

Vnuc = 2.1599791363E+01
Ven = -4.8762248071E+00
Vrep = 4.6494949244E+00
DelSqV = -1.5633978443E+00
DelSqVen = 9.8604595782E+00
DelSqVrep = -1.1423857422E+01
DelSqG = 1.0212967640E+00
DelSqK = 5.4210108034E-01
Stress_EigVals = -1.4899934439E-01 -1.4725378134E-01 6.9523243016E-02
Stress_EigVec1 = 9.1625497517E-01 2.0516908614E-01 3.4406753200E-01
Stress_EigVec2 = -3.9911740475E-01 5.4125368569E-01 7.4010117210E-01
Stress_EigVec3 = 3.4381938694E-02 8.1544472150E-01 -5.7781293554E-01
-DivStress = 5.0082971457E-04 -1.1706602537E-02 1.0311814612E-02
BPL = 2.9319265596E+00 = 1.4778369307E+00 + 1.4540896289E+00
GBL_I = 2.9316561265E+00
GBL_II = 2.9316584999E+00
GBL_III = 2.9317224441E+00 = 1.4777621243E+00 + 1.4539603198E+00
GBL_IV = 2.9317248267E+00 = 1.4777629085E+00 + 1.4539619182E+00

CP# 51 Coords = -2.42588527075056E+00 -1.17550363020721E+00 9.39473270974235E-01

Type = (3,-1) BCP C22 C19
Rho = 2.2575043647E-01
GradRho = -9.5843472048E-17 1.0408340856E-17 5.9847959921E-17
HessRho_EigVals = -4.0299355842E-01 -3.8791012738E-01 3.3441112895E-01
HessRho_EigVec1 = 6.3755261941E-01 4.6428623795E-01 -6.1478853823E-01
HessRho_EigVec2 = 7.6981893506E-01 -3.5275948265E-01 5.3192062812E-01
HessRho_EigVec3 = -3.0090940629E-02 8.1240324756E-01 5.8231906945E-01
DelSqRho = -4.5649255685E-01
Bond Ellipticity = 3.8883828945E-02
V = -2.2672575373E-01
G = 5.6301307258E-02
K = 1.7042444647E-01

L = 1.1412313921E-01
Vnuc = 2.1599785974E+01
Ven = -4.8761611114E+00
Vrep = 4.6494353576E+00
DelSqV = -1.5633770401E+00
DelSqVen = 9.8601415267E+00
DelSqVrep = -1.1423518567E+01
DelSqG = 1.0212782958E+00
DelSqK = 5.4209874436E-01
Stress_EigVals = -1.4899690257E-01 -1.4725141254E-01 6.9522561374E-02
Stress_EigVec1 = 9.1627572149E-01 -2.0511631910E-01 3.4404374408E-01
Stress_EigVec2 = -3.9906183675E-01 -5.4139935441E-01 7.4002458708E-01
Stress_EigVec3 = -3.4473941590E-02 8.1536129089E-01 5.7792517913E-01
-DivStress = 4.9978157357E-04 1.1706796708E-02 1.0314811596E-02
BPL = 2.9319364389E+00 = 1.4540930833E+00 + 1.4778433557E+00
GBL_I = 2.9316660194E+00
GBL_II = 2.9316683930E+00
GBL_III = 2.9317323301E+00 = 1.4539637963E+00 + 1.4777685338E+00
GBL_IV = 2.9317347130E+00 = 1.4539653949E+00 + 1.4777693181E+00

CP# 52 Coords = -2.40784663976122E+00 -3.46350666359338E+00 8.12511215031243E-01

Type = (3,-1) BCP C19 H2O
Rho = 2.7196380747E-01
GradRho = -3.2742905609E-17 -1.5612511284E-17 -4.5102810375E-17
HessRho_EigVals = -6.8612399691E-01 -6.8341518651E-01 4.7348834016E-01
HessRho_EigVec1 = -2.0102560498E-01 5.4670539293E-01 8.1283572725E-01
HessRho_EigVec2 = 9.7919004234E-01 8.8556757138E-02 1.8260493353E-01
HessRho_EigVec3 = 2.7849005844E-02 8.3262891741E-01 -5.5313065252E-01
DelSqRho = -8.9605084325E-01
Bond Ellipticity = 3.9636379921E-03
V = -3.1180964105E-01
G = 4.3898465117E-02

K = 2.6791117593E-01
L = 2.2401271081E-01
Vnuc = 1.8552453012E+01
Ven = -5.0455957590E+00
Vrep = 4.7337861180E+00
DelSqV = -2.2946101611E+00
DelSqVen = 1.6623941166E+01
DelSqVrep = -1.8918551327E+01
DelSqG = 1.6537813422E+00
DelSqK = 6.4082881890E-01
Stress_EigVals = -2.1101152172E-01 -2.1065962035E-01 1.0986150102E-01
Stress_EigVec1 = 9.9196179288E-01 4.6301114478E-02 1.1776250791E-01
Stress_EigVec2 = -1.2370399590E-01 5.5068964815E-01 8.2549272124E-01
Stress_EigVec3 = 2.6629361060E-02 8.3342493256E-01 -5.5199072357E-01
-DivStress = 1.4301720915E-03 1.4861115782E-01 -1.0068604909E-01
BPL = 2.0452422466E+00 = 1.3044165425E+00 + 7.4082570410E-01
GBL_I = 2.0451241774E+00
GBL_II = 2.0709339372E+00
GBL_III = 2.0451649682E+00 = 1.3043396213E+00 + 7.4082534688E-01
GBL_IV = 2.0709764763E+00 = 1.3043395222E+00 + 7.6663695415E-01

CP# 53 Coords = -3.44961534038349E+00 -2.40295606878842E+00 -6.75825782412690E-01

Type = (3,-1) BCP C19 H21
Rho = 2.7103054677E-01
GradRho = -3.1225022568E-17 -1.4398204851E-16 -6.9388939039E-18
HessRho_EigVals = -6.8396598245E-01 -6.8248765827E-01 4.7725942574E-01
HessRho_EigVec1 = -5.2157782175E-01 4.7229980664E-01 7.1055574623E-01
HessRho_EigVec2 = -2.5326523526E-01 -8.8097709812E-01 3.9966995535E-01
HessRho_EigVec3 = 8.1474738200E-01 2.8499916498E-02 5.7911523749E-01
DelSqRho = -8.8919421497E-01
Bond Ellipticity = 2.1660819278E-03
V = -3.0936395805E-01

G = 4.3532702152E-02
K = 2.6583125590E-01
L = 2.2229855374E-01
Vnuc = 1.8637895985E+01
Ven = -5.0514391394E+00
Vrep = 4.7420751813E+00
DelSqV = -2.3257532003E+00
DelSqVen = 1.6572709289E+01
DelSqVrep = -1.8898462489E+01
DelSqG = 1.6482756087E+00
DelSqK = 6.7747759156E-01
Stress_EigVals = -2.1004713659E-01 -2.0974105336E-01 1.1042423191E-01
Stress_EigVec1 = -4.0894912658E-03 9.9917201906E-01 -4.0479036509E-02
Stress_EigVec2 = -5.7967381780E-01 3.0615775217E-02 8.1427325835E-01
Stress_EigVec3 = 8.1483835269E-01 2.6794601012E-02 5.7906865598E-01
-DivStress = 1.3998290093E-01 7.9638977302E-04 1.0078077429E-01
BPL = 2.0473894068E+00 = 1.3081943363E+00 + 7.3919507051E-01
GBL_I = 2.0472466719E+00
GBL_II = 2.0730098524E+00
GBL_III = 2.0472714203E+00 = 1.3080769191E+00 + 7.3919450126E-01
GBL_IV = 2.0730348238E+00 = 1.3080763464E+00 + 7.6495847738E-01

CP# 54 Coords = 8.32970448766861E-01 -1.92333242500408E-04 2.90573178667789E+00

Type = (3,-1) BCP C6 B24
Rho = 1.8601843399E-01
GradRho = -3.7990444124E-14 -4.3833955020E-19 2.5153490402E-14
HessRho_EigVals = -3.9981741571E-01 -3.0242097908E-01 4.4128687571E-01
HessRho_EigVec1 = -4.1802252035E-05 9.9999999201E-01 1.1932602971E-04
HessRho_EigVec2 = 5.4525202712E-01 -7.7234927109E-05 8.3827216401E-01
HessRho_EigVec3 = 8.3827216653E-01 1.0010442386E-04 -5.4525201953E-01
DelSqRho = -2.6095151908E-01
Bond Ellipticity = 3.2205582077E-01

V = -3.2351472103E-01

G = 1.2913842063E-01

K = 1.9437630040E-01

L = 6.5237879770E-02

Vnuc = 2.1371106442E+01

Ven = -3.9754197531E+00

Vrep = 3.6519050321E+00

DelSqV = -3.3816221943E+00

DelSqVen = 5.5768226906E+00

DelSqVrep = -8.9584448849E+00

DelSqG = 5.4205960853E+00

DelSqK = -2.0389738910E+00

Stress_EigVals = -1.4622752129E-01 -1.1819194613E-01 -5.9095253603E-02

Stress_EigVec1 = 5.6336641060E-01 -7.5261466588E-05 8.2620716636E-01

Stress_EigVec2 = -3.6649397523E-05 9.9999999259E-01 1.1608287784E-04

Stress_EigVec3 = 8.2620716897E-01 9.5677189098E-05 -5.6336640367E-01

-DivStress = -4.3932722730E-01 -5.3313284900E-05 2.8029346849E-01

BPL = 2.9709884837E+00 = 1.9810805405E+00 + 9.8990794318E-01

GBL_I = 2.9707152867E+00

GBL_II = 2.9707115413E+00

GBL_III = 2.9709197985E+00 = 1.9810139107E+00 + 9.8990588775E-01

GBL_IV = 2.9709160627E+00 = 1.9810110105E+00 + 9.8990505214E-01

CP# 55 Coords = -8.32978950931140E-01 -2.72684991450471E-04 2.90573047069888E+00

Type = (3,-1) BCP B24 C22

Rho = 1.8601860701E-01

GradRho = 3.8209019282E-14 -5.8529976655E-18 2.5257573810E-14

HessRho_EigVals = -3.9981806342E-01 -3.0242155628E-01 4.4128876989E-01

HessRho_EigVec1 = -5.4095126966E-05 9.9999999191E-01 1.1510458311E-04

HessRho_EigVec2 = -5.4525359185E-01 -1.2598441344E-04 8.3827114033E-01

HessRho_EigVec3 = 8.3827114805E-01 -1.7414803610E-05 5.4525359425E-01

DelSqRho = -2.6095084981E-01

Bond Ellipticity = 3.2205543923E-01

V = -3.2351538406E-01

G = 1.2913883580E-01

K = 1.9437654826E-01

L = 6.5237712451E-02

Vnuc = 2.1371108028E+01

Ven = -3.9754237458E+00

Vrep = 3.6519083617E+00

DelSqV = -3.3816326880E+00

DelSqVen = 5.5768088013E+00

DelSqVrep = -8.9584414893E+00

DelSqG = 5.4206136553E+00

DelSqK = -2.0389809672E+00

Stress_EigVals = -1.4622775879E-01 -1.1819216332E-01 -5.9095461951E-02

Stress_EigVec1 = -5.6336809602E-01 -1.2652452356E-04 8.2620601086E-01

Stress_EigVec2 = -6.1907202620E-05 9.9999999193E-01 1.1092630466E-04

Stress_EigVec3 = 8.2620601822E-01 -1.1344238137E-05 5.6336809931E-01

-DivStress = 4.3932778780E-01 -1.1081382143E-05 2.8029495999E-01

BPL = 2.9709872068E+00 = 9.8990749881E-01 + 1.9810797080E+00

GBL_I = 2.9707139959E+00

GBL_II = 2.9707102505E+00

GBL_III = 2.9709185162E+00 = 9.8990544341E-01 + 1.9810130728E+00

GBL_IV = 2.9709147804E+00 = 9.8990460778E-01 + 1.9810101726E+00

CP# 56 Coords = -3.57119665447210E+00 -3.58534214526134E-04 2.48468368149546E+00

Type = (3,-1) BCP C22 H23

Rho = 2.7238737725E-01

GradRho = -9.0205620751E-17 -4.1914366604E-18 5.5511151231E-17

HessRho_EigVals = -6.8953102476E-01 -6.7453967498E-01 4.7088170832E-01

HessRho_EigVec1 = -6.4124792951E-05 9.9999999619E-01 5.9182816429E-05

HessRho_EigVec2 = 5.4054924710E-01 -1.5128627318E-05 8.4131237435E-01

HessRho_EigVec3 = 8.4131237204E-01 8.5940208674E-05 -5.4054924407E-01

DelSqRho = -8.9318899142E-01

Bond Ellipticity = 2.2224563413E-02

V = -3.1489745639E-01

G = 4.5800104266E-02

K = 2.6909735212E-01

L = 2.2329724786E-01

Vnuc = 1.8554644022E+01

Ven = -5.0540508210E+00

Vrep = 4.7391533646E+00

DelSqV = -2.2982535542E+00

DelSqVen = 1.6572803780E+01

DelSqVrep = -1.8871057335E+01

DelSqG = 1.6666453882E+00

DelSqK = 6.3160816595E-01

Stress_EigVals = -2.1412245253E-01 -2.1029033744E-01 1.0951533358E-01

Stress_EigVec1 = 5.3867058366E-01 -4.2371392733E-05 8.4251646898E-01

Stress_EigVec2 = -4.9505629977E-05 9.9999999542E-01 8.1943346718E-05

Stress_EigVec3 = 8.4251646859E-01 8.5849778967E-05 -5.3867057910E-01

-DivStress = 1.5672745895E-01 1.5878588711E-05 -9.8694520194E-02

BPL = 2.0390775109E+00 = 1.2975222654E+00 + 7.4155524551E-01

GBL_I = 2.0389390500E+00

GBL_II = 2.0647525126E+00

GBL_III = 2.0389628901E+00 = 1.2974077605E+00 + 7.4155512959E-01

GBL_IV = 2.0647773999E+00 = 1.2974076220E+00 + 7.6736977785E-01

CP# 57 Coords = -5.35354641718587E-06 -4.15218634867063E-04 4.42973235927518E+00

Type = (3,-1) BCP H25 B24

Rho = 1.7863575018E-01

GradRho = 7.1329703279E-18 -2.2345787940E-19 -1.1093556629E-15

HessRho_EigVals = -4.2834369334E-01 -3.2148439722E-01 4.7670269734E-01

HessRho_EigVec1 = -4.5936879612E-05 9.9999999131E-01 1.2356078961E-04

HessRho_EigVec2 = 9.9999999894E-01 4.5936816597E-05 5.1282881603E-07

HessRho_EigVec3 = -5.0715282224E-07 -1.2356081304E-04 9.9999999237E-01

DelSqRho = -2.7312539322E-01

Bond Ellipticity = 3.3239341335E-01

V = -3.0758250791E-01

G = 1.1965057980E-01

K = 1.8793192811E-01

L = 6.8281348305E-02

Vnuc = 1.8325932762E+01

Ven = -3.2736667467E+00

Vrep = 2.9660842388E+00

DelSqV = -3.5041712473E+00

DelSqVen = 5.0052775917E+00

DelSqVrep = -8.5094488390E+00

DelSqG = 5.4742634913E+00

DelSqK = -1.9700922440E+00

Stress_EigVals = -1.4387785130E-01 -1.1191934002E-01 -5.1785316587E-02

Stress_EigVec1 = 9.9999999893E-01 4.6315973203E-05 4.1918195078E-07

Stress_EigVec2 = -4.6316025567E-05 9.9999999102E-01 1.2579332173E-04

Stress_EigVec3 = -4.1335570690E-07 -1.2579334101E-04 9.9999999209E-01

-DivStress = 2.0398689483E-07 5.8383187899E-05 -4.7438555488E-01

BPL = 2.2365757634E+00 = 1.2474262532E+00 + 9.8914951019E-01

GBL_I = 2.2365757634E+00

GBL_II = 2.2564966372E+00

GBL_III = 2.2365757634E+00 = 1.2474262532E+00 + 9.8914951019E-01

GBL_IV = 2.2564966372E+00 = 1.2673455805E+00 + 9.8915105676E-01

Number of NACPs = 25

Number of NNACPs = 0

Number of BCPs = 27

Number of RCPs = 4

Number of CCPs = 1

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H3	C1	H2	108.78289861	106.78285417	106.77054850	107.26635941	107.26639945
C4	C1	H2	110.23734741	109.74647750	109.75033213	109.92283331	109.92287490
C4	C1	H3	109.40270980	109.71314195	109.71666493	109.66416301	109.66417724
H5	C4	C1	109.82903216	109.01321291	109.01361778	109.34950314	109.34952770
C6	C1	H2	108.24253390	109.32333476	109.32295871	109.16205399	109.16203927
C6	C1	H3	111.23350130	110.52704983	110.53198998	110.75792774	110.75788513
C6	C1	C4	108.93230123	110.66701245	110.66700131	110.02305593	110.02301985
H7	C6	C1	109.52666683	109.68857212	109.69197031	109.88275665	109.88266682
C8	C6	C1	105.68151206	108.59686369	108.59677013	107.87095194	107.87077896
C8	C6	H7	109.52686381	109.68872433	109.69212245	109.88292855	109.88283872
H9	C8	C6	108.24242997	109.32312426	109.32274822	109.16185343	109.16183872
H10	C8	C6	111.23347889	110.52708740	110.53202729	110.75797772	110.75793512
H10	C8	H9	108.78287039	106.78283700	106.77053149	107.26633905	107.26637909
C11	C4	C1	108.90189819	109.40811746	109.40811053	109.24866686	109.24864231
C11	C4	H5	110.08830863	109.47280320	109.47198724	109.64158570	109.64161478
C14	C8	C6	108.93251091	110.66722717	110.66721603	110.02324354	110.02320746
C14	C8	H9	110.23728778	109.74644923	109.75030410	109.92279271	109.92283429
C14	C8	H10	109.40271150	109.71313496	109.71665774	109.66417905	109.66419328
C14	C11	C4	108.93798970	109.53275599	109.53277217	109.21796831	109.21794732
C11	C14	C8	108.90202080	109.40836418	109.40835724	109.24885038	109.24882583

H12	C11	C4	109.63130977	109.99139942	109.99382978	109.95696068	109.95696028
H12	C11	C14	109.63115433	109.99118723	109.99361709	109.95679551	109.95679511
H13	C11	C4	109.63113051	109.99118780	109.99361803	109.95678434	109.95678394
H13	C11	C14	109.63137096	109.99144252	109.99387257	109.95701549	109.95701509
H13	C11	H12	109.36447211	107.31663084	107.30678508	107.78091041	107.78093355
H15	C14	C8	109.82895999	109.01310202	109.01350667	109.34941325	109.34943781
H15	C14	C11	110.08821323	109.47270005	109.47188442	109.64149097	109.64152005
C16	C14	C8	109.26652659	110.50767650	110.50768772	109.98966242	109.98963342
C16	C14	C11	108.90196981	109.40825135	109.40824441	109.24877291	109.24874836
C16	C14	H15	109.82911358	109.01329976	109.01370465	109.34957843	109.34960299
H17	C16	C14	109.40266238	109.71307683	109.71659969	109.66411939	109.66413362
H18	C16	C14	110.23732957	109.74657172	109.75042667	109.92288488	109.92292646
H18	C16	H17	108.78283875	106.78278839	106.77048276	107.26629614	107.26633618
C19	C4	C1	109.26655312	110.50781132	110.50782254	109.98974116	109.98971216
C19	C4	H5	109.82897154	109.01311565	109.01352064	109.34943403	109.34945859
C19	C4	C11	108.90204023	109.40833450	109.40832756	109.24883802	109.24881347
C22	C16	C14	108.93246601	110.66711661	110.66710547	110.02315679	110.02312071
C22	C16	H17	111.23341382	110.52702106	110.53196078	110.75792167	110.75787907
C22	C16	H18	108.24258178	109.32329105	109.32291515	109.16201088	109.16199616
C22	C19	C4	108.93244142	110.66724742	110.66723628	110.02325448	110.02321840
C19	C22	C16	105.68151197	108.59682740	108.59673384	107.87091219	107.87073920
H20	C19	C4	109.40279118	109.71321646	109.71673950	109.66424460	109.66425883
H20	C19	C22	111.23353436	110.52708579	110.53202617	110.75795429	110.75791169
H21	C19	C4	110.23740747	109.74646528	109.75032013	109.92283956	109.92288115
H21	C19	C22	108.24231429	109.32309087	109.32271464	109.16182778	109.16181307
H21	C19	H20	108.78280129	106.78275035	106.77044428	107.26626307	107.26630311
B24	C6	C1	108.65199130	107.36243557	107.36246377	107.64671941	107.64679747
B24	C6	H7	114.43160779	113.98117487	113.97449102	113.71542527	113.71560907
B24	C6	C8	108.65273441	107.36340472	107.36343291	107.64752252	107.64760058
B24	C22	C16	108.65327755	107.36403287	107.36406106	107.64807536	107.64815342
B24	C22	C19	108.65131960	107.36173501	107.36176320	107.64609836	107.64617641
C22	B24	C6	114.86057808	112.68895354	112.68905911	114.59108886	114.59123951

H23	C22	C16	109.52685725	109.68872969	109.69212773	109.88293763	109.88284780
H23	C22	C19	109.52663017	109.68850505	109.69190311	109.88269896	109.88260913
H23	C22	B24	114.43176721	113.98133761	113.97465399	113.71557295	113.71575675
H25	B24	C6	122.56967940	123.65548544	123.65543262	122.70442665	122.70435133
H25	B24	C22	122.56974252	123.65556100	123.65550826	122.70448448	122.70440916

Total time for electron density critical point search, analysis and connectivity = 197 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7861425935E+01	3.7861425935E+01	-1.7968264382E+02	-8.9877032107E+01		
H2	-6.2605251616E-01	6.2605251616E-01	-1.5543285836E+01	-1.2949754722E+00		
H3	-6.2930234617E-01	6.2930234617E-01	-1.5509277283E+01	-1.3014208364E+00		
C4	-3.7863841906E+01	3.7863841906E+01	-1.8532377336E+02	-8.9850439949E+01		

H5	-6.3354705014E-01	6.3354705014E-01	-1.5592159097E+01	-1.3036231498E+00
C6	-3.8173850679E+01	3.8173850679E+01	-1.9507261987E+02	-9.1789407748E+01
H7	-6.3170901110E-01	6.3170901110E-01	-1.5257073844E+01	-1.3028167002E+00
C8	-3.7861383434E+01	3.7861383434E+01	-1.7968614820E+02	-8.9877424151E+01
H9	-6.2605287206E-01	6.2605287206E-01	-1.5543371149E+01	-1.2949791950E+00
H10	-6.2930204899E-01	6.2930204899E-01	-1.5509296296E+01	-1.3014211981E+00
C11	-3.7883067735E+01	3.7883067735E+01	-1.8077370164E+02	-8.9921618811E+01
H12	-6.2812140430E-01	6.2812140430E-01	-1.5708887892E+01	-1.2998823630E+00
H13	-6.2812078699E-01	6.2812078699E-01	-1.5708957083E+01	-1.2998844352E+00
C14	-3.7863788902E+01	3.7863788902E+01	-1.8532655508E+02	-8.9850907150E+01
H15	-6.3354763508E-01	6.3354763508E-01	-1.5592140796E+01	-1.3036229693E+00
C16	-3.7861409723E+01	3.7861409723E+01	-1.7968404109E+02	-8.9877125866E+01
H17	-6.2930191982E-01	6.2930191982E-01	-1.5509222825E+01	-1.3014186444E+00
H18	-6.2605386830E-01	6.2605386830E-01	-1.5543356766E+01	-1.2949795078E+00
C19	-3.7861430982E+01	3.7861430982E+01	-1.7968250424E+02	-8.9876921886E+01
H20	-6.2930127698E-01	6.2930127698E-01	-1.5509259691E+01	-1.3014188125E+00
H21	-6.2605219759E-01	6.2605219759E-01	-1.5543296991E+01	-1.2949754964E+00
C22	-3.8173891561E+01	3.8173891561E+01	-1.9506974514E+02	-9.1788995816E+01
H23	-6.3171031696E-01	6.3171031696E-01	-1.5257047093E+01	-1.3028163737E+00
B24	-2.3952751917E+01	2.3952751917E+01	-9.8433453737E+01	-5.2653025172E+01
H25	-8.2932808263E-01	8.2932808263E-01	-2.2776138849E+01	-1.6716814071E+00

Total	-3.7499434611E+02	3.7499434611E+02	-1.9988379577E+03	-8.8523281522E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
C1	-3.7861422351E+01	-3.7861425935E+01	3.5837395941E-06			
H2	-6.2605382871E-01	-6.2605251616E-01	-1.3125532183E-06			
H3	-6.2926322507E-01	-6.2930234617E-01	3.9121099131E-05			
C4	-3.7864205114E+01	-3.7863841906E+01	-3.6320772523E-04			
H5	-6.3348870371E-01	-6.3354705014E-01	5.8346426823E-05			
C6	-3.8173881097E+01	-3.8173850679E+01	-3.0418320645E-05			
H7	-6.3167690983E-01	-6.3170901110E-01	3.2101274708E-05			
C8	-3.7861380527E+01	-3.7861383434E+01	2.9072370112E-06			
H9	-6.2605413686E-01	-6.2605287206E-01	-1.2648028504E-06			
H10	-6.2926310807E-01	-6.2930204899E-01	3.8940918541E-05			
C11	-3.7882899273E+01	-3.7883067735E+01	1.6846178564E-04			
H12	-6.2810239084E-01	-6.2812140430E-01	1.9013458821E-05			
H13	-6.2810173099E-01	-6.2812078699E-01	1.9056001810E-05			
C14	-3.7864151701E+01	-3.7863788902E+01	-3.6279885697E-04			
H15	-6.3348931804E-01	-6.3354763508E-01	5.8317038963E-05			
C16	-3.7861406077E+01	-3.7861409723E+01	3.6460245681E-06			
H17	-6.2926296334E-01	-6.2930191982E-01	3.8956482975E-05			
H18	-6.2605518618E-01	-6.2605386830E-01	-1.3178816700E-06			
C19	-3.7861427575E+01	-3.7861430982E+01	3.4070254982E-06			
H20	-6.2926227254E-01	-6.2930127698E-01	3.9004439250E-05			
H21	-6.2605355804E-01	-6.2605219759E-01	-1.3604519160E-06			
C22	-3.8173921969E+01	-3.8173891561E+01	-3.0408433224E-05			
H23	-6.3167816645E-01	-6.3171031696E-01	3.2150508447E-05			

H25 -8.2930485005E-01 -8.2932808263E-01 2.3232576106E-05

IQA Atomic Energy Components:

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$$

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

H5 6.3354705014E-01 -7.8491835881E+00 -7.7960795484E+00
7.2821219512E+00

C6 4.6988606549E+01	3.8173850679E+01 -9.1371689702E+01 -9.7536309935E+01
H7 7.0994228508E+00	6.3170901110E-01 -7.6696076611E+00 -7.6285369220E+00
C8 4.5369811675E+01	3.7861383434E+01 -8.9693054713E+01 -8.9843074101E+01
H9 7.2629418431E+00	6.2605287206E-01 -7.8282808664E+00 -7.7716855743E+00
H10 7.2011835096E+00	6.2930204899E-01 -7.7660576575E+00 -7.7546481478E+00
C11 4.5930486565E+01	3.7883067735E+01 -9.0274055305E+01 -9.0386850821E+01
H12 7.3123676651E+00	6.2812140430E-01 -7.8782855025E+00 -7.8544439461E+00
H13 7.3123682832E+00	6.2812078699E-01 -7.8782861039E+00 -7.8544785413E+00
C14 4.8440691554E+01	3.7863788902E+01 -9.2752506620E+01 -9.2663277542E+01
H15 7.2821200493E+00	6.3354763508E-01 -7.8491820758E+00 -7.7960703979E+00
C16 4.5369799285E+01	3.7861409723E+01 -8.9693042981E+01 -8.9842020547E+01
H17 7.2011779713E+00	6.2930191982E-01 -7.7660522923E+00 -7.7546114126E+00
H18 7.2629409599E+00	6.2605386830E-01 -7.8282800292E+00 -7.7716783828E+00
C19 4.5369837780E+01	3.7861430982E+01 -8.9693076540E+01 -8.9841252121E+01
H20 7.2011890852E+00	6.2930127698E-01 -7.7660626821E+00 -7.7546298453E+00
H21 7.2629439791E+00	6.2605219759E-01 -7.8282823263E+00 -7.7716484957E+00
C22 4.6988600934E+01	3.8173891561E+01 -9.1371683988E+01 -9.7534872569E+01
H23 7.0994226099E+00	6.3171031696E-01 -7.6696073740E+00 -7.6285235463E+00
B24 3.7374250361E+01	2.3952751917E+01 -6.6060788026E+01 -4.9216726869E+01

H25 8.2932808263E-01 -6.8920606536E+00 -1.1388069424E+01
 6.3088427377E+00

 Total 3.7499434611E+02 -9.9941903449E+02 -9.9941897884E+02
 5.6319577110E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

C1	3.7861425935E+01	-8.9877032107E+01				
H2	6.2605251616E-01	-1.2949754722E+00				
H3	6.2930234617E-01	-1.3014208364E+00				
C4	3.7863841906E+01	-8.9850439949E+01				
H5	6.3354705014E-01	-1.3036231498E+00				
C6	3.8173850679E+01	-9.1789407748E+01				
H7	6.3170901110E-01	-1.3028167002E+00				
C8	3.7861383434E+01	-8.9877424151E+01				
H9	6.2605287206E-01	-1.2949791950E+00				
H10	6.2930204899E-01	-1.3014211981E+00				
C11	3.7883067735E+01	-8.9921618811E+01				
H12	6.2812140430E-01	-1.2998823630E+00				

H13	6.2812078699E-01 -1.2998844352E+00
C14	3.7863788902E+01 -8.9850907150E+01
H15	6.3354763508E-01 -1.3036229693E+00
C16	3.7861409723E+01 -8.9877125866E+01
H17	6.2930191982E-01 -1.3014186444E+00
H18	6.2605386830E-01 -1.2949795078E+00
C19	3.7861430982E+01 -8.9876921886E+01
H20	6.2930127698E-01 -1.3014188125E+00
H21	6.2605219759E-01 -1.2949754964E+00
C22	3.8173891561E+01 -9.1788995816E+01
H23	6.3171031696E-01 -1.3028163737E+00
B24	2.3952751917E+01 -5.2653025172E+01
H25	8.2932808263E-01 -1.6716814071E+00

Total 3.7499434611E+02 -8.8523281522E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A VeeX(A,A')	E_IQA_Inter(A)	Vne(A,A')/2	Ven(A,A')/2	Vee(A,A')	Vnn(A)	VeeC(A,A')
C1	-4.4754535614E+01	-4.4902805857E+01		4.5369812087E+01		
H2	-7.1807953275E+00	-7.1241551818E+00		7.2629446421E+00		
H3	-7.1153462127E+00	-7.1039282235E+00		7.2011828498E+00		
C4	-4.7827296470E+01	-4.7736666706E+01		4.8440703321E+01		
H5	-7.1973720132E+00	-7.1442679734E+00		7.2821219512E+00		
C6	-4.5476985828E+01	-5.1641606060E+01		4.6988606549E+01		
H7	-7.0181993110E+00	-6.9771285719E+00		7.0994228508E+00		
C8	-4.4754342638E+01	-4.4904362026E+01		4.5369811675E+01		
H9	-7.1807912689E+00	-7.1241959768E+00		7.2629418431E+00		
H10	-7.1153470584E+00	-7.1039375488E+00		7.2011835096E+00		
C11	-4.5313245900E+01	-4.5426041415E+01		4.5930486565E+01		
H12	-7.2283443210E+00	-7.2045027646E+00		7.3123676651E+00		
H13	-7.2283438862E+00	-7.2045363237E+00		7.3123682832E+00		
C14	-4.7827053045E+01	-4.7737823967E+01		4.8440691554E+01		
H15	-7.1973705912E+00	-7.1442589132E+00		7.2821200493E+00		
C16	-4.4754480048E+01	-4.4903457613E+01		4.5369799285E+01		
H17	-7.1153429701E+00	-7.1039020904E+00		7.2011779713E+00		
H18	-7.1807902753E+00	-7.1241886289E+00		7.2629409599E+00		
C19	-4.4754615597E+01	-4.4902791178E+01		4.5369837780E+01		
H20	-7.1153532758E+00	-7.1039204390E+00		7.2011890852E+00		
H21	-7.1807945781E+00	-7.1241607475E+00		7.2629439791E+00		
C22	-4.5477186080E+01	-5.1640374661E+01		4.6988600934E+01		
H23	-7.0181991871E+00	-6.9771153594E+00		7.0994226099E+00		
B24	-3.9734275440E+01	-2.2890214283E+01		3.7374250361E+01		
H25	-6.0562199500E+00	-1.0552228721E+01		6.3088427377E+00		
Total	-5.5680262689E+02	-5.5680257123E+02		5.6319577110E+02		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other

Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$
C1 3.4879635703E+01	5.9744352078E+00	3.8905739720E+00	6.5120364297E+01	2.0838612358E+00	
H2 5.5416126222E+01	1.0170228946E+00	4.5342820362E-01	4.4583873778E+01	5.6359469098E-01	
H3 5.5018142893E+01	1.0226817732E+00	4.6002125388E-01	4.4981857107E+01	5.6266051932E-01	
C4 3.5615393821E+01	5.9489354042E+00	3.8301986318E+00	6.4384606179E+01	2.1187367724E+00	
H5 5.4951077335E+01	1.0199275196E+00	4.5946635954E-01	4.5048922665E+01	5.6046116006E-01	
C6 3.0844618096E+01	6.6139224470E+00	4.5738833271E+00	6.9155381904E+01	2.0400391199E+00	
H7 5.5102572684E+01	1.0222276756E+00	4.5895392766E-01	4.4897427316E+01	5.6327374794E-01	
C8 3.4879856985E+01	5.9746303684E+00	3.8906878405E+00	6.5120143015E+01	2.0839425279E+00	

H9	1.0170289590E+00 5.5415982518E+01	4.5343236888E-01	4.4584017482E+01	5.6359659012E-01
H10	1.0226830792E+00 5.5018147978E+01	4.6002178934E-01	4.4981852022E+01	5.6266128986E-01
C11	5.9715233206E+00 3.4866169181E+01	3.8894818970E+00	6.5133830819E+01	2.0820414236E+00
H12	1.0212508126E+00 5.5204165948E+01	4.5747781927E-01	4.4795834052E+01	5.6377299333E-01
H13	1.0212556384E+00 5.5204180928E+01	4.5747982804E-01	4.4795819072E+01	5.6377581036E-01
C14	5.9491720656E+00 3.5614515632E+01	3.8304032503E+00	6.4385484368E+01	2.1187688153E+00
H15	1.0199261916E+00 5.4951049456E+01	4.5946604564E-01	4.5048950544E+01	5.6046014596E-01
C16	5.9744872268E+00 3.4880315479E+01	3.8905672338E+00	6.5119684521E+01	2.0839199930E+00
H17	1.0226787306E+00 5.5018214735E+01	4.6001915055E-01	4.4981785265E+01	5.6265958005E-01
H18	1.0170278292E+00 5.5415913154E+01	4.5343257062E-01	4.4584086846E+01	5.6359525858E-01
C19	5.9743844004E+00 3.4880351518E+01	3.8904981205E+00	6.5119648482E+01	2.0838862799E+00
H20	1.0226798378E+00 5.5018242625E+01	4.6001936336E-01	4.4981757375E+01	5.6266047444E-01
H21	1.0170237706E+00 5.5416138580E+01	4.5342846849E-01	4.4583861420E+01	5.6359530211E-01
C22	6.6136825008E+00 3.0843098545E+01	4.5738178896E+00	6.9156901455E+01	2.0398646112E+00
H23	1.0222253180E+00 5.5102559767E+01	4.5895300119E-01	4.4897440233E+01	5.6327231681E-01
B24	3.0826928164E+00 2.9348944497E+01	2.1779550127E+00	7.0651055503E+01	9.0473780370E-01
H25	1.6362916680E+00 2.6796652748E+01	1.1978202718E+00	7.3203347252E+01	4.3847139621E-01

Total	7.3999797456E+01 3.7781603220E+01	4.6041487597E+01	6.2218396780E+01	2.7958309859E+01

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$DI(A,A')/2$	$DI\_Bond(A,A')/2$	$DI\_NonBond(A,A')/2$
C1	5.9744352078E+00	3.8905739720E+00	2.0838612358E+00	1.9143184333E+00	1.6954280250E-01
H2	1.0170228946E+00	4.5342820362E-01	5.6359469098E-01	4.6705128361E-01	9.6543407360E-02
H3	1.0226817732E+00	4.6002125388E-01	5.6266051932E-01	4.7196998120E-01	9.0690538122E-02
C4	5.9489354042E+00	3.8301986318E+00	2.1187367724E+00	1.9088361416E+00	2.0990063079E-01
H5	1.0199275196E+00	4.5946635954E-01	5.6046116006E-01	4.6636033628E-01	9.4100823777E-02
C6	6.6139224470E+00	4.5738833271E+00	2.0400391199E+00	1.7415711215E+00	2.9846799842E-01
H7	1.0222276756E+00	4.5895392766E-01	5.6327374794E-01	4.8380876980E-01	7.9464978140E-02
C8	5.9746303684E+00	3.8906878405E+00	2.0839425279E+00	1.9144082411E+00	1.6953428680E-01

H9	1.0170289590E+00	4.5343236888E-01	5.6359659012E-01	4.6707677767E-01
9.6519812456E-02				
H10	1.0226830792E+00	4.6002178934E-01	5.6266128986E-01	4.7198667244E-01
9.0674617419E-02				
C11	5.9715233206E+00	3.8894818970E+00	2.0820414236E+00	1.9001071875E+00
1.8193423608E-01				
H12	1.0212508126E+00	4.5747781927E-01	5.6377299333E-01	4.6927568965E-01
9.4497303679E-02				
H13	1.0212556384E+00	4.5747982804E-01	5.6377581036E-01	4.6936969838E-01
9.4406111981E-02				
C14	5.9491720656E+00	3.8304032503E+00	2.1187688153E+00	1.9089592230E+00
2.0980959231E-01				
H15	1.0199261916E+00	4.5946604564E-01	5.6046014596E-01	4.6642243418E-01
9.4037711786E-02				
C16	5.9744872268E+00	3.8905672338E+00	2.0839199930E+00	1.9143030663E+00
1.6961692668E-01				
H17	1.0226787306E+00	4.6001915055E-01	5.6265958005E-01	4.7199026299E-01
9.0669317061E-02				
H18	1.0170278292E+00	4.5343257062E-01	5.6359525858E-01	4.6702239388E-01
9.6572864694E-02				
C19	5.9743844004E+00	3.8904981205E+00	2.0838862799E+00	1.9141825428E+00
1.6970373711E-01				
H20	1.0226798378E+00	4.6001936336E-01	5.6266047444E-01	4.7197320561E-01
9.0687268826E-02				
H21	1.0170237706E+00	4.5342846849E-01	5.6359530211E-01	4.6701290626E-01
9.6582395845E-02				
C22	6.6136825008E+00	4.5738178896E+00	2.0398646112E+00	1.7414236014E+00
2.9844100981E-01				
H23	1.0222253180E+00	4.5895300119E-01	5.6327231681E-01	4.8379436110E-01
7.9477955708E-02				
B24	3.0826928164E+00	2.1779550127E+00	9.0473780370E-01	8.2444185158E-01
8.0295952118E-02				
H25	1.6362916680E+00	1.1978202718E+00	4.3847139621E-01	2.8662826479E-01
1.5184313143E-01				

Total	7.3999797456E+01	4.6041487597E+01	2.7958309859E+01	2.4564294448E+01
3.3940154109E+00				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

C1	1.5901651040E+01	2.0216523404E+02	2.1806688508E+02
H2	2.9045368226E-01	3.6830881971E+01	3.7121335653E+01
H3	2.9292837768E-01	3.7034956344E+01	3.7327884722E+01
C4	1.5779816906E+01	2.0135632535E+02	2.1713614225E+02
H5	2.9039289285E-01	3.6936961573E+01	3.7227354465E+01
C6	1.9585043404E+01	2.2182312591E+02	2.4140816932E+02
H7	2.9299774655E-01	3.7018312413E+01	3.7311310159E+01
C8	1.5902760099E+01	2.0217124835E+02	2.1807400845E+02
H9	2.9045776728E-01	3.6831099236E+01	3.7121557004E+01
H10	2.9292944557E-01	3.7035002945E+01	3.7327932391E+01
C11	1.5884804436E+01	2.0207579677E+02	2.1796060120E+02
H12	2.9273770148E-01	3.6982916958E+01	3.7275654660E+01
H13	2.9274162546E-01	3.6983089176E+01	3.7275830802E+01
C14	1.5781122508E+01	2.0136365789E+02	2.1714478039E+02
H15	2.9039169534E-01	3.6936914298E+01	3.7227305993E+01
C16	1.5901965195E+01	2.0216681858E+02	2.1806878378E+02
H17	2.9292631773E-01	3.7034847349E+01	3.7327773667E+01
H18	2.9045651737E-01	3.6831059248E+01	3.7121515766E+01
C19	1.5901385422E+01	2.0216364519E+02	2.1806503061E+02

H20	2.9292734364E-01	3.7034886736E+01	3.7327814080E+01
H21	2.9045444074E-01	3.6830913186E+01	3.7121367627E+01
C22	1.9583489166E+01	2.2181592211E+02	2.4139941128E+02
H23	2.9299579978E-01	3.7018228307E+01	3.7311224107E+01
B24	3.6625199938E+00	1.0885576780E+02	1.1251828780E+02
H25	7.3981507549E-01	5.8984830807E+01	5.9724645882E+01

Total	1.5871016460E+02	2.5422824425E+03	2.7009926071E+03

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B

$= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$
C1	H2	5.6090861050E+00	9.3410256723E-01	7.8174968406E+00	4.5923379512E+01 (Bonded)
C1	H3	5.6379760110E+00	9.4393996240E-01	7.8998259214E+00	4.6150229091E+01 (Bonded)
H2	H3	1.0209149902E+00	3.8351573981E-02	1.8854823321E+00	1.8750492571E+00
C1	C4	3.5060640734E+01	9.6177678848E-01	8.0491021748E+00	8.0836042345E+00 (Bonded)
H2	C4	6.0305181372E+00	3.9370734663E-02	1.9355874323E+00	3.3090571663E-01
H3	C4	6.0639086577E+00	3.9918300165E-02	1.9516481672E+00	3.3550793085E-01
C1	H5	6.0727430339E+00	4.1495697123E-02	3.4727715407E-01	2.0342473521E+00
H2	H5	1.0354895860E+00	3.6001045903E-03	1.7699230811E-01	1.7648825633E-01

H3	H5	1.0411469504E+00	3.8286678439E-03	1.8718764450E-01	1.8769313360E-01
C4	H5	5.6011225948E+00	9.3272067256E-01	7.8393914977E+00	4.5724850768E+01 (Bonded)
C1	C6	3.9020042355E+01	9.8881754844E-01	8.2754060764E+00	7.4752732313E+00 (Bonded)
H2	C6	6.7025308673E+00	4.7959368829E-02	2.3578313273E+00	3.6256373743E-01
H3	C6	6.7416966927E+00	4.4482486314E-02	2.1747960842E+00	3.3627916468E-01
C4	C6	3.9324280154E+01	4.3034502567E-02	3.6169919190E-01	3.2533268202E-01
H5	C6	6.7402073557E+00	1.1028320947E-02	5.4064238559E-01	8.3372015887E-02
C1	H7	6.0864075288E+00	4.1650973323E-02	3.4857665934E-01	2.0372650006E+00
H2	H7	1.0376144611E+00	4.0289768816E-03	1.9807700018E-01	1.9706847006E-01
H3	H7	1.0437755503E+00	3.2761232704E-03	1.6017315240E-01	1.6024430509E-01
C4	H7	6.0760012008E+00	1.0330419437E-02	8.6825782556E-02	5.0528955943E-01
H5	H7	1.0416990925E+00	1.7980903008E-03	8.8147945135E-02	8.7949599864E-02
C6	H7	6.2771257998E+00	9.6761753960E-01	7.3150051831E+00	4.7328866294E+01 (Bonded)
C1	C8	3.5671899203E+01	4.6285647630E-02	3.8736421118E-01	3.8735155797E-01
H2	C8	6.0716912260E+00	9.2892908801E-03	4.5669035227E-01	7.7739460915E-02
H3	C8	6.1043940586E+00	1.1503041548E-02	5.6239594021E-01	9.6265717193E-02
C4	C8	3.5538498543E+01	8.3831649310E-03	7.0459370975E-02	7.0156347875E-02
H5	C8	6.0933154429E+00	7.4897848763E-04	3.6717240845E-02	6.2679901638E-03
C6	C8	3.9021299719E+01	9.8888437464E-01	7.4757784247E+00	8.2756950110E+00 (Bonded)
H7	C8	6.0866015389E+00	4.1661950397E-02	2.0378019199E+00	3.4865713716E-01
C1	H9	6.0715335953E+00	9.2800493790E-03	7.7664658300E-02	4.5623329094E-01
H2	H9	1.0306961018E+00	7.2912679306E-03	3.5846134681E-01	3.5845920935E-01
H3	H9	1.0397190525E+00	7.5585335125E-04	3.6954474552E-02	3.7159873599E-02
C4	H9	6.0498180783E+00	8.4300589087E-04	7.0853508535E-03	4.1444537218E-02
H5	H9	1.0371888672E+00	2.1391265788E-04	1.0486659776E-02	1.0516547046E-02
C6	H9	6.7025692345E+00	4.7962853276E-02	3.6259007919E-01	2.3579885731E+00
H7	H9	1.0376206120E+00	4.0290734713E-03	1.9707319453E-01	1.9808056770E-01
C8	H9	5.6092953263E+00	9.3415355534E-01	7.8176681881E+00	4.5925612396E+01 (Bonded)
C1	H10	6.1042034407E+00	1.1500708102E-02	9.6249333220E-02	5.6228113754E-01
H2	H10	1.0397141757E+00	7.5585954812E-04	3.7160399836E-02	3.6954730331E-02
H3	H10	1.0446981171E+00	2.3624554580E-03	1.1550296093E-01	1.1550281343E-01
C4	H10	6.0835489651E+00	6.5322398855E-04	5.4902595521E-03	3.1936775030E-02

H5	H10	1.0428946172E+00	3.3599826951E-04	1.6471673872E-02	1.6427291912E-02
C6	H10	6.7417108952E+00	4.4471357029E-02	3.3619502939E-01	2.1742491850E+00
H7	H10	1.0437769355E+00	3.2760227692E-03	1.6023938930E-01	1.6016803426E-01
C8	H10	5.6381667098E+00	9.4397334489E-01	7.8998472431E+00	4.6151802259E+01
(Bonded)					
H9	H10	1.0209224210E+00	3.8351772875E-02	1.8854808674E+00	1.8750565867E+00
C1	C11	3.5653362061E+01	4.6234220405E-02	3.8693381715E-01	3.8712249725E-01
H2	C11	6.0688549638E+00	8.6419377425E-03	4.2486446413E-01	7.2359574589E-02
H3	C11	6.1014889465E+00	1.0958223462E-02	5.3575920435E-01	9.1754003743E-02
C4	C11	3.5043462907E+01	9.6148718396E-01	8.0811701475E+00	8.0506022697E+00
(Bonded)					
H5	C11	6.0699912893E+00	4.1059358612E-02	2.0128566895E+00	3.4379300229E-01
C6	C11	3.9491031531E+01	8.3212036067E-03	6.2906721945E-02	6.9674044293E-02
H7	C11	6.1039603721E+00	5.9206342300E-04	2.8959469457E-02	4.9573901935E-03
C8	C11	3.5654555805E+01	4.6177543967E-02	3.8644686884E-01	3.8664794131E-01
H9	C11	6.0689173853E+00	8.5895221320E-03	4.2228503210E-01	7.1920694861E-02
H10	C11	6.1015014164E+00	1.0948881157E-02	5.3530176552E-01	9.1675779942E-02
C1	H12	6.0959347931E+00	1.0924035382E-02	9.1423163883E-02	5.3483606806E-01
H2	H12	1.0382727813E+00	7.2535252197E-04	3.5660579807E-02	3.5512947114E-02
H3	H12	1.0432144809E+00	2.4002221130E-03	1.1734941288E-01	1.1751384104E-01
C4	H12	6.0555914098E+00	3.9527411660E-02	3.3222256567E-01	1.9352450530E+00
H5	H12	1.0397663312E+00	3.6709539090E-03	1.7996150896E-01	1.7972832255E-01
C6	H12	6.7541032866E+00	7.4077372105E-04	5.6001089141E-03	3.6267962381E-02
H7	H12	1.0437777241E+00	3.4624062053E-04	1.6935592178E-02	1.6951791678E-02
C8	H12	6.0961334668E+00	1.0925303748E-02	9.1430792154E-02	5.3489816671E-01
H9	H12	1.0382789525E+00	7.2539664861E-04	3.5662536557E-02	3.5515107536E-02
H10	H12	1.0432158226E+00	2.4002061416E-03	1.1734848216E-01	1.1751305908E-01
C11	H12	5.6291473540E+00	9.3855137931E-01	7.8585591056E+00	4.5951071359E+01
(Bonded)					
C1	H13	6.0971098937E+00	8.6314970853E-03	7.2236929393E-02	4.2259238338E-01
H2	H13	1.0347868586E+00	7.7070137007E-03	3.7890069838E-01	3.7733028886E-01
H3	H13	1.0440422363E+00	7.5458173472E-04	3.6892303867E-02	3.6943822210E-02
C4	H13	6.0556085133E+00	3.9550621337E-02	3.3241763988E-01	1.9363722388E+00

H5	H13	1.0397712165E+00	3.6710272300E-03	1.7996510337E-01	1.7973106301E-01
C6	H13	6.7539192288E+00	1.1727243519E-03	8.8655738048E-03	5.7415807941E-02
H7	H13	1.0438826637E+00	1.4622750975E-04	7.1523943853E-03	7.1592020768E-03
C8	H13	6.0973078392E+00	8.6342236775E-03	7.2257387864E-02	4.2272587552E-01
H9	H13	1.0347930437E+00	7.7070301266E-03	3.7889924659E-01	3.7733109306E-01
H10	H13	1.0440435732E+00	7.5457538418E-04	3.6891946270E-02	3.6943511292E-02
C11	H13	5.6290821626E+00	9.3873939676E-01	7.8601333894E+00	4.5960059434E+01
(Bonded)					
H12	H13	1.0242161781E+00	3.7483944973E-02	1.8351978040E+00	1.8351891320E+00
C1	C14	3.5538772422E+01	8.3412484550E-03	6.9807840950E-02	7.0104279747E-02
H2	C14	6.0500295326E+00	8.2932415316E-04	4.0772147685E-02	6.9700804080E-03
H3	C14	6.0837846165E+00	6.5044123672E-04	3.1800764117E-02	5.4666534229E-03
C4	C14	3.5370818422E+01	4.0843808714E-02	3.4328670543E-01	3.4327304929E-01
H5	C14	6.0624665104E+00	1.0515596251E-02	5.1550703600E-01	8.8378652822E-02
C6	C14	3.9325848073E+01	4.3029186047E-02	3.2529249014E-01	3.6164012045E-01
H7	C14	6.0762433855E+00	1.0329893820E-02	5.0526385007E-01	8.6817911018E-02
C8	C14	3.5063201486E+01	9.6180520729E-01	8.0490770808E+00	8.0835215109E+00
(Bonded)					
H9	C14	6.0308183899E+00	3.9323765710E-02	1.9332667650E+00	3.3049780101E-01
H10	C14	6.0641306284E+00	3.9973956609E-02	1.9543667741E+00	3.3596235046E-01
C11	C14	3.5044901520E+01	9.6143641506E-01	8.0501771780E+00	8.0804219853E+00
(Bonded)					
H12	C14	6.0558376075E+00	3.9518397681E-02	1.9348037325E+00	3.3213359140E-01
H13	C14	6.0558707136E+00	3.9509604507E-02	1.9343640819E+00	3.3205968891E-01
C1	H15	6.0931100345E+00	7.4582788310E-04	6.2418275298E-03	3.6562836078E-02
H2	H15	1.0371813301E+00	2.1391513645E-04	1.0516731609E-02	1.0486794937E-02
H3	H15	1.0428919320E+00	3.3598833156E-04	1.6426827013E-02	1.6471208129E-02
C4	H15	6.0622173472E+00	1.0515367327E-02	8.8380244637E-02	5.1549648463E-01
H5	H15	1.0393878948E+00	1.7257920269E-03	8.4603660248E-02	8.4603770407E-02
C6	H15	6.7401980592E+00	1.1029347331E-02	8.3379775162E-02	5.4069340616E-01
H7	H15	1.0416977296E+00	1.7981010495E-03	8.7950125612E-02	8.8148586842E-02
C8	H15	6.0729387921E+00	4.1486411426E-02	3.4718810092E-01	2.0337947867E+00
H9	H15	1.0354943545E+00	3.6002367497E-03	1.7699775005E-01	1.7649496499E-01

H10	H15	1.0411468786E+00	3.8287590805E-03	1.8719186610E-01	1.8769785069E-01
C11	H15	6.0699774402E+00	4.1071196415E-02	3.4389212107E-01	2.0134396368E+00
H12	H15	1.0397650862E+00	3.6707314690E-03	1.7971743198E-01	1.7995083856E-01
H13	H15	1.0397699893E+00	3.6707692232E-03	1.7971843117E-01	1.7995268939E-01
C14	H15	5.6012939739E+00	9.3284486835E-01	7.8401234497E+00	4.5730998774E+01
(Bonded)					
C1	C16	3.5693249533E+01	1.8746060207E-03	1.5688562647E-02	1.5688426048E-02
H2	C16	6.0757932925E+00	7.9400134852E-04	3.9035569048E-02	6.6449330158E-03
H3	C16	6.1098699457E+00	2.5849074173E-04	1.2637887391E-02	2.1632880941E-03
C4	C16	3.5537654194E+01	8.3687824195E-03	7.0338487905E-02	7.0037662663E-02
H5	C16	6.0931697732E+00	7.4832978828E-04	3.6685439598E-02	6.2627114251E-03
C6	C16	3.9507940482E+01	1.3709393246E-02	1.0364041426E-01	1.1473280238E-01
H7	C16	6.1069923367E+00	5.8770816810E-04	2.8746441822E-02	4.9184820872E-03
C8	C16	3.5671701227E+01	4.7303187167E-02	3.9586705997E-01	3.9587654447E-01
H9	C16	6.0707962757E+00	1.0860498247E-02	5.3393259608E-01	9.0890630736E-02
H10	C16	6.1057383183E+00	8.5373507901E-03	4.1739963063E-01	7.1448397712E-02
C11	C16	3.5653693022E+01	4.6193562473E-02	3.8678206542E-01	3.8659018522E-01
H12	C16	6.0971384829E+00	8.6229045953E-03	4.2217369567E-01	7.2164390582E-02
H13	C16	6.0960168084E+00	1.0923917081E-02	5.3482774882E-01	9.1421377822E-02
C14	C16	3.5062336538E+01	9.6183195525E-01	8.0837463150E+00	8.0494937786E+00
(Bonded)					
H15	C16	6.0727952882E+00	4.1481431552E-02	2.0335506576E+00	3.4715474297E-01
C1	H17	6.1097987619E+00	2.5810484824E-04	2.1600773903E-03	1.2619058191E-02
H2	H17	1.0400569186E+00	6.1528473358E-05	3.0249305932E-03	3.0082014770E-03
H3	H17	1.0458487933E+00	5.2208625761E-05	2.5525352621E-03	2.5525428563E-03
C4	H17	6.0835238245E+00	6.5176615920E-04	5.4780066929E-03	3.1865635790E-02
H5	H17	1.0428901839E+00	3.3599436348E-04	1.6471482386E-02	1.6427170793E-02
C6	H17	6.7633623686E+00	1.1108875724E-03	8.3980994733E-03	5.4312636957E-02
H7	H17	1.0453441316E+00	1.3274004343E-04	6.4926848780E-03	6.4898212632E-03
C8	H17	6.1058574969E+00	8.5398082002E-03	7.1467251308E-02	4.1752155123E-01
H9	H17	1.0396920651E+00	8.0363934302E-04	3.9509167163E-02	3.9290899428E-02
H10	H17	1.0422800447E+00	7.1923770735E-03	3.5164251858E-01	3.5164401382E-01
C11	H17	6.1014731763E+00	1.0953425910E-02	9.1713833485E-02	5.3552624015E-01

H12	H17	1.0440342437E+00	7.5448187061E-04	3.6939107480E-02	3.6887531149E-02
H13	H17	1.0432163090E+00	2.4002218656E-03	1.1751327363E-01	1.1734974992E-01
C14	H17	6.0641020105E+00	3.9979451358E-02	3.3600853124E-01	1.9546437293E+00
H15	H17	1.0411426183E+00	3.8284092547E-03	1.8768070112E-01	1.8717555867E-01
C16	H17	5.6379907501E+00	9.4398052597E-01	7.9000966119E+00	4.6152349596E+01
(Bonded)					
C1	H18	6.0757700238E+00	7.9369255972E-04	6.6424066218E-03	3.9020198707E-02
H2	H18	1.0342852700E+00	1.1063340427E-04	5.4390813057E-03	5.4390549154E-03
H3	H18	1.0400650607E+00	6.1526032426E-05	3.0080731875E-03	3.0247959131E-03
C4	H18	6.0498155104E+00	8.3469963772E-04	7.0155379156E-03	4.1036224071E-02
H5	H18	1.0371877127E+00	2.1391709829E-04	1.0486877458E-02	1.0516777031E-02
C6	H18	6.7258525994E+00	1.3811787037E-03	1.0441449191E-02	6.7902699613E-02
H7	H18	1.0394835693E+00	3.0084911079E-04	1.4715367132E-02	1.4790603666E-02
C8	H18	6.0709344999E+00	1.0861707900E-02	9.0898576399E-02	5.3399265920E-01
H9	H18	1.0330593780E+00	2.5747528874E-03	1.2658208327E-01	1.2658222388E-01
H10	H18	1.0396953276E+00	8.0364881951E-04	3.9291195672E-02	3.9509676945E-02
C11	H18	6.0689045765E+00	8.6016464522E-03	7.2022212678E-02	4.2288156751E-01
H12	H18	1.0347872707E+00	7.7064526843E-03	3.7730460477E-01	3.7887127879E-01
H13	H18	1.0382826907E+00	7.2542863983E-04	3.5516505983E-02	3.5664148955E-02
C14	H18	6.0308005876E+00	3.9345927698E-02	3.3068406212E-01	1.9343584595E+00
H15	H18	1.0354933164E+00	3.6000083292E-03	1.7648376710E-01	1.7698671688E-01
C16	H18	5.6091973810E+00	9.3404478777E-01	7.8169452232E+00	4.5920316089E+01
(Bonded)					
H17	H18	1.0209168875E+00	3.8351683732E-02	1.8750602014E+00	1.8854785794E+00
C1	C19	3.5669920207E+01	4.7304599842E-02	3.9589181401E-01	3.9589518075E-01
H2	C19	6.0706553790E+00	1.0860674613E-02	5.3394445057E-01	9.0893671092E-02
H3	C19	6.1056265527E+00	8.5349593689E-03	4.1728324453E-01	7.1429613471E-02
C4	C19	3.5060383059E+01	9.6168763812E-01	8.0828549377E+00	8.0484245210E+00
(Bonded)					
H5	C19	6.0726944094E+00	4.1489306543E-02	2.0339340662E+00	3.4722662422E-01
C6	C19	3.9507257569E+01	1.3715047574E-02	1.0368315991E-01	1.1478209849E-01
H7	C19	6.1068870487E+00	5.8806002362E-04	2.8763652054E-02	4.9215114412E-03
C8	C19	3.5693798530E+01	1.8798824910E-03	1.5732207476E-02	1.5732855178E-02

H9	C19	6.0757249542E+00	7.9398644604E-04	3.9034603637E-02	6.6449226634E-03
H10	C19	6.1097726069E+00	2.5845601424E-04	1.2636173390E-02	2.1630346904E-03
C11	C19	3.5653086181E+01	4.6179184284E-02	3.8666167579E-01	3.8647650694E-01
H12	C19	6.0970320700E+00	8.6257073240E-03	4.2231091606E-01	7.2189088832E-02
H13	C19	6.0959116781E+00	1.0924153468E-02	5.3483932216E-01	9.1424929631E-02
C14	C19	3.5538467009E+01	8.3475497869E-03	7.0157239486E-02	6.9861170855E-02
H15	C19	6.0930572786E+00	7.4770010137E-04	3.6654618125E-02	6.2575493244E-03
C16	C19	3.5670734783E+01	4.6297009661E-02	3.8745592637E-01	3.8746259496E-01
H17	C19	6.1041251790E+00	1.1501351423E-02	5.6231498117E-01	9.6255535735E-02
H18	C19	6.0714761430E+00	9.2781090587E-03	4.5613840606E-01	7.7649080113E-02
C1	H20	6.1056659772E+00	8.5369040202E-03	7.1445280795E-02	4.1737911049E-01
H2	H20	1.0396869907E+00	8.0363629316E-04	3.9509252812E-02	3.9290707778E-02
H3	H20	1.0422800860E+00	7.1918879245E-03	3.5161905262E-01	3.5161971805E-01
C4	H20	6.0639014509E+00	3.9909686797E-02	3.3543553666E-01	1.9512307431E+00
H5	H20	1.0411450454E+00	3.8285297461E-03	1.8768636362E-01	1.8718124699E-01
C6	H20	6.7633684623E+00	1.1133460385E-03	8.4166850113E-03	5.4432775408E-02
H7	H20	1.0453452582E+00	1.3275050050E-04	6.4931963624E-03	6.4903254953E-03
C8	H20	6.1100047977E+00	2.5843664828E-04	2.1627835727E-03	1.2635266616E-02
H9	H20	1.0400642453E+00	6.1531104011E-05	3.0250418863E-03	3.0083268359E-03
H10	H20	1.0458512595E+00	5.2212033496E-05	2.5526986101E-03	2.5527067009E-03
C11	H20	6.1014804654E+00	1.0952071072E-02	9.1702489334E-02	5.3545942080E-01
H12	H20	1.0440353933E+00	7.5444412755E-04	3.6937259596E-02	3.6885645911E-02
H13	H20	1.0432174440E+00	2.4002133287E-03	1.1751285567E-01	1.1734920549E-01
C14	H20	6.0837735946E+00	6.4945695069E-04	5.4583809607E-03	3.1752701417E-02
H15	H20	1.0428899559E+00	3.3599248971E-04	1.6471411974E-02	1.6427061397E-02
C16	H20	6.1042359171E+00	1.1503421815E-02	9.6271206033E-02	5.6241559625E-01
H17	H20	1.0446917024E+00	2.3624318823E-03	1.1550215193E-01	1.1550202688E-01
H18	H20	1.0397159527E+00	7.5580538695E-04	3.7157556817E-02	3.6952199458E-02
C19	H20	5.6379092639E+00	9.4394641122E-01	7.8999470737E+00	4.6150631719E+01
(Bonded)					
C1	H21	6.0707120678E+00	1.0861108932E-02	9.0896532927E-02	5.3396534308E-01
H2	H21	1.0330490496E+00	2.5748188154E-03	1.2658607928E-01	1.2658597025E-01

H3	H21	1.0396898663E+00	8.0361368716E-04	3.9289528190E-02	3.9508107401E-02
C4	H21	6.0305521375E+00	3.9313156751E-02	3.3042178205E-01	1.9327550588E+00
H5	H21	1.0354904848E+00	3.6000938954E-03	1.7648773203E-01	1.7699162986E-01
C6	H21	6.7258255726E+00	1.3815457172E-03	1.0444223744E-02	6.7921014099E-02
H7	H21	1.0394794353E+00	3.0081940201E-04	1.4713913994E-02	1.4789202117E-02
C8	H21	6.0759440567E+00	7.9409697207E-04	6.6455740615E-03	3.9040236572E-02
H9	H21	1.0342873019E+00	1.1064963924E-04	5.4398470300E-03	5.4398747816E-03
H10	H21	1.0400622336E+00	6.1535538299E-05	3.0085340977E-03	3.0252753219E-03
C11	H21	6.0688860725E+00	8.5901824074E-03	7.1926223396E-02	4.2231964757E-01
H12	H21	1.0347833405E+00	7.7060233184E-03	3.7728358320E-01	3.7885168180E-01
H13	H21	1.0382785654E+00	7.2538949621E-04	3.5514589537E-02	3.5662366858E-02
C14	H21	6.0500355618E+00	8.2768867087E-04	6.9563349467E-03	4.0691707254E-02
H15	H21	1.0371822230E+00	2.1391618790E-04	1.0486846483E-02	1.0516774243E-02
C16	H21	6.0715496376E+00	9.2917784087E-03	7.7762141385E-02	4.5681225342E-01
H17	H21	1.0397106423E+00	7.5587290439E-04	3.6955540473E-02	3.7161024464E-02
H18	H21	1.0306960085E+00	7.2909382630E-03	3.5844340016E-01	3.5844483058E-01
C19	H21	5.6090780436E+00	9.3402581253E-01	7.8169209573E+00	4.5919566461E+01
(Bonded)					
H20	H21	1.0209139770E+00	3.8351455421E-02	1.8750470090E+00	1.8854748792E+00
C1	C22	3.9506161712E+01	1.3711748551E-02	1.1475351288E-01	1.0366198067E-01
H2	C22	6.7255750710E+00	1.3828999328E-03	6.7987650037E-02	1.0454840647E-02
H3	C22	6.7631328913E+00	1.1193120754E-03	5.4724358286E-02	8.4620941151E-03
C4	C22	3.9322851201E+01	4.3037560222E-02	3.6172489108E-01	3.2536760131E-01
H5	C22	6.7399618589E+00	1.1029859050E-02	5.4071778820E-01	8.3386668843E-02
C6	C22	4.3677230439E+01	1.3030542063E-01	9.8508427994E-01	9.8512001907E-01
H7	C22	6.7555253071E+00	1.0327965633E-02	5.0516953704E-01	7.8080295141E-02
C8	C22	3.9507454109E+01	1.3708415364E-02	1.1472186996E-01	1.0363678149E-01
H9	C22	6.7256154611E+00	1.3823356617E-03	6.7959503484E-02	1.0450574710E-02
H10	C22	6.7631430939E+00	1.1161817929E-03	5.4571245754E-02	8.4384289141E-03
C11	C22	3.9489587037E+01	8.3445026264E-03	6.9869128683E-02	6.3085146780E-02
H12	C22	6.7536412398E+00	1.1747767981E-03	5.7516566135E-02	8.8814121174E-03
H13	C22	6.7538894086E+00	7.4227192547E-04	3.6341142098E-02	5.6116386399E-03

C14	C22	3.9324415332E+01	4.3039705462E-02	3.6172853119E-01	3.2538381951E-01
H15	C22	6.7399524458E+00	1.1031119349E-02	5.4078027607E-01	8.3396196808E-02
C16	C22	3.9018987191E+01	9.8874886356E-01	8.2747592055E+00	7.4750251727E+00
(Bonded)					
H17	C22	6.7414395873E+00	4.4465674323E-02	2.1739805959E+00	3.3616426490E-01
H18	C22	6.7023793360E+00	4.7839641623E-02	2.3519337549E+00	3.6167174352E-01
C19	C22	3.9018328950E+01	9.8870522373E-01	8.2745363996E+00	7.4746952519E+00
(Bonded)					
H20	C22	6.7414378519E+00	4.4483790600E-02	2.1748639680E+00	3.3630122549E-01
H21	C22	6.7023493547E+00	4.7845919577E-02	2.3522517841E+00	3.6171920538E-01
C1	H23	6.1069253922E+00	5.8707596025E-04	4.9132339697E-03	2.8715585004E-02
H2	H23	1.0394761377E+00	3.0082832581E-04	1.4789653576E-02	1.4714384417E-02
H3	H23	1.0453448306E+00	1.3274051872E-04	6.4898251929E-03	6.4927231005E-03
C4	H23	6.0759875438E+00	1.0329682992E-02	8.6819592835E-02	5.0525470314E-01
H5	H23	1.0416966943E+00	1.7980775768E-03	8.8147321364E-02	8.7949180338E-02
C6	H23	6.7557551595E+00	1.0327634178E-02	7.8074956739E-02	5.0515448975E-01
H7	H23	1.0442554122E+00	1.3831971804E-03	6.7656022893E-02	6.7656178931E-02
C8	H23	6.1071250413E+00	5.8677391937E-04	4.9105457844E-03	2.8700811310E-02
H9	H23	1.0394823357E+00	3.0083070760E-04	1.4789682483E-02	1.4714500918E-02
H10	H23	1.0453461637E+00	1.3274430575E-04	6.4900020566E-03	6.4929083348E-03
C11	H23	6.1039462450E+00	5.9216067328E-04	4.9582044772E-03	2.8964293040E-02
H12	H23	1.0438753337E+00	1.4620598922E-04	7.1581822709E-03	7.1513582497E-03
H13	H23	1.0437802465E+00	3.4624639932E-04	1.6951994501E-02	1.6935913894E-02
C14	H23	6.0762296755E+00	1.0329262280E-02	8.6812603221E-02	5.0523412493E-01
H15	H23	1.0416953213E+00	1.7981085499E-03	8.8148954537E-02	8.7950695323E-02
C16	H23	6.0864418233E+00	4.1660564036E-02	3.4865388823E-01	2.0377388088E+00
H17	H23	1.0437700472E+00	3.2760868223E-03	1.6017184695E-01	1.6024289189E-01
H18	H23	1.0376172847E+00	4.0286228658E-03	1.9805863469E-01	1.9705160862E-01
C19	H23	6.0863415675E+00	4.1650852194E-02	3.4857860997E-01	2.0372637745E+00
H20	H23	1.0437711594E+00	3.2761259841E-03	1.6017358820E-01	1.6024480740E-01
H21	H23	1.0376129871E+00	4.0289203365E-03	1.9807404964E-01	1.9706615878E-01
C22	H23	6.2768793364E+00	9.6758872220E-01	7.3150527114E+00	4.7327565908E+01
(Bonded)					

C1	B24	1.8405902459E+01	2.2892076415E-02	1.9158360262E-01	3.7129999286E-01
H2	B24	3.1322926254E+00	5.7530917423E-03	2.8283983443E-01	9.3312763953E-02
H3	B24	3.1515336266E+00	2.1602583060E-03	1.0561732704E-01	3.5038494502E-02
C4	B24	1.8336959836E+01	3.5611989415E-03	2.9931396961E-02	5.7761171055E-02
H5	B24	3.1435706492E+00	1.1051775306E-03	5.4179219078E-02	1.7925521555E-02
C6	B24	2.0119779825E+01	5.3782278033E-01	4.0658382725E+00	8.7232626207E+00
(Bonded)					
H7	B24	3.1444224785E+00	1.3582867509E-02	6.6437584470E-01	2.2030848219E-01
C8	B24	1.8406523470E+01	2.2853294786E-02	1.9125279203E-01	3.7067097092E-01
H9	B24	3.1323119353E+00	5.7518613760E-03	2.8277765963E-01	9.3292807922E-02
H10	B24	3.1515380903E+00	2.1593827906E-03	1.0557438734E-01	3.5024294005E-02
C11	B24	1.8408138704E+01	4.6667871643E-04	3.9075349067E-03	7.5693353866E-03
H12	B24	3.1480940053E+00	2.1707688102E-04	1.0627990614E-02	3.5208970525E-03
H13	B24	3.1481088787E+00	2.1708309328E-04	1.0628244541E-02	3.5209978128E-03
C14	B24	1.8337714365E+01	3.5112506921E-03	2.9510414671E-02	5.6951031148E-02
H15	B24	3.1435687930E+00	1.1007022115E-03	5.3959895362E-02	1.7852933735E-02
C16	B24	1.8406086273E+01	2.2845164589E-02	1.9118933326E-01	3.7053910250E-01
H17	B24	3.1515250030E+00	2.1587466097E-03	1.0554373261E-01	3.5013975414E-02
H18	B24	3.1323089268E+00	5.7509127249E-03	2.8273133536E-01	9.3277421194E-02
C19	B24	1.8405740630E+01	2.2902487510E-02	1.9167236300E-01	3.7146885652E-01
H20	B24	3.1515274564E+00	2.1606661717E-03	1.0563746794E-01	3.5045109914E-02
H21	B24	3.1322949224E+00	5.7538986545E-03	2.8287926108E-01	9.3325851734E-02
C22	B24	2.0119049339E+01	5.3780439327E-01	4.0658467745E+00	8.7229643902E+00
(Bonded)					
H23	B24	3.1444163069E+00	1.3580675265E-02	6.6427014800E-01	2.2027292491E-01
C1	H25	9.7722641725E+00	7.3087580491E-03	6.1166937082E-02	2.2333298495E-01
H2	H25	1.6632435888E+00	1.8049996120E-03	8.8739379496E-02	5.5155191684E-02
H3	H25	1.6727020130E+00	1.4073031050E-03	6.8804546139E-02	4.3002819501E-02
C4	H25	9.7337133142E+00	9.6024241034E-04	8.0707079931E-03	2.9342030798E-02
H5	H25	1.6686966170E+00	4.0457066791E-04	1.9833304825E-02	1.2362425227E-02
C6	H25	1.0761957295E+01	1.2069779613E-01	9.1245245991E-01	3.6881504224E+00
H7	H25	1.6685058638E+00	8.3135292332E-03	4.0663784750E-01	2.5403567701E-01
C8	H25	9.7725826603E+00	7.3104617163E-03	6.1179196582E-02	2.2338504373E-01

H9	H25	1.6632534845E+00	1.8050544923E-03	8.8741548425E-02	5.5156868656E-02
H10	H25	1.6727043834E+00	1.4068361186E-03	6.8781626841E-02	4.2988549845E-02
C11	H25	9.7709682760E+00	3.7115754726E-04	3.1077291951E-03	1.1341423858E-02
H12	H25	1.6710253808E+00	7.7629514009E-05	3.8007075760E-03	2.3721172553E-03
H13	H25	1.6710332745E+00	7.7635024681E-05	3.8009594152E-03	2.3722856444E-03
C14	H25	9.7341008942E+00	9.5957641882E-04	8.0647895895E-03	2.9321680162E-02
H15	H25	1.6686944588E+00	4.0454105816E-04	1.9831879086E-02	1.2361520445E-02
C16	H25	9.7723483239E+00	7.3106917267E-03	6.1182587301E-02	2.2339207214E-01
H17	H25	1.6726973114E+00	1.4067489683E-03	6.8777658426E-02	4.2985886800E-02
H18	H25	1.6632516290E+00	1.8050679901E-03	8.8742310597E-02	5.5157281107E-02
C19	H25	9.7721805362E+00	7.3097592651E-03	6.1175836498E-02	2.2336357900E-01
H20	H25	1.6726987470E+00	1.4075013371E-03	6.8814368148E-02	4.3008876860E-02
H21	H25	1.6632450250E+00	1.8049940284E-03	8.8739028554E-02	5.5155021067E-02
C22	H25	1.0761564218E+01	1.2069870612E-01	9.1249244357E-01	3.6881782290E+00
H23	H25	1.6685021170E+00	8.3133074125E-03	4.0662793545E-01	2.5402889885E-01
B24	H25	4.7575563057E+00	5.7325652957E-01	9.2979833495E+00	1.7516942144E+01
(Bonded)					

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	H2	4.9260310350E+01	3.8859928495E+01	3.1099979774E+01
C1	H3	4.7983749941E+01	3.7362070227E+01	2.9627794411E+01

C1	C4	5.1514329914E+01	4.2735976311E+01	3.6065274157E+01
C1	C6	4.7990884868E+01	4.0083443334E+01	3.4124359002E+01

C1	Total	1.9674927507E+02	1.5904141837E+02	1.3091740734E+02
H2	C1	4.9260310350E+01	3.8859928495E+01	3.1099979774E+01

H2	Total	4.9260310350E+01	3.8859928495E+01	3.1099979774E+01
H3	C1	4.7983749941E+01	3.7362070227E+01	2.9627794411E+01

H3	Total	4.7983749941E+01	3.7362070227E+01	2.9627794411E+01
C4	C1	5.1514329914E+01	4.2735976311E+01	3.6065274157E+01
C4	H5	4.5739753669E+01	3.5581582861E+01	2.8267895251E+01
C4	C11	5.0500989464E+01	4.2295548575E+01	3.5991491846E+01
C4	C19	5.1514018722E+01	4.2735708239E+01	3.6065039820E+01

C4	Total	1.9926909177E+02	1.6334881599E+02	1.3638970107E+02
H5	C4	4.5739753669E+01	3.5581582861E+01	2.8267895251E+01

H5	Total	4.5739753669E+01	3.5581582861E+01	2.8267895251E+01
C6	C1	4.7990884868E+01	4.0083443334E+01	3.4124359002E+01
C6	H7	4.5472444408E+01	3.5273489459E+01	2.8043472865E+01
C6	C8	4.7990967635E+01	4.0083511020E+01	3.4124406125E+01
C6	B24	4.2670178999E+01	3.5574841578E+01	3.0480831387E+01

C6	Total	1.8412447591E+02	1.5101528539E+02	1.2677306938E+02
H7	C6	4.5472444408E+01	3.5273489459E+01	2.8043472865E+01

H7	Total	4.5472444408E+01	3.5273489459E+01	2.8043472865E+01
C8	C6	4.7990967635E+01	4.0083511020E+01	3.4124406125E+01
C8	H9	4.9252779669E+01	3.8847768105E+01	3.1100962442E+01
C8	H10	4.7985177045E+01	3.7362084269E+01	2.9629193978E+01
C8	C14	5.1524448611E+01	4.2753815543E+01	3.6070244112E+01
C8	Total	1.9675337296E+02	1.5904717894E+02	1.3092480666E+02
H9	C8	4.9252779669E+01	3.8847768105E+01	3.1100962442E+01
H9	Total	4.9252779669E+01	3.8847768105E+01	3.1100962442E+01
H10	C8	4.7985177045E+01	3.7362084269E+01	2.9629193978E+01
H10	Total	4.7985177045E+01	3.7362084269E+01	2.9629193978E+01
C11	C4	5.0500989464E+01	4.2295548575E+01	3.5991491846E+01
C11	C14	5.0500889843E+01	4.2295463959E+01	3.5991419392E+01
C11	H12	4.9464940548E+01	3.9056100415E+01	3.1290427771E+01
C11	H13	4.9462131225E+01	3.9055637780E+01	3.1290421252E+01
C11	Total	1.9992895108E+02	1.6270275073E+02	1.3456376026E+02
H12	C11	4.9464940548E+01	3.9056100415E+01	3.1290427771E+01
H12	Total	4.9464940548E+01	3.9056100415E+01	3.1290427771E+01
H13	C11	4.9462131225E+01	3.9055637780E+01	3.1290421252E+01
H13	Total	4.9462131225E+01	3.9055637780E+01	3.1290421252E+01

C14	C8	5.1524448611E+01	4.2753815543E+01	3.6070244112E+01
C14	C11	5.0500889843E+01	4.2295463960E+01	3.5991419393E+01
C14	H15	4.5739753076E+01	3.5582809993E+01	2.8267895640E+01
C14	C16	5.1524781983E+01	4.2754108474E+01	3.6070505755E+01

C14	Total	1.9928987351E+02	1.6338619797E+02	1.3640006490E+02
H15	C14	4.5739753076E+01	3.5582809993E+01	2.8267895640E+01

H15	Total	4.5739753076E+01	3.5582809993E+01	2.8267895640E+01
C16	C14	5.1524781983E+01	4.2754108474E+01	3.6070505755E+01
C16	H17	4.7960865791E+01	3.7370481240E+01	2.9635074031E+01
C16	H18	4.9254928162E+01	3.8845592794E+01	3.1102132383E+01
C16	C22	4.7968946546E+01	4.0068481711E+01	3.4110192966E+01

C16	Total	1.9670952248E+02	1.5903866422E+02	1.3091790514E+02
H17	C16	4.7960865791E+01	3.7370481240E+01	2.9635074031E+01

H17	Total	4.7960865791E+01	3.7370481240E+01	2.9635074031E+01
H18	C16	4.9254928162E+01	3.8845592794E+01	3.1102132383E+01

H18	Total	4.9254928162E+01	3.8845592794E+01	3.1102132383E+01
C19	C4	5.1514018722E+01	4.2735708240E+01	3.6065039820E+01
C19	C22	4.7968904407E+01	4.0070068372E+01	3.4110134084E+01
C19	H20	4.7962033406E+01	3.7370396074E+01	2.9636476911E+01
C19	H21	4.9260301489E+01	3.8859924971E+01	3.1100883269E+01

C19	Total	1.9670525802E+02	1.5903609766E+02	1.3091253408E+02
H20	C19	4.7962033406E+01	3.7370396074E+01	2.9636476911E+01

H20	Total	4.7962033406E+01	3.7370396074E+01	2.9636476911E+01
H21	C19	4.9260301489E+01	3.8859924971E+01	3.1100883269E+01

H21	Total	4.9260301489E+01	3.8859924971E+01	3.1100883269E+01
C22	C16	4.7968946546E+01	4.0068481711E+01	3.4110192966E+01
C22	C19	4.7968904407E+01	4.0070068372E+01	3.4110134084E+01
C22	B24	4.2670189214E+01	3.5574848155E+01	3.0480835741E+01
C22	H23	4.5472442548E+01	3.5273488652E+01	2.8043472472E+01

C22	Total	1.8408048271E+02	1.5098688689E+02	1.2674463526E+02
H23	C22	4.5472442548E+01	3.5273488652E+01	2.8043472472E+01

H23	Total	4.5472442548E+01	3.5273488652E+01	2.8043472472E+01
B24	C6	4.2670178999E+01	3.5574841578E+01	3.0480831387E+01
B24	C22	4.2670189214E+01	3.5574848155E+01	3.0480835741E+01
B24	H25	5.3719708155E+01	4.0853741393E+01	3.2314133754E+01

B24	Total	1.3906007637E+02	1.1200343113E+02	9.3275800882E+01
H25	B24	5.3719708155E+01	4.0853741393E+01	3.2314133754E+01

H25	Total	5.3719708155E+01	4.0853741393E+01	3.2314133754E+01

Total Total 2.6166616994E+03 2.1051618240E+03 1.7282699012E+03

Some Properties of Interatomic Surfaces:

 $N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta \rho\_IAS(A B)$	$V\_IAS(A B)$

C1	H2	9.9155085244E-01	5.6179504719E-01	3.6764206530E-01	-1.9415298189E-01	7.7661192756E-01	-9.2943711249E-01

C1	H3	9.8822594753E-01	5.5649797703E-01	3.7251174897E-01	-1.8398622806E-01	7.3594491222E-01	-9.2900972600E-01

C1	C4	1.1995909142E+00	8.3002378817E-01	3.1777612435E-01	-5.1224766382E-01	2.0489906553E+00	-1.1477999125E+00

C1	C6	1.1678039749E+00	7.9722265187E-01	2.9930000908E-01	-4.9792264279E-01	1.9916905712E+00	-1.0965226610E+00

C1	Total	4.3471716891E+00	2.7455394643E+00	1.3572299477E+00	-1.3883095166E+00	5.5532380663E+00	-4.1027694120E+00

H2	C1	9.9155085244E-01	5.6179504719E-01	3.6764206530E-01	-1.9415298189E-01	7.7661192756E-01	-9.2943711249E-01

H2	Total	9.9155085244E-01	5.6179504719E-01	3.6764206530E-01	-1.9415298189E-01	7.7661192756E-01	-9.2943711249E-01

H3	C1	9.8822594753E-01	5.5649797703E-01	3.7251174897E-01	-1.8398622806E-01
7.3594491222E-01 -9.2900972600E-01					

H3	Total	9.8822594753E-01	5.5649797703E-01	3.7251174897E-01	-1.8398622806E-01
7.3594491222E-01 -9.2900972600E-01					

C4	C1	1.1995909142E+00	8.3002378817E-01	3.1777612435E-01	-5.1224766382E-01
2.0489906553E+00 -1.1477999125E+00					

C4	H5	9.8401177627E-01	5.6135222906E-01	3.7465395441E-01	-1.8669827465E-01
7.4679309859E-01 -9.3600618348E-01					

C4	C11	1.2039955302E+00	8.3729205989E-01	3.2011526051E-01	-5.1717679938E-01
2.0687071975E+00 -1.1574073204E+00					

C4	C19	1.1995901766E+00	8.3002205797E-01	3.1777858805E-01	-5.1224346992E-01
2.0489738797E+00 -1.1478006460E+00					

C4	Total	4.5871883973E+00	3.0586901351E+00	1.3303239273E+00	-1.7283662078E+00
6.9134648311E+00 -4.3890140624E+00					

H5	C4	9.8401177627E-01	5.6135222906E-01	3.7465395441E-01	-1.8669827465E-01
7.4679309859E-01 -9.3600618348E-01					

H5	Total	9.8401177627E-01	5.6135222906E-01	3.7465395441E-01	-1.8669827465E-01
7.4679309859E-01 -9.3600618348E-01					

C6	C1	1.1678039749E+00	7.9722265187E-01	2.9930000908E-01	-4.9792264279E-01
1.9916905712E+00 -1.0965226610E+00					

C6	H7	9.8650567952E-01	5.5565998015E-01	3.7664568833E-01	-1.7901429183E-01
7.1605716732E-01 -9.3230566848E-01					

C6	C8	1.1678025742E+00	7.9722108332E-01	2.9930044403E-01	-4.9792063930E-01
1.9916825572E+00 -1.0965215273E+00					

C6	B24	9.9293099875E-01	7.2256221449E-01	4.6426909195E-01	-2.5829312254E-01
1.0331724901E+00 -1.1868313064E+00					

C6	Total	4.3150432274E+00	2.8726659298E+00	1.4395152334E+00	-1.4331506965E+00
5.7326027858E+00 -4.3121811632E+00					

H7 C6 9.8650567952E-01 5.5565998015E-01 3.7664568833E-01 -1.7901429183E-01
7.1605716732E-01 -9.3230566848E-01

H7 Total 9.8650567952E-01 5.5565998015E-01 3.7664568833E-01 -1.7901429183E-01
7.1605716732E-01 -9.3230566848E-01

C8 C6 1.1678025742E+00 7.9722108332E-01 2.9930044403E-01 -4.9792063930E-01
1.9916825572E+00 -1.0965215273E+00

C8 H9 9.9154863387E-01 5.6179466793E-01 3.6764030471E-01 -1.9415436321E-01
7.7661745286E-01 -9.2943497264E-01

C8 H10 9.8822557236E-01 5.5649792806E-01 3.7251156551E-01 -1.8398636255E-01
7.3594545019E-01 -9.2900949357E-01

C8 C14 1.1996394326E+00 8.3007513348E-01 3.1776584394E-01 -5.1230928955E-01
2.0492371582E+00 -1.1478409774E+00

C8 Total 4.3472162130E+00 2.7455888128E+00 1.3572181582E+00 -1.3883706546E+00
5.5534826184E+00 -4.1028069709E+00

H9 C8 9.9154863387E-01 5.6179466793E-01 3.6764030471E-01 -1.9415436321E-01
7.7661745286E-01 -9.2943497264E-01

H9 Total 9.9154863387E-01 5.6179466793E-01 3.6764030471E-01 -1.9415436321E-01
7.7661745286E-01 -9.2943497264E-01

H10 C8 9.8822557236E-01 5.5649792806E-01 3.7251156551E-01 -1.8398636255E-01
7.3594545019E-01 -9.2900949357E-01

H10 Total 9.8822557236E-01 5.5649792806E-01 3.7251156551E-01 -1.8398636255E-01
7.3594545019E-01 -9.2900949357E-01

C11 C4 1.2039955302E+00 8.3729205989E-01 3.2011526051E-01 -5.1717679938E-01
2.0687071975E+00 -1.1574073204E+00

C11 C14 1.2039933935E+00 8.3728981891E-01 3.2011455851E-01 -5.1717526039E-01
2.0687010416E+00 -1.1574043774E+00

C11 H12 9.9597172275E-01 5.6349238620E-01 3.7016814566E-01 -1.9332424054E-01
7.7329696216E-01 -9.3366053185E-01

C11	H13	9.9597194750E-01	5.6349256181E-01	3.7016830674E-01	-1.9332425507E-01
7.7329702028E-01 -9.3366086854E-01					

C11	Total	4.3999325940E+00	2.8015668268E+00	1.3805662714E+00	-1.4210005554E+00
5.6840022215E+00 -4.1821330982E+00					

H12	C11	9.9597172275E-01	5.6349238620E-01	3.7016814566E-01	-1.9332424054E-01
7.7329696216E-01 -9.3366053185E-01					

H12	Total	9.9597172275E-01	5.6349238620E-01	3.7016814566E-01	-1.9332424054E-01
7.7329696216E-01 -9.3366053185E-01					

H13	C11	9.9597194750E-01	5.6349256181E-01	3.7016830674E-01	-1.9332425507E-01
7.7329702028E-01 -9.3366086854E-01					

H13	Total	9.9597194750E-01	5.6349256181E-01	3.7016830674E-01	-1.9332425507E-01
7.7329702028E-01 -9.3366086854E-01					

C14	C8	1.1996394326E+00	8.3007513348E-01	3.1776584394E-01	-5.1230928954E-01
2.0492371582E+00 -1.1478409774E+00					

C14	C11	1.2039933935E+00	8.3728981891E-01	3.2011455851E-01	-5.1717526040E-01
2.0687010416E+00 -1.1574043774E+00					

C14	H15	9.8401182574E-01	5.6135244105E-01	3.7465387433E-01	-1.8669856672E-01
7.4679426686E-01 -9.3600631538E-01					

C14	C16	1.1996437053E+00	8.3007995616E-01	3.1776614537E-01	-5.1231381078E-01
2.0492552431E+00 -1.1478461015E+00					

C14	Total	4.5872883571E+00	3.0587973496E+00	1.3303004222E+00	-1.7284969274E+00
6.9139877098E+00 -4.3890977717E+00					

H15	C14	9.8401182574E-01	5.6135244105E-01	3.7465387433E-01	-1.8669856672E-01
7.4679426686E-01 -9.3600631538E-01					

H15	Total	9.8401182574E-01	5.6135244105E-01	3.7465387433E-01	-1.8669856672E-01
7.4679426686E-01 -9.3600631538E-01					

C16	C14	1.1996437053E+00	8.3007995616E-01	3.1776614537E-01	-5.1231381078E-01
2.0492552431E+00 -1.1478461015E+00					

C16	H17	9.8822555762E-01	5.5649796333E-01	3.7251137953E-01	-1.8398658379E-01
7.3594633517E-01 -9.2900934286E-01					

C16	H18	9.9154953575E-01	5.6179494631E-01	3.6764068300E-01	-1.9415426330E-01
7.7661705321E-01 -9.2943562931E-01					

C16	C22	1.1677457867E+00	7.9716015198E-01	2.9931664460E-01	-4.9784350737E-01
1.9913740295E+00 -1.0964767966E+00					

C16	Total	4.3471645854E+00	2.7455330178E+00	1.3572348525E+00	-1.3882981652E+00
5.5531926610E+00 -4.1027678703E+00					

H17	C16	9.8822555762E-01	5.5649796333E-01	3.7251137953E-01	-1.8398658379E-01
7.3594633517E-01 -9.2900934286E-01					

H17	Total	9.8822555762E-01	5.5649796333E-01	3.7251137953E-01	-1.8398658379E-01
7.3594633517E-01 -9.2900934286E-01					

H18	C16	9.9154953575E-01	5.6179494631E-01	3.6764068300E-01	-1.9415426330E-01
7.7661705321E-01 -9.2943562931E-01					

H18	Total	9.9154953575E-01	5.6179494631E-01	3.6764068300E-01	-1.9415426330E-01
7.7661705321E-01 -9.2943562931E-01					

C19	C4	1.1995901766E+00	8.3002205797E-01	3.1777858805E-01	-5.1224346992E-01
2.0489738797E+00 -1.1478006460E+00					

C19	C22	1.1677423412E+00	7.9715765599E-01	2.9931084532E-01	-4.9784681067E-01
1.9913872427E+00 -1.0964685013E+00					

C19	H20	9.8822635717E-01	5.5649791826E-01	3.7251146107E-01	-1.8398645719E-01
7.3594582877E-01 -9.2900937933E-01					

C19	H21	9.9155009234E-01	5.6179454582E-01	3.6764161044E-01	-1.9415293538E-01
7.7661174150E-01 -9.2943615626E-01					

C19	Total	4.3471089673E+00	2.7454721780E+00	1.3572425049E+00	-1.3882296732E+00
5.5529186927E+00 -4.1027146829E+00					

H20 C19 9.8822635717E-01 5.5649791826E-01 3.7251146107E-01 -1.8398645719E-01
7.3594582877E-01 -9.2900937933E-01

H20 Total 9.8822635717E-01 5.5649791826E-01 3.7251146107E-01 -1.8398645719E-01
7.3594582877E-01 -9.2900937933E-01

H21 C19 9.9155009234E-01 5.6179454582E-01 3.6764161044E-01 -1.9415293538E-01
7.7661174150E-01 -9.2943615626E-01

H21 Total 9.9155009234E-01 5.6179454582E-01 3.6764161044E-01 -1.9415293538E-01
7.7661174150E-01 -9.2943615626E-01

C22 C16 1.1677457867E+00 7.9716015198E-01 2.9931664460E-01 -4.9784350737E-01
1.9913740295E+00 -1.0964767966E+00

C22 C19 1.1677423412E+00 7.9715765599E-01 2.9931084532E-01 -4.9784681067E-01
1.9913872427E+00 -1.0964685013E+00

C22 B24 9.9293152250E-01 7.2256314812E-01 4.6426975243E-01 -2.5829339569E-01
1.0331735827E+00 -1.1868329006E+00

C22 H23 9.8650575913E-01 5.5566003573E-01 3.7664587547E-01 -1.7901416026E-01
7.1605664104E-01 -9.3230591120E-01

C22 Total 4.3149254095E+00 2.8725409918E+00 1.4395431178E+00 -1.4329978740E+00
5.7319914959E+00 -4.3120841097E+00

H23 C22 9.8650575913E-01 5.5566003573E-01 3.7664587547E-01 -1.7901416026E-01
7.1605664104E-01 -9.3230591120E-01

H23 Total 9.8650575913E-01 5.5566003573E-01 3.7664587547E-01 -1.7901416026E-01
7.1605664104E-01 -9.3230591120E-01

B24 C6 9.9293099875E-01 7.2256221449E-01 4.6426909195E-01 -2.5829312254E-01
1.0331724902E+00 -1.1868313064E+00

B24 C22 9.9293152250E-01 7.2256314812E-01 4.6426975243E-01 -2.5829339569E-01
1.0331735827E+00 -1.1868329006E+00

B24 H25 8.8264593858E-01 5.6379059445E-01 4.0542456278E-01 -1.5836603167E-01
6.3346412668E-01 -9.6921515724E-01

B24 Total 2.8685084598E+00 2.0089159571E+00 1.3339634072E+00 -6.7495254990E-01
 2.6998101996E+00 -3.3428793642E+00

H25 B24 8.8264593858E-01 5.6379059445E-01 4.0542456278E-01 -1.5836603167E-01
 6.3346412668E-01 -9.6921515724E-01

H25 Total 8.8264593858E-01 5.6379059445E-01 4.0542456278E-01 -1.5836603167E-01
 6.3346412668E-01 -9.6921515724E-01

Total Total 5.7196275098E+01 3.6053281885E+01 1.9292109069E+01 -1.6761172817E+01
 6.7044691267E+01 -5.5345390954E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	6.6728949095E+00
H2	3.9535220073E+01
H3	4.2906586992E+01
C4	2.1994507795E+00
H5	4.4191850901E+01
C6	6.1079981016E+00
H7	4.5532854986E+01
C8	7.0547585103E+00
H9	4.0129639535E+01
H10	4.2599029572E+01
C11	7.1061724975E+00
H12	4.0297463366E+01
H13	3.9686986007E+01
C14	2.6988854746E+00
H15	4.3954165373E+01
C16	7.0190621719E+00
H17	4.2986766266E+01
H18	3.9869915664E+01

C19 7.3333047075E+00
H20 4.2463257659E+01
H21 4.0227347959E+01
C22 6.0028604235E+00
H23 4.5826730003E+01
B24 3.0166675535E+00
H25 7.8322706232E+01

Total 7.2374257572E+02

0.001 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 7.6439908394E+00 -8.1421784817E-03 2.3721605948E-02 -3.1156204905E-03 -1.0651737623E-03 1.8592048703E-03 1.3472551389E-05
H2 3.5237540731E+01 1.6375880210E-01 1.1256274972E-02 -2.8136278468E-03 4.6472823785E-03 3.3883649871E-03 1.5419291753E-05
H3 3.7356319171E+01 2.6016821076E-01 2.2239094211E-02 -2.6248169619E-03 6.9645033701E-03 4.4389152432E-03 2.6494993432E-05
C4 3.2499411711E+00 5.9060114906E-03 5.3148417714E-03 -1.6239768227E-04 1.8172671995E-03 7.8848142778E-04 1.1545262187E-06
H5 3.8268437115E+01 2.1477991702E-01 1.1807372083E-02 2.9883546194E-04 5.6124559353E-03 2.7392373162E-03 9.9643643217E-06
C6 8.2600029241E+00 5.6585299855E-03 2.6528179112E-02 -1.2430070868E-02 6.8505181384E-04 5.6261228342E-03 6.4153782483E-05
H7 3.9304212813E+01 1.8950007134E-02 7.4888772195E-03 -1.1343061318E-02 4.8213679343E-04 3.1574421387E-03 1.5252139820E-05
C8 7.9178396868E+00 -6.9696061103E-03 2.3109694066E-02 -3.1075734696E-03 -8.8024087200E-04 2.0887188133E-03 1.5150663827E-05
H9 3.5199187412E+01 1.6417121822E-01 1.1248749259E-02 -2.7411029460E-03 4.6640627326E-03 3.3729937061E-03 1.5341831206E-05
H10 3.7421978196E+01 2.6055261264E-01 2.1880009848E-02 -2.6621895530E-03 6.9625558350E-03 4.4276877233E-03 2.6343465635E-05

C11 8.1597357551E+00 -9.5874266028E-03 2.5691980841E-03 -3.0085653625E-03 -
1.1749677797E-03 1.2652420471E-03 2.3198715517E-06

H12 3.5284284018E+01 1.8289945398E-01 1.1815554557E-02 -2.6954023045E-03 5.1835954468E-
03 3.3597648633E-03 1.5468102557E-05

H13 3.5143663276E+01 1.8267735386E-01 1.1815464906E-02 -2.7527277383E-03 5.1980168496E-
03 3.3397456937E-03 1.5351049727E-05

C14 3.0850322128E+00 5.4014133911E-03 4.2014941233E-03 -2.6630774709E-04 1.7508450540E-
03 7.4636362142E-04 9.5127120914E-07

H15 3.8328833574E+01 2.1492435054E-01 1.1792092103E-02 3.0701919989E-04 5.6073804104E-
03 2.7389116753E-03 9.9648445606E-06

C16 7.7052113816E+00 -9.5057229082E-03 2.3732408669E-02 -3.1048798687E-03 -
1.2336745142E-03 1.6611481754E-03 9.1330144205E-06

H17 3.7559255994E+01 2.6239266365E-01 2.2798417469E-02 -2.6254074316E-03 6.9860985450E-
03 4.4776315258E-03 2.7142923937E-05

H18 3.4755603987E+01 1.6380647619E-01 1.1242361129E-02 -2.7629512460E-03 4.7130953687E-
03 3.3616962960E-03 1.5252227568E-05

C19 7.6577997223E+00 -8.9553621313E-03 2.4024537656E-02 -3.1054440102E-03 -
1.1694432417E-03 1.7730392330E-03 1.1767430463E-05

H20 3.7241502762E+01 2.6153501496E-01 2.2310404318E-02 -2.6225960712E-03 7.0226761961E-
03 4.4364766517E-03 2.6591983286E-05

H21 3.5216800052E+01 1.6403530427E-01 1.1245439905E-02 -2.8129845211E-03 4.6578707899E-
03 3.3761474168E-03 1.5379807942E-05

C22 8.2369250053E+00 5.1165628722E-03 2.7300685808E-02 -1.2463127447E-02 6.2117390518E-
04 5.7303337525E-03 6.7961134399E-05

H23 3.9378165235E+01 1.8622692938E-02 7.4937413231E-03 -1.0892591053E-02 4.7291926443E-
04 3.1586143234E-03 1.5265704673E-05

B24 3.5671932249E+00 5.2526055137E-02 2.9041368642E-02 -1.0724673311E-02 1.4724757484E-
02 1.0222551929E-02 1.3825793229E-04

H25 6.5586910696E+01 -4.0256689860E-01 2.8075971454E-02 -1.4220401430E-02 -
6.1379152383E-03 5.9184864004E-03 6.8624462265E-05

Total 6.4676636696E+02 2.1621554563E+00 2.9041368642E-02 -1.4220401430E-02
3.3430239523E-03 4.0909654982E-05

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP- _IDS(A)

C1	1.8238131015E-02	1.1165689429E-04	1.4960519894E+00	5.0479762664E-03
6.1479388500E+00 -1.3190154748E-02				
H2	1.7947191489E-01	1.3043713165E-03	2.9459608605E+01	1.7161535850E-01
5.7779321257E+00 -7.8565563980E-03				
H3	2.7106349504E-01	2.8016978117E-03	3.2885490394E+01	2.6561585290E-01
4.4708287776E+00 -5.4476421374E-03				
C4	5.9362487603E-03	1.4484943253E-05	3.0860505952E+00	5.9211301255E-03
1.6389057593E-01 -1.5118634828E-05				
H5	2.1477991702E-01	1.5867634695E-03	3.8268437115E+01	2.1477991702E-01
0.0000000000E+00 NULL				
C6	4.4669771029E-02	5.3378681713E-04	2.9118348245E+00	2.5164150507E-02
5.3481680996E+00 -1.9505620522E-02				
H7	1.2388201419E-01	6.0860984501E-04	2.0274007851E+01	7.1416010662E-02
1.9030204962E+01 -5.2466003528E-02				
C8	1.9952830862E-02	1.2609545949E-04	1.6347351240E+00	6.4916123757E-03
6.2831045628E+00 -1.3461218486E-02				
H9	1.7946050118E-01	1.3057248525E-03	2.9289981948E+01	1.7181585970E-01
5.9092054636E+00 -7.6446414755E-03				
H10	2.7160833836E-01	2.7999367101E-03	3.3029350307E+01	2.6608047550E-01
4.3926278887E+00 -5.5278628579E-03				
C11	1.3730966632E-02	3.0194456196E-05	1.7306853780E+00	2.0717700146E-03
6.4290503770E+00 -1.1659196617E-02				
H12	1.9460476712E-01	1.4938577007E-03	3.0670865184E+01	1.8875211055E-01
4.6134188344E+00 -5.8526565735E-03				
H13	1.9403703161E-01	1.4890520860E-03	3.0773201064E+01	1.8835719274E-01
4.3704622124E+00 -5.6798388724E-03				
C14	5.4207968317E-03	1.2391740244E-05	3.0125437905E+00	5.4111051114E-03
7.2488422271E-02 -9.6917203116E-06				
H15	2.1492435054E-01	1.5871034617E-03	3.8328833574E+01	2.1492435054E-01
0.0000000000E+00 NULL				
C16	1.7426526647E-02	8.2098774752E-05	1.4612123116E+00	3.9604018695E-03
6.2439990700E+00 -1.3466124778E-02				
H17	2.7344689085E-01	2.8525690343E-03	3.2926396117E+01	2.6791977725E-01
4.6328598769E+00 -5.5271135989E-03				
H18	1.7858932428E-01	1.3021359255E-03	2.9252321644E+01	1.7119790023E-01
5.5032823430E+00 -7.3914240474E-03				
C19	1.8244077717E-02	1.0058541345E-04	1.3377126054E+00	4.6443577931E-03
6.3200871169E+00 -1.3599719924E-02				

H20	2.7223333778E-01	2.8270011430E-03	3.2758568891E+01	2.6688417637E-01
4.4829338711E+00 -5.3491614126E-03				
H21	1.7959293167E-01	1.3056828734E-03	2.9512692111E+01	1.7181411797E-01
5.7041079407E+00 -7.7788136995E-03				
C22	4.5513684929E-02	5.6296904265E-04	2.8644862910E+00	2.5315123901E-02
5.3724387143E+00 -2.0198561029E-02				
H23	1.2425595930E-01	6.0994247130E-04	2.0221971274E+01	7.1439326120E-02
1.9156193961E+01 -5.2816633183E-02				
B24	5.7656440233E-02	1.2666261829E-03	3.0668712433E+00	5.5091247685E-02
5.0032198159E-01 -2.5651925483E-03				
H25	6.1818103748E-01	6.9717879795E-03	1.0864589345E+01	1.0780706944E-01
5.4722321351E+01 -5.1037396804E-01				

Total	3.7369212860E+00	3.3687126405E-02	4.6111849958E+02	2.9495383711E+00
1.8564786738E+02 -7.8738291483E-01				

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

C1	1.1112201086E-05	3.3741984250E-03	3.9157517077E-03	4.1467588172E-05
7.9070541349E-05				
H2	1.0663411477E-05	5.8254459792E-03	2.6680102882E-03	9.8636829992E-06
1.2903162407E-03				
H3	4.0326902215E-05	8.0769923063E-03	3.7970939758E-03	1.9682408215E-05
2.7926428466E-03				
C4	2.2496901001E-04	1.9186756480E-03	7.4901982107E-04	1.0118158673E-06
1.4483243140E-05				
H5	2.9883546194E-04	5.6124559353E-03	2.7392373162E-03	9.9643643217E-06
1.5867634695E-03				
C6	1.3709523692E-04	8.6420253978E-03	6.7120610564E-03	6.4155382969E-05
4.0427910610E-04				
H7	1.3021091737E-05	3.5225403475E-03	1.8921428864E-03	4.7539558055E-06
3.4794751634E-04				
C8	9.5359412138E-05	3.9710484471E-03	4.4429555045E-03	4.0959215960E-05
9.2735976227E-05				

H9	2.9221600747E-05	5.8660281869E-03	2.6411312140E-03	9.7038905562E-06
1.2921034552E-03				
H10	1.3446689357E-05	8.0558797865E-03	3.7979442894E-03	1.9593834617E-05
2.7906839516E-03				
C11	1.1090669849E-04	1.1970806716E-03	6.8441588476E-04	6.1467757794E-07
3.5438893368E-06				
H12	4.6677754397E-06	6.1541175778E-03	2.7432720985E-03	1.0501417051E-05
1.4836902280E-03				
H13	3.9284740432E-07	6.1208189667E-03	2.7642997124E-03	1.0600943044E-05
1.4791252296E-03				
C14	8.6644170781E-05	1.7961913544E-03	7.2705774696E-04	8.8629754726E-07
1.2389390392E-05				
H15	3.0701919989E-04	5.6073804104E-03	2.7389116753E-03	9.9648445606E-06
1.5871034617E-03				
C16	4.4721604924E-05	2.7103534771E-03	2.6275774200E-03	2.5964237748E-05
4.8673352836E-05				
H17	1.0165079490E-05	8.1369299056E-03	3.8225388011E-03	2.0146543741E-05
2.8433975274E-03				
H18	6.3453030089E-06	5.8524551424E-03	2.6581884097E-03	9.8127314641E-06
1.2889732086E-03				
C19	6.3919180709E-05	3.4718651632E-03	3.6953671181E-03	3.7945063178E-05
6.6884173352E-05				
H20	7.2889010798E-05	8.1470035293E-03	3.7871276871E-03	1.9656594483E-05
2.8182282313E-03				
H21	2.2885871372E-06	5.8217026534E-03	2.6653749835E-03	9.8721167794E-06
1.2916034495E-03				
C22	1.7600743111E-06	8.8375790034E-03	6.9652799589E-03	7.0123540827E-05
4.2459232883E-04				
H23	5.0197334953E-05	3.5327577689E-03	1.8848312517E-03	4.7266011240E-06
3.4795902651E-04				
B24	3.6967060648E-04	1.7963338958E-02	8.1290951429E-03	8.3984995636E-05
1.2471939238E-03				
H25	3.5115710171E-06	9.9227928474E-03	6.4926923786E-03	5.9670641285E-05
1.7180442311E-03				

Total 3.9284740432E-07 6.3964867466E-03 1.8402525397E-05 2.7352427999E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
C1	-9.5306257436E-05	-2.1454596524E-03	6.9243778695E-04	6.9737325330E-07	3.2586352938E-05
H2	-4.7137286484E-05	-1.3597522828E-03	6.5791298680E-04	5.8361802180E-07	1.4055075815E-05
H3	-5.7861305331E-06	-1.2184859695E-03	6.2488818850E-04	5.4063569845E-07	9.0549651500E-06
C4	-4.7735573674E-05	-9.2248347672E-05	3.6251510205E-05	1.8637071513E-09	1.7001131204E-09
H5	NULL	NULL	NULL	NULL	NULL
C6	-5.9786040341E-07	-3.6471592064E-03	2.6570036434E-03	1.0913570119E-05	1.2950771102E-04
H7	-6.1143261143E-07	-2.7569857305E-03	1.8749665448E-03	6.0963245446E-06	2.6066232866E-04
C8	-2.9355082766E-06	-2.1424469944E-03	7.0435117679E-04	7.1931576734E-07	3.3359483266E-05
H9	-4.0736510407E-06	-1.2936834779E-03	6.8241864623E-04	6.3149792654E-07	1.3621397369E-05
H10	-5.8936313444E-05	-1.2584409602E-03	6.1683021619E-04	5.2275528676E-07	9.2527584941E-06
C11	-2.2017670938E-05	-1.8135176945E-03	8.2161067458E-04	8.5648846524E-07	2.6650566859E-05
H12	-2.7681389008E-06	-1.2686159188E-03	6.6079316237E-04	5.9450475329E-07	1.0167472722E-05
H13	-1.0201130140E-05	-1.2995968381E-03	6.5753579142E-04	5.8239966871E-07	9.9268563843E-06
C14	-2.4044535372E-05	-1.3370025182E-04	1.2004439136E-04	1.4541169900E-08	2.3498519103E-09
H15	NULL	NULL	NULL	NULL	NULL
C16	-9.4276851176E-05	-2.1566506700E-03	6.9519661724E-04	7.0206526998E-07	3.3425421917E-05
H17	-3.1483818731E-05	-1.1930241246E-03	6.4189761725E-04	5.5635765111E-07	9.1715069018E-06
H18	-8.3431540121E-05	-1.3430937369E-03	6.6343585575E-04	5.8789308133E-07	1.3162716959E-05

C19	-8.3785431792E-05	-2.1518247570E-03	6.9436492860E-04	7.0205141153E-07
3.3701240102E-05				
H20	-4.2910477665E-06	-1.1932278205E-03	6.2145563075E-04	5.3316500661E-07
8.7729116810E-06				
H21	-2.9459329827E-05	-1.3637213356E-03	6.7571868315E-04	6.0855961207E-07
1.4079423924E-05				
C22	-1.7054796514E-04	-3.7596633676E-03	2.7646601116E-03	1.1621709836E-05
1.3837671383E-04				
H23	-2.2772156968E-05	-2.7571569430E-03	1.8795130293E-03	6.0742597480E-06
2.6198344479E-04				
B24	-7.8170563990E-04	-5.1270834437E-03	3.1801545187E-03	1.2552522302E-05
1.9432259076E-05				
H25	-7.4718628673E-06	-9.3266139929E-03	2.2319922394E-03	9.0215974809E-06
5.2537437484E-03				

Total	-5.9786040341E-07	-4.2412709930E-03	1.6133738197E-05	6.3346984062E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	8.9724301275E+00
H2	3.1648067700E+01
H3	3.3097563104E+01
C4	4.6034743752E+00
H5	3.3734804000E+01
C6	1.1072190821E+01
H7	3.4274299665E+01
C8	8.5297594305E+00
H9	3.1334957617E+01
H10	3.3040905078E+01
C11	8.3488272871E+00
H12	3.1561594760E+01
H13	3.1353144484E+01

C14	4.7722416927E+00
H15	3.3656936532E+01
C16	8.6951836777E+00
H17	3.3318364131E+01
H18	3.1444784819E+01
C19	8.7091698698E+00
H20	3.3134642031E+01
H21	3.1312644081E+01
C22	1.0841057855E+01
H23	3.4427433011E+01
B24	5.6101323311E+00
H25	5.6170775756E+01

Total	5.9366538424E+02

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A | \text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.0342216998E+02	6.0050887138E+01	5.9730265012E+00	9.9466082617E-02	
	9.9976421100E+01				

H2 9.9112868516E+01	8.8795530423E+01	6.7262137203E+01	1.0080005641E+00	1.4986151288E-02
H3 9.9074372708E+01	9.0890336933E+01	6.8662439184E+01	1.0132155515E+00	1.4756474771E-02
C4 9.9993580166E+01	2.0146854255E+02	5.0569267143E+01	5.9485534927E+00	1.1763179158E-01
H5 9.9054307976E+01	8.9931604570E+01	6.8059781706E+01	1.0102821463E+00	1.4844040357E-02
C6 9.9984846392E+01	1.9023247401E+02	7.3514443561E+01	6.6129201992E+00	8.9954026433E-02
H7 9.9019994817E+01	9.1005299394E+01	6.9019430515E+01	1.0122097915E+00	1.4665577272E-02
C8 9.9977123495E+01	2.0380813147E+02	6.0149117907E+01	5.9732635816E+00	9.9307584043E-02
H9 9.9113428117E+01	8.9382419204E+01	6.7281421482E+01	1.0080122665E+00	1.4982029873E-02
H10 9.9072006480E+01	9.0584206617E+01	6.8598633073E+01	1.0131926461E+00	1.4769866405E-02
C11 9.9977142780E+01	2.0703512358E+02	5.9345093567E+01	5.9701583962E+00	1.0060070745E-01
H12 9.9126883436E+01	8.9762403914E+01	6.7114677633E+01	1.0123341026E+00	1.5083646951E-02
H13 9.9126785893E+01	8.9149117232E+01	6.7114030403E+01	1.0123378903E+00	1.5083848850E-02
C14 9.9993412140E+01	2.0198875898E+02	5.0639704040E+01	5.9487801424E+00	1.1747264829E-01
H15 9.9052514978E+01	8.9693918449E+01	6.8012568348E+01	1.0102625440E+00	1.4854056663E-02
C16 9.9976985354E+01	2.0372858465E+02	6.0144650385E+01	5.9731122201E+00	9.9312443947E-02
H17 9.9071021464E+01	9.0947632057E+01	6.8573972187E+01	1.0131782646E+00	1.4774968291E-02
H18 9.9112337457E+01	8.9124843826E+01	6.7254824341E+01	1.0080000545E+00	1.4987773210E-02
C19 9.9976631161E+01	2.0403856273E+02	6.0095148546E+01	5.9729882563E+00	9.9392187235E-02
H20 9.9073945369E+01	9.0425291065E+01	6.8650878571E+01	1.0132092643E+00	1.4758868137E-02

H21	8.9487649448E+01	6.7255750441E+01	1.0079949982E+00	1.4987491651E-02
9.9112235902E+01				
C22	1.9008334313E+02	7.3436821262E+01	6.6126581616E+00	9.0045539118E-02
9.9984511813E+01				
H23	9.1299172551E+01	6.8970689875E+01	1.0121878377E+00	1.4675622929E-02
9.9018075553E+01				
B24	1.4207674392E+02	2.7494322055E+01	3.0821776567E+00	1.1210233336E-01
9.9983288646E+01				
H25	1.3204241439E+02	1.2030053401E+02	1.6170190227E+00	1.3441494969E-02
9.8822175466E+01				

Total	3.3404042751E+03	1.6475712246E+03	7.3839075553E+01	4.4816924726E-02
9.9782807645E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.6668540921E+02	5.6624107186E+01	5.9707530709E+00	1.0544542541E-01	
9.9938368460E+01					
H2	7.4097469226E+01	5.0586535289E+01	9.9715434738E-01	1.9711853000E-02	
9.8046401204E+01					
H3	7.4718389398E+01	5.1049753934E+01	1.0017853888E+00	1.9623706513E-02	
9.7956707076E+01					
C4	1.6659875716E+02	4.9149988973E+01	5.9475954103E+00	1.2100908941E-01	
9.9977475059E+01					
H5	7.3850019976E+01	5.0423969371E+01	9.9888444251E-01	1.9809714606E-02	
9.7936806627E+01					
C6	1.5927528831E+02	6.9834503735E+01	6.6104447534E+00	9.4658720259E-02	
9.9947418590E+01					
H7	7.4577702272E+01	5.0710638770E+01	1.0003641529E+00	1.9726908931E-02	
9.7861188528E+01					
C8	1.6696501863E+02	5.6586872917E+01	5.9709046645E+00	1.0551748765E-01	
9.9937641269E+01					
H9	7.4046955517E+01	5.0587500553E+01	9.9716259180E-01	1.9711639850E-02	
9.8046627157E+01					
H10	7.4784062465E+01	5.1002159673E+01	1.0017382638E+00	1.9641095010E-02	
9.7951974034E+01					

C11	1.7086248649E+02 9.9938219782E+01	5.5843735978E+01	5.9678341003E+00	1.0686666993E-01
H12	7.4340384433E+01 9.8078420643E+01	5.0631248649E+01	1.0016266678E+00	1.9782776339E-02
H13	7.4199301056E+01 9.8074968220E+01	5.0595796246E+01	1.0015961430E+00	1.9796034795E-02
C14	1.6647123018E+02 9.9977517623E+01	4.9205375107E+01	5.9478345502E+00	1.2087774023E-01
H15	7.3911643567E+01 9.7938152869E+01	5.0434489548E+01	9.9889687297E-01	1.9805828946E-02
C16	1.6674387560E+02 9.9937467120E+01	5.6578680149E+01	5.9707512083E+00	1.0553005465E-01
H17	7.4929737234E+01 9.7951365803E+01	5.0996825323E+01	1.0017277843E+00	1.9642944006E-02
H18	7.3601196781E+01 9.8044638100E+01	5.0564177900E+01	9.9714125491E-01	1.9720309839E-02
C19	1.6669389738E+02 9.9937637478E+01	5.6574738056E+01	5.9706586238E+00	1.0553577142E-01
H20	7.4611898836E+01 9.7956774259E+01	5.1049760132E+01	1.0017841806E+00	1.9623680465E-02
H21	7.4076725023E+01 9.8044159817E+01	5.0562182698E+01	9.9713241053E-01	1.9720913088E-02
C22	1.5922381190E+02 9.9948112113E+01	6.9839333941E+01	6.6102508010E+00	9.4649396378E-02
H23	7.4651653887E+01 9.7861065157E+01	5.0709260645E+01	1.0003605845E+00	1.9727374680E-02
B24	1.1557062435E+02 9.9942309409E+01	2.5588501722E+01	3.0809143927E+00	1.2040229734E-01
H25	1.0644065209E+02 9.7531445389E+01	8.7400809714E+01	1.5958989140E+00	1.8259543810E-02

Total	2.7519281910E+03 9.9515401537E+01	1.3431309462E+03	7.3641195575E+01	5.4828008976E-02

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.3988983748E+02 9.9861835837E+01	5.3492371250E+01	5.9661806789E+00	1.1153329979E-01
H2	6.2748047474E+01 9.6418045711E+01	3.9070181670E+01	9.8059359921E-01	2.5098260548E-02
H3	6.2725357515E+01 9.6279329274E+01	3.9077387700E+01	9.8463115175E-01	2.5196954293E-02
C4	1.4099317545E+02 9.9937182329E+01	4.7532006905E+01	5.9451984218E+00	1.2507779092E-01
H5	6.2002699251E+01 9.6292200117E+01	3.8573251575E+01	9.8211064813E-01	2.5460924553E-02
C6	1.3784526020E+02 9.9862944383E+01	6.6033409565E+01	6.6048576949E+00	1.0002296926E-01
H7	6.2317772530E+01 9.6188050115E+01	3.8677429584E+01	9.8326086899E-01	2.5422084135E-02
C8	1.3945456609E+02 9.9862897587E+01	5.3522528115E+01	5.9664390058E+00	1.1147528370E-01
H9	6.2435920059E+01 9.6420320376E+01	3.9081723043E+01	9.8062258087E-01	2.5091590250E-02
H10	6.2670099056E+01 9.6284255826E+01	3.9103275216E+01	9.8468279188E-01	2.5181593778E-02
C11	1.4291258755E+02 9.9863353818E+01	5.2755194355E+01	5.9633634618E+00	1.1303841327E-01
H12	6.2852022531E+01 9.6469727550E+01	3.9170830003E+01	9.8519787652E-01	2.5151314803E-02
H13	6.2643565736E+01 9.6462560223E+01	3.9136929286E+01	9.8512933542E-01	2.5171349756E-02
C14	1.4117230659E+02 9.9936817531E+01	4.7575115378E+01	5.9454132317E+00	1.2496897137E-01
H15	6.1924832172E+01 9.6289754751E+01	3.8558336423E+01	9.8208442882E-01	2.5470093368E-02
C16	1.3961308882E+02 9.9862156185E+01	5.3492660490E+01	5.9662517661E+00	1.1153402563E-01
H17	6.2953438162E+01 9.6286979841E+01	3.9117216628E+01	9.8470646307E-01	2.5173224170E-02
H18	6.2546917202E+01 9.6417303055E+01	3.9064554202E+01	9.8059080462E-01	2.5101804555E-02
C19	1.3962170395E+02 9.9862440987E+01	5.3491880285E+01	5.9661660964E+00	1.1153405086E-01

H20	6.2771118942E+01	3.9075263936E+01	9.8462608435E-01	2.5198194079E-02
9.6279015922E+01				
H21	6.2413527350E+01	3.9067977010E+01	9.8059306160E-01	2.5099663117E-02
9.6417909830E+01				
C22	1.3758569311E+02	6.5955276048E+01	6.6045757568E+00	1.0013718617E-01
9.9862304483E+01				
H23	6.2470905483E+01	3.8670971084E+01	9.8324844682E-01	2.5426008690E-02
9.6187056758E+01				
B24	9.8885933213E+01	2.3656991836E+01	3.0780551570E+00	1.3011185777E-01
9.9849558173E+01				
H25	8.8484909510E+01	6.6235187326E+01	1.5658909052E+00	2.3641375051E-02
9.5697541972E+01				

Total	2.3219352854E+03	1.1291879489E+03	7.3334470318E+01	6.4944432314E-02
9.9100906813E+01				

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	H2	1.7030684550E-02		
C1	H3	2.2689563250E-02		
C1	C4	-1.2057951054E-02		
C1	C6	-2.1013991209E-03		
C1		2.5560897625E-02	2.5564792700E-02	
H2	C1	-1.7026789475E-02		
H2		-1.7026789475E-02	-1.7022894400E-02	
H3	C1	-2.2685668175E-02		
H3		-2.2685668175E-02	-2.2681773100E-02	
C4	C1	1.2061846129E-02		
C4	H5	1.9935309650E-02		

C4	C11	7.1255997015E-03
C4	C19	1.1937944944E-02
C4		5.1060700425E-02 5.1064595500E-02
H5	C4	-1.9931414575E-02
H5		-1.9931414575E-02 -1.9927519500E-02
C6	C1	2.1052941959E-03
C6	H7	2.2235465850E-02
C6	C8	2.3035447384E-03
C6	B24	-6.4057064696E-01
C6		-6.1392634218E-01 -6.1392244710E-01
H7	C6	-2.2231570775E-02
H7		-2.2231570775E-02 -2.2227675700E-02
C8	C6	-2.2996496560E-03
C8	H9	1.7036749450E-02
C8	H10	2.2690868950E-02
C8	C14	-1.2062232019E-02
C8		2.5365736725E-02 2.5369631800E-02
H9	C8	-1.7032854375E-02
H9		-1.7032854375E-02 -1.7028959300E-02
H10	C8	-2.2686973875E-02
H10		-2.2686973875E-02 -2.2683078800E-02
C11	C4	-7.1217046265E-03
C11	C14	-6.9275423485E-03
C11	H12	2.1258602750E-02
C11	H13	2.1263428750E-02
C11		2.8472784525E-02 2.8476679600E-02
H12	C11	-2.1254707675E-02
H12		-2.1254707675E-02 -2.1250812600E-02
H13	C11	-2.1259533675E-02
H13		-2.1259533675E-02 -2.1255638600E-02
C14	C8	1.2066127101E-02
C14	C11	6.9314374235E-03

C14	H15	1.9933982050E-02
C14	C16	1.1892492851E-02
C14		5.0824039425E-02 5.0827934500E-02
H15	C14	-1.9930086975E-02
H15		-1.9930086975E-02 -1.9926191900E-02
C16	C14	-1.1888597776E-02
C16	H17	2.2686520650E-02
C16	H18	1.7035619750E-02
C16	C22	-2.3246648994E-03
C16		2.5508877725E-02 2.5512772800E-02
H17	C16	-2.2682625575E-02
H17		-2.2682625575E-02 -2.2678730500E-02
H18	C16	-1.7031724675E-02
H18		-1.7031724675E-02 -1.7027829600E-02
C19	C4	-1.1934049876E-02
C19	C22	-2.1734344987E-03
C19	H20	2.2687628450E-02
C19	H21	1.7031560250E-02
C19		2.5611704325E-02 2.5615599400E-02
H20	C19	-2.2683733375E-02
H20		-2.2683733375E-02 -2.2679838300E-02
H21	C19	-1.7027665175E-02
H21		-1.7027665175E-02 -1.7023770100E-02
C22	C16	2.3285599744E-03
C22	C19	2.1773295664E-03
C22	B24	-6.4042539387E-01
C22	H23	2.2233108150E-02
C22		-6.1368639618E-01 -6.1368250110E-01
H23	C22	-2.2229213075E-02
H23		-2.2229213075E-02 -2.2225318000E-02
B24	C6	6.4057454203E-01
B24	C22	6.4042928894E-01

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B24   H25   6.3629945755E-01
B24               1.9173032885E+00 1.9173071836E+00
H25   B24   -6.3629556247E-01
H25               -6.3629556247E-01 -6.3629166740E-01

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Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

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Atom A  Mu_Intra_X(A)  Mu_Bond_X(A)  Mu_X(A)
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C1  -2.4508727866E-02 -3.3012150166E-02 -5.7520878032E-02
H2  -1.2756877609E-01 -1.0619526639E-02 -1.3818830273E-01
H3  -7.6235528204E-03 -4.9241229154E-04 -8.1159651119E-03
C4  -4.3019170676E-04 -1.4749610618E-04 -5.7768781294E-04
H5  -1.1095560138E-05 -6.3229118355E-07 -1.1727851322E-05
C6  8.2319337534E-01 -1.0746266214E+00 -2.5143324610E-01
H7  -1.3008180939E-01 -1.4350260821E-02 -1.4443207021E-01
C8  -2.4623523637E-02 -3.3012639373E-02 -5.7636163010E-02
H9  -1.2756630118E-01 -1.0623333760E-02 -1.3818963494E-01
H10 -7.6011028345E-03 -4.9072695383E-04 -8.0918297883E-03
C11 -8.2852533137E-04 -5.1374527760E-06 -8.3366278415E-04
H12 1.1906953630E-01 1.3050015944E-02 1.3211955224E-01
H13 -1.1907963963E-01 -1.3053004586E-02 -1.3213264422E-01
C14 2.9031885138E-04 -2.0507111155E-04 8.5247739830E-05
H15 3.4846716079E-06 5.9872039986E-07 4.0833920078E-06
C16 2.4383046794E-02 3.2804926068E-02 5.7187972862E-02
H17 7.6212407222E-03 4.9230792085E-04 8.1135486431E-03
H18 1.2756233644E-01 1.0622625163E-02 1.3818496160E-01

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C19	2.4138781643E-02	3.2858205385E-02	5.6996987028E-02
H20	7.6061598492E-03	4.9073898590E-04	8.0968988351E-03
H21	1.2756650443E-01	1.0620067752E-02	1.3818657218E-01
C22	-8.2438109559E-01	1.0743792415E+00	2.4999814591E-01
H23	1.3007943063E-01	1.4348784664E-02	1.4442821529E-01
B24	-1.3103374934E-04	-1.2160130665E-04	-2.5263505599E-04
H25	6.8689546128E-07	3.6933272157E-07	1.0562281828E-06

Total	-2.9204728187E-03	-1.0927328624E-03	-4.0132056811E-03

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	2.9641285072E-02	2.7622539584E-02	5.7263824656E-02
H2	1.4361875685E-02	3.3947706199E-04	1.4701352747E-02
H3	1.2603074006E-01	1.4495415485E-02	1.4052615554E-01
C4	3.8122808753E-02	1.2770759983E-02	5.0893568736E-02
H5	1.2340631407E-01	1.2440660403E-02	1.3584697447E-01
C6	4.6638331121E-04	-3.5785653770E-04	1.0852677351E-04
H7	-2.2724053727E-06	-8.7135020381E-08	-2.3595403931E-06
C8	-2.9077899472E-02	-2.7865097953E-02	-5.6942997425E-02
H9	-1.4387254377E-02	-3.4195188661E-04	-1.4729206264E-02
H10	-1.2602215335E-01	-1.4494855608E-02	-1.4051700896E-01
C11	1.7700714606E-05	-2.3295537176E-04	-2.1525465715E-04
H12	3.0196316482E-06	-4.3284704702E-08	2.9763469435E-06
H13	-8.5643624274E-06	-1.3693393725E-06	-9.9337017999E-06
C14	-3.9499653374E-02	-1.2999589470E-02	-5.2499242844E-02
H15	-1.2341757395E-01	-1.2441102401E-02	-1.3585867635E-01
C16	-2.9244992902E-02	-2.7884786663E-02	-5.7129779565E-02
H17	-1.2601706980E-01	-1.4492084405E-02	-1.4050915421E-01
H18	-1.4381546073E-02	-3.4070888705E-04	-1.4722254960E-02
C19	2.9540749498E-02	2.7709377467E-02	5.7250126965E-02
H20	1.2603088873E-01	1.4494177851E-02	1.4052506658E-01

H21	1.4374714464E-02	3.4073671208E-04	1.4715451176E-02
C22	4.4711827692E-04	-1.9197768104E-04	2.5514059588E-04
H23	1.0948475327E-05	1.4661916457E-06	1.2414666973E-05
B24	1.8683404479E-04	-7.9131972996E-07	1.8604272506E-04
H25	-3.7339345040E-05	1.0011362400E-04	6.2774278964E-05

Total	5.4506137566E-04	-1.3305335798E-03	-7.8547220414E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	-3.9462839285E-03	-1.1689432158E-02	-1.5635716087E-02
H2	9.0449155180E-02	7.5336232111E-03	9.7982778391E-02
H3	-8.7006691319E-02	-9.5974226562E-03	-9.6604113975E-02
C4	2.7702605115E-02	1.0264240844E-03	2.8729029199E-02
H5	8.7260131516E-02	8.8145875620E-03	9.6074719078E-02
C6	-7.1288245436E-01	7.0041523778E-01	-1.2467216579E-02
H7	-7.9711496831E-02	-9.2254050356E-03	-8.8936901867E-02
C8	-4.2477646405E-03	-1.1524445024E-02	-1.5772209664E-02
H9	9.0448406204E-02	7.5361837524E-03	9.7984589956E-02
H10	-8.7023787165E-02	-9.6001887036E-03	-9.6623975869E-02
C11	5.1621343917E-02	4.4493539697E-02	9.6114883614E-02
H12	9.8824148821E-02	9.7449788272E-03	1.0856912765E-01
H13	9.8817228009E-02	9.7471541469E-03	1.0856438216E-01
C14	2.7093740055E-02	8.9617128950E-04	2.7989911344E-02
H15	8.7243523112E-02	8.8122166597E-03	9.6055739772E-02
C16	-4.6490469844E-03	-1.1357068807E-02	-1.6006115792E-02
H17	-8.7029616866E-02	-9.5982517591E-03	-9.6627868625E-02
H18	9.0452912884E-02	7.5357492282E-03	9.7988662112E-02
C19	-4.2747191108E-03	-1.1523881711E-02	-1.5798600821E-02
H20	-8.7011275194E-02	-9.5966989903E-03	-9.6607974184E-02
H21	9.0452613254E-02	7.5339621021E-03	9.7986575356E-02
C22	-7.1369774026E-01	7.0034070409E-01	-1.3357036166E-02

H23 -7.9713251278E-02 -9.2243502609E-03 -8.8937601539E-02
B24 -7.6300780799E-02 5.5748855073E-02 -2.0551925726E-02
H25 3.0116667546E-01 -8.0640636277E-01 -5.0523968731E-01

Total -8.8596242521E-01 6.6083587963E-01 -2.2512654558E-01

Atom A |Mu_Intra(A)| |Mu_Bond(A)| |Mu(A)|

C1 3.8663376458E-02 4.4603246248E-02 8.2657562518E-02
H2 1.5703854871E-01 1.3024786731E-02 1.7003753011E-01
H3 1.5333633076E-01 1.7391666440E-02 1.7072148113E-01
C4 4.7127146553E-02 1.2812790955E-02 5.8445240872E-02
H5 1.5114049433E-01 1.5246868057E-02 1.6638735606E-01
C6 1.0889669161E+00 1.2827330232E+00 2.5174217071E-01
H7 1.5256211806E-01 1.7059838326E-02 1.6961838174E-01
C8 3.8339087867E-02 4.4711417729E-02 8.2542079207E-02
H9 1.5703842991E-01 1.3029436550E-02 1.7004206712E-01
H10 1.5333786040E-01 1.7392678781E-02 1.7072404701E-01
C11 5.1627995461E-02 4.4494149833E-02 9.6118740006E-02
H12 1.5473773578E-01 1.6287035596E-02 1.7100535539E-01
H13 1.5474109085E-01 1.6290731861E-02 1.7101245814E-01
C14 4.7899662336E-02 1.3032056765E-02 5.9494646006E-02
H15 1.5114010023E-01 1.5245858184E-02 1.6638595223E-01
C16 3.8359043506E-02 4.4527603949E-02 8.2404318430E-02
H17 1.5333799074E-01 1.7389344851E-02 1.7072081619E-01
H18 1.5703728218E-01 1.3028574916E-02 1.7004001384E-01
C19 3.8387626699E-02 4.4500237195E-02 8.2315425989E-02
H20 1.5333819026E-01 1.7390188263E-02 1.7072186381E-01
H21 1.5703986982E-01 1.3025456826E-02 1.7003953124E-01
C22 1.0903984846E+00 1.2824850460E+00 2.5035484511E-01
H23 1.5256100688E-01 1.7058026299E-02 1.6961546655E-01
B24 7.6301122059E-02 5.5748987699E-02 2.0554320407E-02

H25 3.0116667778E-01 8.0640636899E-01 5.0523969122E-01

Total 8.8596740636E-01 6.6083812253E-01 2.2516368337E-01

Bond Contributions to Atomic Dipole Moments:

 $\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	H2	-1.8112401480E-02	
C1	H3	-4.9623219266E-04	
C1	C4	-1.4486834469E-02	
C1	C6	8.3317975850E-05	
C1		-3.3012150166E-02	
H2	C1	-1.0619526639E-02	
H2		-1.0619526639E-02	
H3	C1	-4.9241229154E-04	
H3		-4.9241229154E-04	
C4	C1	-1.4290922622E-02	
C4	H5	-1.0767137266E-06	
C4	C11	4.4692889447E-07	
C4	C19	1.4144056301E-02	
C4		-1.4749610618E-04	
H5	C4	-6.3229118355E-07	
H5		-6.3229118355E-07	
C6	C1	9.8438207778E-05	
C6	H7	-2.4423777249E-02	
C6	C8	1.0801545267E-04	
C6	B24	-1.0504092979E+00	

C6		-1.0746266214E+00
H7	C6	-1.4350260821E-02
H7		-1.4350260821E-02
C8	C6	9.1492544978E-05
C8	H9	-1.8118896289E-02
C8	H10	-4.9336166861E-04
C8	C14	-1.4491873961E-02
C8		-3.3012639373E-02
H9	C8	-1.0623333760E-02
H9		-1.0623333760E-02
H10	C8	-4.9072695383E-04
H10		-4.9072695383E-04
C11	C4	4.3907125917E-07
C11	C14	-4.4806208958E-07
C11	H12	2.2399666767E-02
C11	H13	-2.2404795229E-02
C11		-5.1374527760E-06
H12	C11	1.3050015944E-02
H12		1.3050015944E-02
H13	C11	-1.3053004586E-02
H13		-1.3053004586E-02
C14	C8	-1.4295912883E-02
C14	C11	-4.5531265600E-07
C14	H15	1.0250932266E-06
C14	C16	1.4090271991E-02
C14		-2.0507111155E-04
H15	C14	5.9872039986E-07
H15		5.9872039986E-07
C16	C14	1.4283344353E-02
C16	H17	4.9610711300E-04
C16	H18	1.8117655569E-02
C16	C22	-9.2180966563E-05

C16		3.2804926068E-02
H17	C16	4.9230792085E-04
H17		4.9230792085E-04
H18	C16	1.0622625163E-02
H18		1.0622625163E-02
C19	C4	1.4337908835E-02
C19	C22	-8.6474266155E-05
C19	H20	4.9341711753E-04
C19	H21	1.8113353699E-02
C19		3.2858205385E-02
H20	C19	4.9073898590E-04
H20		4.9073898590E-04
H21	C19	1.0620067752E-02
H21		1.0620067752E-02
C22	C16	-1.0888865063E-04
C22	C19	-1.0210099116E-04
C22	B24	1.0501689711E+00
C22	H23	2.4421260072E-02
C22		1.0743792415E+00
H23	C22	1.4348784664E-02
H23		1.4348784664E-02
B24	C6	-5.3358282477E-01
B24	C22	5.3346095694E-01
B24	H25	2.6652855908E-07
B24		-1.2160130665E-04
H25	B24	3.6933272157E-07
H25		3.6933272157E-07

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	H2	3.7461255922E-04
C1	H3	2.4565388488E-02

C1	C4	1.4966454478E-04
C1	C6	2.5328739924E-03
C1		2.7622539584E-02
H2	C1	3.3947706199E-04
H2		3.3947706199E-04
H3	C1	1.4495415485E-02
H3		1.4495415485E-02
C4	C1	3.0595851863E-07
C4	H5	2.1212855191E-02
C4	C11	-8.4442124912E-03
C4	C19	1.8113251407E-06
C4		1.2770759983E-02
H5	C4	1.2440660403E-02
H5		1.2440660403E-02
C6	C1	2.4742554963E-03
C6	H7	-1.6678749861E-07
C6	C8	-2.7075383076E-03
C6	B24	-1.2440693893E-04
C6		-3.5785653770E-04
H7	C6	-8.7135020381E-08
H7		-8.7135020381E-08
C8	C6	-2.7721196579E-03
C8	H9	-3.7878081489E-04
C8	H10	-2.4564349768E-02
C8	C14	-1.4984771171E-04
C8		-2.7865097953E-02
H9	C8	-3.4195188661E-04
H9		-3.4195188661E-04
H10	C8	-1.4494855608E-02
H10		-1.4494855608E-02
C11	C4	-8.4273154511E-03
C11	C14	8.1967200241E-03

C11	H12	-3.9248352555E-08
C11	H13	-2.3206964509E-06
C11		-2.3295537176E-04
H12	C11	-4.3284704702E-08
H12		-4.3284704702E-08
H13	C11	-1.3693393725E-06
H13		-1.3693393725E-06
C14	C8	-3.9294294173E-07
C14	C11	8.2132810673E-03
C14	H15	-2.1213594676E-02
C14	C16	1.1170823858E-06
C14		-1.2999589470E-02
H15	C14	-1.2441102401E-02
H15		-1.2441102401E-02
C16	C14	-1.4615546943E-04
C16	H17	-2.4559697881E-02
C16	H18	-3.7666849056E-04
C16	C22	-2.8022648224E-03
C16		-2.7884786663E-02
H17	C16	-1.4492084405E-02
H17		-1.4492084405E-02
H18	C16	-3.4070888705E-04
H18		-3.4070888705E-04
C19	C4	1.4967007038E-04
C19	C22	2.6197093683E-03
C19	H20	2.4563246311E-02
C19	H21	3.7675171734E-04
C19		2.7709377467E-02
H20	C19	1.4494177851E-02
H20		1.4494177851E-02
H21	C19	3.4073671208E-04
H21		3.4073671208E-04

C22	C16	-2.7369345468E-03
C22	C19	2.5589209898E-03
C22	B24	-1.6443680540E-05
C22	H23	2.4795564470E-06
C22		-1.9197768104E-04
H23	C22	1.4661916457E-06
H23		1.4661916457E-06
B24	C6	-6.4840073908E-05
B24	C22	-1.3365757691E-05
B24	H25	7.7414511869E-05
B24		-7.9131972996E-07
H25	B24	1.0011362400E-04
H25		1.0011362400E-04

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	H2	1.2964731730E-02	
C1	H3	-1.6497057048E-02	
C1	C4	-9.9518123995E-03	
C1	C6	1.7947055592E-03	
C1		-1.1689432158E-02	
H2	C1	7.5336232111E-03	
H2		7.5336232111E-03	
H3	C1	-9.5974226562E-03	
H3		-9.5974226562E-03	
C4	C1	-1.0008472148E-02	
C4	H5	1.5012159948E-02	
C4	C11	5.9284548323E-03	
C4	C19	-9.9057185485E-03	
C4		1.0264240844E-03	
H5	C4	8.8145875620E-03	
H5		8.8145875620E-03	

C6	C1	1.7995042710E-03
C6	H7	-1.5352952889E-02
C6	C8	1.9685468050E-03
C6	B24	7.1200013959E-01
C6		7.0041523778E-01
H7	C6	-9.2254050356E-03
H7		-9.2254050356E-03
C8	C6	1.9635979381E-03
C8	H9	1.2969167301E-02
C8	H10	-1.6501741055E-02
C8	C14	-9.9554692076E-03
C8		-1.1524445024E-02
H9	C8	7.5361837524E-03
H9		7.5361837524E-03
H10	C8	-9.6001887036E-03
H10		-9.6001887036E-03
C11	C4	5.9860724910E-03
C11	C14	5.8240712776E-03
C11	H12	1.6339876168E-02
C11	H13	1.6343519760E-02
C11		4.4493539697E-02
H12	C11	9.7449788272E-03
H12		9.7449788272E-03
H13	C11	9.7471541469E-03
H13		9.7471541469E-03
C14	C8	-1.0012124623E-02
C14	C11	5.7681031891E-03
C14	H15	1.5008117319E-02
C14	C16	-9.8679245956E-03
C14		8.9617128950E-04
H15	C14	8.8122166597E-03
H15		8.8122166597E-03

C16	C14	-9.8120429056E-03
C16	H17	-1.6498417536E-02
C16	H18	1.2968416797E-02
C16	C22	1.9849748375E-03
C16		-1.1357068807E-02
H17	C16	-9.5982517591E-03
H17		-9.5982517591E-03
H18	C16	7.5357492282E-03
H18		7.5357492282E-03
C19	C4	-9.8496066424E-03
C19	C22	1.8562133280E-03
C19	H20	-1.6495813383E-02
C19	H21	1.2965324986E-02
C19		-1.1523881711E-02
H20	C19	-9.5966989903E-03
H20		-9.5966989903E-03
H21	C19	7.5339621021E-03
H21		7.5339621021E-03
C22	C16	1.9899432185E-03
C22	C19	1.8610606654E-03
C22	B24	7.1184090149E-01
C22	H23	-1.5351201283E-02
C22		7.0034070409E-01
H23	C22	-9.2243502609E-03
H23		-9.2243502609E-03
B24	C6	3.4261098846E-01
B24	C22	3.4253414270E-01
B24	H25	-6.2939627609E-01
B24		5.5748855073E-02
H25	B24	-8.0640636277E-01
H25		-8.0640636277E-01

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	H2	2.2277425587E-02	
C1	H3	2.9594888903E-02	
C1	C4	1.7576385932E-02	
C1	C6	3.1053760788E-03	
C1		4.4603246248E-02	
H2	C1	1.3024786731E-02	
H2		1.3024786731E-02	
H3	C1	1.7391666440E-02	
H3		1.7391666440E-02	
C4	C1	1.7447062338E-02	
C4	H5	2.5987500319E-02	
C4	C11	1.0317524000E-02	
C4	C19	1.7267819546E-02	
C4		1.2812790955E-02	
H5	C4	1.5246868057E-02	
H5		1.5246868057E-02	
C6	C1	3.0610204120E-03	
C6	H7	2.8848467162E-02	
C6	C8	3.3492697037E-03	
C6	B24	1.2689775046E+00	
C6		1.2827330232E+00	
H7	C6	1.7059838326E-02	
H7		1.7059838326E-02	
C8	C6	3.3983430000E-03	
C8	H9	2.2285357931E-02	
C8	H10	2.9596590059E-02	
C8	C14	1.7582611648E-02	
C8		4.4711417729E-02	
H9	C8	1.3029436550E-02	
H9		1.3029436550E-02	

H10	C8	1.7392678781E-02
H10		1.7392678781E-02
C11	C4	1.0336958439E-02
C11	C14	1.0055149208E-02
C11	H12	2.7726100059E-02
C11	H13	2.7732390679E-02
C11		4.4494149833E-02
H12	C11	1.6287035596E-02
H12		1.6287035596E-02
H13	C11	1.6290731861E-02
H13		1.6290731861E-02
C14	C8	1.7453245107E-02
C14	C11	1.0036383836E-02
C14	H15	2.5985768905E-02
C14	C16	1.7202084230E-02
C14		1.3032056765E-02
H15	C14	1.5245858184E-02
H15		1.5245858184E-02
C16	C14	1.7329497203E-02
C16	H17	2.9590921977E-02
C16	H18	2.2283876608E-02
C16	C22	3.4353035631E-03
C16		4.4527603949E-02
H17	C16	1.7389344851E-02
H17		1.7389344851E-02
H18	C16	1.3028574916E-02
H18		1.3028574916E-02
C19	C4	1.7395769080E-02
C19	C22	3.2118348170E-03
C19	H20	2.9592370452E-02
C19	H21	2.2278581105E-02
C19		4.4500237195E-02

H20	C19	1.7390188263E-02
H20		1.7390188263E-02
H21	C19	1.3025456826E-02
H21		1.3025456826E-02
C22	C16	3.3856375270E-03
C22	C19	3.1657618427E-03
C22	B24	1.2686892201E+00
C22	H23	2.8845403975E-02
C22		1.2824850460E+00
H23	C22	1.7058026299E-02
H23		1.7058026299E-02
B24	C6	6.3410797543E-01
B24	C22	6.3396390408E-01
B24	H25	6.2939628085E-01
B24		5.5748987699E-02
H25	B24	8.0640636899E-01
H25		8.0640636899E-01

Atomic Traceless Quadrupole Moment Tensors:

 $Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$

C1 -1.5825912974E-02 -1.5365972883E-02 1.7329012940E-02 3.8885795251E-02 -1.7940101274E-02 -2.3059882278E-02

H2 1.8100512332E-01 9.5053897507E-03 -2.6011209350E-01 -1.9068575554E-01 4.3121194895E-04 9.6806322265E-03

H3 -1.8804920890E-01 7.9570934550E-03 1.7959754818E-02 2.1149132459E-01 -2.7638346078E-01 -2.3442115689E-02

C4 1.3349370949E-02 -2.0824221109E-03 6.5175414701E-04 1.2858569935E-02 2.4516507828E-02 -2.6207940884E-02

H5 -1.8927971587E-01 -2.3772448401E-05 -1.2888486787E-05 1.8922988877E-01 2.6825008624E-01 4.9827105296E-05

C6 -8.6858084774E-01 1.5085610471E-03 2.2657645047E+00 1.0375211200E+00 1.9069754631E-03 -1.6894027231E-01

H7 2.2293114431E-01 2.6907760265E-06 2.6662547503E-01 -2.0070457717E-01 6.6792503181E-06 -2.2226567147E-02

C8 -1.8261281029E-02 1.7732123080E-02 1.7930023904E-02 3.7603571269E-02 1.5962534650E-02 -1.9342290241E-02

H9 1.8101713681E-01 -9.4206004687E-03 -2.6012476677E-01 -1.9069707328E-01 -4.9708853990E-04 9.6799364665E-03

H10 -1.8804765788E-01 -7.9901857206E-03 1.7912031388E-02 2.1140977956E-01 2.7642757096E-01 -2.3362121679E-02

C11 4.9589799503E-02 4.1695576985E-03 7.3500246164E-04 -6.8735269734E-02 1.1333454137E-03 1.9145470231E-02

H12 1.9481427622E-01 -4.8928451646E-06 2.6763341662E-01 -1.8424033542E-01 -3.6011591357E-07 -1.0573940798E-02

H13 1.9477702455E-01 4.5041296084E-05 -2.6767003508E-01 -1.8421891710E-01 -2.5442592285E-05 -1.0558107449E-02

C14 1.9467989191E-02 1.6358594642E-03 -9.2083135496E-04 1.3321010746E-02 -2.6221494752E-02 -3.2788999936E-02

H15 -1.8926699825E-01 -1.7016136538E-05 1.4577327112E-05 1.8929376561E-01 -2.6821201334E-01 -2.6767362789E-05

C16 -1.7119662913E-02 -1.5002804765E-02 -1.6630002139E-02 3.7025786689E-02 1.6191980042E-02 -1.9906123776E-02

H17 -1.8804330349E-01 7.9723722007E-03 -1.7962097458E-02 2.1141533635E-01 2.7640712374E-01 -2.3372032860E-02

H18 1.8100788570E-01 9.4835362242E-03 2.6011010221E-01 -1.9067283799E-01 -4.9090740944E-04 9.6649522963E-03

C19 -1.7541541040E-02 1.5050968287E-02 -1.7089772173E-02 3.6279339913E-02 -1.7492807184E-02 -1.8737798873E-02

H20 -1.8803797832E-01 -8.0057846262E-03 -1.7931370527E-02 2.1148908188E-01 -2.7638871911E-01 -2.3451103558E-02

H21 1.8101027979E-01 -9.4611464960E-03 2.6010660538E-01 -1.9068506762E-01 4.7813285056E-04 9.6747878282E-03

C22 -8.6617770859E-01 -1.0491089239E-03 -2.2589546727E+00 1.0325686107E+00 2.6958144758E-03 -1.6639090207E-01

H23 2.2292374574E-01 4.0044105708E-05 -2.6660496917E-01 -2.0070363148E-01 -2.8285959689E-05 -2.2220114253E-02

B24 2.7840750938E-02 5.9700071745E-04 -6.1317471184E-04 -3.2322068119E-01 -1.1193200088E-03 2.9537993025E-01

H25 1.1920871790E-02 8.7454591606E-06 9.5998423290E-06 -7.2995038202E-01 -1.7044780919E-04 7.1802951023E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
C1	1	-3.7437664799E-02	-5.9381460311E-01	6.8879358521E-02	8.0164820907E-01
C1	2	-1.2171819404E-02	7.4988361602E-01	4.0852219389E-01	5.2036927227E-01
C1	3	4.9609484203E-02	-2.9164838343E-01	9.1014573068E-01	-2.9423794686E-01
H2	1	-1.9317536208E-01	-2.2941046045E-01	9.2718735582E-01	-2.9613248359E-01
H2	2	-1.7612116097E-01	5.3939730607E-01	3.7436169603E-01	7.5425716221E-01
H2	3	3.6929652306E-01	8.1019836265E-01	1.3301418997E-02	-5.8600485101E-01
H3	1	-2.1858034261E-01	5.3591121348E-01	-4.6343617049E-01	-7.0570963374E-01
H3	2	-1.7577292690E-01	8.4425560314E-01	2.9973369806E-01	4.4428840500E-01
H3	3	3.9435326951E-01	-5.6256412650E-03	8.3389845073E-01	-5.5188923348E-01
C4	1	-3.8064530433E-02	-2.9012438263E-02	-4.3456689489E-01	9.0017214592E-01
C4	2	1.3172110863E-02	9.9012848459E-01	1.1104814932E-01	8.5521298689E-02
C4	3	2.4892419570E-02	1.3712717609E-01	-8.9376726411E-01	-4.2705528351E-01

H5	1	-1.8979887713E-01 -6.1883014565E-03 -5.7767863710E-01 8.1624083282E-01
H5	2	-1.8927969726E-01 9.9998085116E-01 -3.5363562770E-03 5.0785323604E-03
H5	3	3.7907857439E-01 -4.7241259690E-05 8.1625663025E-01 5.7768945926E-01
C6	1	-2.8113710885E+00 7.5913963833E-01 2.4966889619E-05 -6.5092780620E-01
C6	2	1.0375131056E+00 -2.1667499280E-03 9.9999455602E-01 -2.4886000991E-03
C6	3	1.7738579829E+00 6.5092420043E-01 3.2995927564E-03 7.5913555969E-01
H7	1	-2.0070457951E-01 2.8771342799E-04 9.9999984946E-01 -4.6723390528E-04
H7	2	-1.9310080556E-01 -5.3957757403E-01 5.4862470609E-04 8.4193571050E-01
H7	3	3.9380538508E-01 8.4193584009E-01 9.8727276948E-06 5.3957765065E-01
C8	1	-3.6753555864E-02 7.0352282016E-01 -1.5243002295E-02 -7.1050917826E-01
C8	2	-1.2256735277E-02 6.3652553602E-01 -4.3110921519E-01 6.3951550925E-01
C8	3	4.9010291141E-02 3.1605519060E-01 9.0217099015E-01 2.9359261066E-01
H9	1	-1.9318636582E-01 2.2934753541E-01 9.2713277376E-01 2.9635203362E-01
H9	2	-1.7612700248E-01 5.3941940430E-01 -3.7450362982E-01 7.5417089411E-01
H9	3	3.6931336830E-01 8.1020146523E-01 -1.3109198403E-02 -5.8600489303E-01
H10	1	-2.1856678767E-01 5.3562002798E-01 4.6368425533E-01 -7.0576773586E-01
H10	2	-1.7579415359E-01 8.4444094927E-01 -2.9957832220E-01 4.4404089009E-01
H10	3	3.9436094126E-01 5.5379447111E-03 8.3381637081E-01 5.5201412205E-01
C11	1	-6.8895929862E-02 -3.5087945513E-02 9.9930516165E-01 -1.2570997217E-02
C11	2	1.9139786613E-02 -2.5726546620E-02 1.1671397974E-02 9.9960088199E-01
C11	3	4.9756143249E-02 9.9905304207E-01 3.5397349628E-02 2.5299145453E-02
H12	1	-1.9453943174E-01 -5.6646088632E-01 -2.4029661598E-04 8.2408859143E-01
H12	2	-1.8424033486E-01 -1.2991824435E-04 9.999997110E-01 2.0228772359E-04
H12	3	3.7877976659E-01 8.2408861623E-01 -7.5239402127E-06 5.6646090116E-01
H13	1	-1.9457482413E-01 5.6651534938E-01 -4.3941976116E-04 8.2405106991E-01
H13	2	-1.8421891982E-01 1.7351645407E-04 9.9999989927E-01 4.1395490492E-04
H13	3	3.7879374395E-01 8.2405116881E-01 9.1525387959E-05 -5.6651536856E-01
C14	1	-4.4650031980E-02 2.5725203155E-03 4.1206056719E-01 9.1115282533E-01
C14	2	1.8910786883E-02 9.5829628218E-01 -2.6139311587E-01 1.1550703242E-01
C14	3	2.5739245096E-02 2.8576496934E-01 8.7285722082E-01 -3.9554854868E-01
H15	1	-1.8979268602E-01 -3.9412729877E-03 5.7757162827E-01 8.1633049715E-01
H15	2	-1.8926699096E-01 9.9999223238E-01 2.3084317667E-03 3.1947326337E-03

H15	3	3.7905967698E-01 -3.9256322663E-05 8.1633674752E-01 -5.7757624008E-01
C16	1	-3.5254852347E-02 6.6174013716E-01 -3.0460231019E-02 7.4911425376E-01
C16	2	-1.1728418733E-02 -6.9170389269E-01 -4.1024392029E-01 5.9434472379E-01
C16	3	4.6983271080E-02 -2.8921569062E-01 9.1146700444E-01 2.9254432845E-01
H17	1	-2.1858491137E-01 5.3597547277E-01 -4.6350976805E-01 7.0561249104E-01
H17	2	-1.7575852446E-01 -8.4421491129E-01 -2.9981458704E-01 4.4431114880E-01
H17	3	3.9434343583E-01 -5.6103600912E-03 8.3382846457E-01 5.5199512275E-01
H18	1	-1.9318876951E-01 -2.3037821290E-01 9.2646262999E-01 2.9764555136E-01
H18	2	-1.7610089718E-01 -5.3896822734E-01 -3.7615494694E-01 7.5367148401E-01
H18	3	3.6928966669E-01 8.1020931181E-01 1.3207994404E-02 5.8599182584E-01
C19	1	-3.5320552746E-02 6.7566185887E-01 3.7842723105E-02 7.3623975767E-01
C19	2	-1.1944365398E-02 -6.7659193088E-01 4.2841643530E-01 5.9890125816E-01
C19	3	4.7264918144E-02 2.9275315803E-01 9.0278861660E-01 -3.1506872614E-01
H20	1	-2.1858823415E-01 5.3572758806E-01 4.6354122298E-01 7.0578005496E-01
H20	2	-1.7576495093E-01 -8.4437277420E-01 2.9956252879E-01 4.4418116747E-01
H20	3	3.9435318509E-01 5.5289764408E-03 8.3390156849E-01 -5.5188549943E-01
H21	1	-1.9318122145E-01 2.2958633977E-01 9.2700530604E-01 -2.9656580242E-01
H21	2	-1.7610979042E-01 -5.3931031117E-01 3.7481625302E-01 7.5409360476E-01
H21	3	3.6929101187E-01 8.1020645570E-01 -1.3188595372E-02 5.8599621167E-01
C22	1	-2.8021764069E+00 7.5929773659E-01 -2.4974209761E-04 6.5074333253E-01
C22	2	1.0325587408E+00 2.5996090819E-03 9.9999311110E-01 -2.6494884059E-03
C22	3	1.7696176662E+00 -6.5073818793E-01 3.7034288270E-03 7.5929315510E-01
H23	1	-2.0070363616E-01 8.6923766941E-05 9.9999995466E-01 2.8831942611E-04
H23	2	-1.9307975590E-01 5.3957438745E-01 -2.8964889829E-04 8.4193788162E-01
H23	3	3.9378339205E-01 8.4193792696E-01 8.2385365534E-05 -5.3957438817E-01
B24	1	-3.2322371798E-01 -1.6973817434E-03 9.9999692548E-01 1.8077419670E-03
B24	2	2.7840352118E-02 9.9999592384E-01 1.6932240723E-03 2.2989775057E-03
B24	3	2.9538336586E-01 -2.2959095253E-03 -1.8116368408E-03 9.9999572338E-01
H25	1	-7.2995040219E-01 -1.1789901354E-05 9.9999999300E-01 1.1771428575E-04
H25	2	1.1920871762E-02 9.999999984E-01 1.1791501475E-05 -1.3592571977E-05
H25	3	7.1802953043E-01 1.3593959910E-05 -1.1771412548E-04 9.9999999298E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1 8.7820355430E+00	1.3770057000E+02		1.4979505351E+01	5.9744352073E+00	5.9673171522E+00
H2 1.6917412698E+00	2.9667823544E+00		1.2949754722E+00	1.0170228944E+00	1.1401148242E+00
H3 1.7049478393E+00	2.9791547531E+00		1.3014208364E+00	1.0226817731E+00	1.1473017634E+00
C4 8.4247565850E+00	1.3767070027E+02		1.4975073325E+01	5.9489354045E+00	5.8622966470E+00
H5 1.6792925584E+00	2.9927520822E+00		1.3036231498E+00	1.0199275195E+00	1.1375038359E+00
C6 1.1762218303E+01	1.3784665152E+02		1.5298234625E+01	6.6139224471E+00	7.3155939558E+00
H7 1.6993449933E+00	2.9843151217E+00		1.3028167002E+00	1.0222276757E+00	1.1446437748E+00
C8 8.7836163378E+00	1.3770059149E+02		1.4979570692E+01	5.9746303682E+00	5.9678855270E+00
H9 1.6917660821E+00	2.9667853486E+00		1.2949791950E+00	1.0170289593E+00	1.1401263483E+00
H10 1.7049587426E+00	2.9791545958E+00		1.3014211981E+00	1.0226830788E+00	1.1473057236E+00
C11 8.7153322645E+00	1.3771572251E+02		1.4986936469E+01	5.9715233204E+00	5.9451575781E+00
H12 1.6953934958E+00	2.9760027461E+00		1.2998823630E+00	1.0212508126E+00	1.1444134432E+00
H13 1.6954275972E+00	2.9760040639E+00		1.2998844352E+00	1.0212556386E+00	1.1444261772E+00

C14	1.3767072539E+02 8.4268275145E+00	1.4975151192E+01	5.9491720655E+00	5.8630039657E+00
H15	2.9927524170E+00 1.6792746898E+00	1.3036229693E+00	1.0199261919E+00	1.1374986499E+00
C16	1.3770057472E+02 8.7825550044E+00	1.4979520978E+01	5.9744872272E+00	5.9674865699E+00
H17	2.9791528136E+00 1.7049399061E+00	1.3014186444E+00	1.0226787305E+00	1.1472969882E+00
H18	2.9667864075E+00 1.6917520469E+00	1.2949795078E+00	1.0170278296E+00	1.1401213571E+00
C19	1.3770056324E+02 8.7816525016E+00	1.4979486981E+01	5.9743844006E+00	5.9671766984E+00
H20	2.9791522751E+00 1.7049485698E+00	1.3014188125E+00	1.0226798383E+00	1.1473003405E+00
H21	2.9667812103E+00 1.6917539625E+00	1.2949754964E+00	1.0170237701E+00	1.1401179862E+00
C22	1.3784663257E+02 1.1759402548E+01	1.5298165969E+01	6.6136825011E+00	7.3147678053E+00
H23	2.9843158962E+00 1.6993225941E+00	1.3028163737E+00	1.0222253180E+00	1.1446361798E+00
B24	9.2265828946E+01 2.2223574808E+00	1.0530605034E+01	3.0826928164E+00	1.9729777600E+00
H25	3.1621749432E+00 3.8541000736E+00	1.6716814071E+00	1.6362916674E+00	2.2319664398E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)

C1	-1.3595389089E+02	-2.6921315458E+01	-1.2416957889E+01	-1.3375206602E+01	-
2.2684930607E+01					
H2	-2.2920280108E+00	-1.8388840083E+00	-2.1069282784E+00	-3.1658549777E+00	-
5.9770548325E+00					
H3	-2.3060591378E+00	-1.8570682429E+00	-2.1396290782E+00	-3.2370093676E+00	-
6.1502251645E+00					
C4	-1.3582392934E+02	-2.6714990590E+01	-1.1968462804E+01	-1.2289601903E+01	-
1.9813670195E+01					
H5	-2.3179780685E+00	-1.8641877097E+00	-2.1450578914E+00	-3.2416970519E+00	-
6.1520407731E+00					
C6	-1.3617876895E+02	-2.7452721367E+01	-1.3597006080E+01	-1.6120275140E+01	-
2.9388475160E+01					
H7	-2.3087431044E+00	-1.8616491455E+00	-2.1527244470E+00	-3.2768775161E+00	-
6.2739095879E+00					
C8	-1.3595396217E+02	-2.6921519453E+01	-1.2417503408E+01	-1.3376483755E+01	-
2.2686902730E+01					
H9	-2.2920329706E+00	-1.8388917546E+00	-2.1069425160E+00	-3.1658851108E+00	-
5.9771251435E+00					
H10	-2.3060591989E+00	-1.8570691407E+00	-2.1396323738E+00	-3.2370193256E+00	-
6.1502470557E+00					
C11	-1.3595133767E+02	-2.6920258942E+01	-1.2404523790E+01	-1.3322217357E+01	-
2.2498743529E+01					
H12	-2.2993697448E+00	-1.8453262700E+00	-2.1135992259E+00	-3.1715565409E+00	-
5.9715709201E+00					
H13	-2.2993716727E+00	-1.8453302526E+00	-2.1136086777E+00	-3.1715785506E+00	-
5.9716065285E+00					
C14	-1.3582408356E+02	-2.6715481601E+01	-1.1970022675E+01	-1.2294567556E+01	-
1.9829594640E+01					
H15	-2.3179782683E+00	-1.8641860977E+00	-2.1450504661E+00	-3.2416706448E+00	-
6.1519531840E+00					
C16	-1.3595388156E+02	-2.6921292117E+01	-1.2416876150E+01	-1.3374849558E+01	-
2.2683166985E+01					
H17	-2.3060566028E+00	-1.8570642857E+00	-2.1396224379E+00	-3.2369986501E+00	-
6.1502108381E+00					
H18	-2.2920338092E+00	-1.8388911178E+00	-2.1069379618E+00	-3.1658718566E+00	-
5.9771037829E+00					
C19	-1.3595383505E+02	-2.6921145860E+01	-1.2416444920E+01	-1.3373651056E+01	-
2.2680198771E+01					

H20 -2.3060562411E+00 -1.8570650866E+00 -2.1396255829E+00 -3.2370063322E+00 -
6.1502235588E+00

H21 -2.2920274902E+00 -1.8388842623E+00 -2.1069302948E+00 -3.1658658471E+00 -
5.9771156308E+00

C22 -1.3617867970E+02 -2.7452425514E+01 -1.3596038042E+01 -1.6117137511E+01 -
2.9378381052E+01

H23 -2.3087419303E+00 -1.8616449137E+00 -2.1527120862E+00 -3.2768416351E+00 -
6.2738021238E+00

B24 -9.0967571172E+01 -1.9408653485E+01 -7.0032103542E+00 -4.5590822291E+00 -
5.5569392253E+00

H25 -2.7569888335E+00 -2.6479730174E+00 -3.6434678528E+00 -6.4491294352E+00 -
1.3952392797E+01

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
C1	2.9872176037E+00	2.9872176037E+00	5.9744352073E+00	0.0000000000E+00
H2	5.0851144720E-01	5.0851144720E-01	1.0170228944E+00	0.0000000000E+00
H3	5.1134088655E-01	5.1134088655E-01	1.0226817731E+00	0.0000000000E+00
C4	2.9744677022E+00	2.9744677022E+00	5.9489354045E+00	0.0000000000E+00
H5	5.0996375976E-01	5.0996375976E-01	1.0199275195E+00	0.0000000000E+00
C6	3.3069612235E+00	3.3069612235E+00	6.6139224471E+00	0.0000000000E+00
H7	5.1111383787E-01	5.1111383787E-01	1.0222276757E+00	0.0000000000E+00
C8	2.9873151841E+00	2.9873151841E+00	5.9746303682E+00	0.0000000000E+00
H9	5.0851447963E-01	5.0851447963E-01	1.0170289593E+00	0.0000000000E+00
H10	5.1134153939E-01	5.1134153939E-01	1.0226830788E+00	0.0000000000E+00
C11	2.9857616602E+00	2.9857616602E+00	5.9715233204E+00	0.0000000000E+00
H12	5.1062540632E-01	5.1062540632E-01	1.0212508126E+00	0.0000000000E+00

H13	5.1062781931E-01	5.1062781931E-01	1.0212556386E+00	0.0000000000E+00
C14	2.9745860327E+00	2.9745860327E+00	5.9491720655E+00	0.0000000000E+00
H15	5.0996309593E-01	5.0996309593E-01	1.0199261919E+00	0.0000000000E+00
C16	2.9872436136E+00	2.9872436136E+00	5.9744872272E+00	0.0000000000E+00
H17	5.1133936527E-01	5.1133936527E-01	1.0226787305E+00	0.0000000000E+00
H18	5.0851391479E-01	5.0851391479E-01	1.0170278296E+00	0.0000000000E+00
C19	2.9871922003E+00	2.9871922003E+00	5.9743844006E+00	0.0000000000E+00
H20	5.1133991916E-01	5.1133991916E-01	1.0226798383E+00	0.0000000000E+00
H21	5.0851188507E-01	5.0851188507E-01	1.0170237701E+00	0.0000000000E+00
C22	3.3068412505E+00	3.3068412505E+00	6.6136825011E+00	0.0000000000E+00
H23	5.1111265901E-01	5.1111265901E-01	1.0222253180E+00	0.0000000000E+00
B24	1.5413464082E+00	1.5413464082E+00	3.0826928164E+00	0.0000000000E+00
H25	8.1814583371E-01	8.1814583371E-01	1.6362916674E+00	0.0000000000E+00

Total	3.6999898728E+01	3.6999898728E+01	7.3999797456E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional

of the corresponding DFT model and atomic contributions $VeeX(A)$ to $VeeX$ are explicitly calculated and unambiguous. However, since $VeeX$ is at least partly just a one-electron functional for DFT models, the partitioning of $VeeX(A)$ into interatomic ($VeeX(A,B)$ and $VeeX(A,A')$) and intraatomic ($VeeX(A,A)$) contributions is ambiguous. Currently, interatomic contributions $VeeX(A,B)$ and $VeeX(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$. For wavefunctions of non-supported DFT models, $VeeX$ is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E\_IQA(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 16 sec (NProc = 1)

Boradamantan2

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\boradamantan\boradamantan2.wfn

Sum File: D:\calc\ellipticity\boradamantan\boradamantan2.sum

Wfn Title: boradamantan2

Total memory allocated for AIMSum = 1.305 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted SCF

Restricted, closed-shell, single-determinant wavefunction.

Number of electrons (from MO Occs)	=	74.0000000000
Number of Alpha electrons (from MO Occs)	=	37.0000000000
Number of Beta electrons (from MO Occs)	=	37.0000000000
Number of electron pairs ($N*(N-1)/2$)	=	2701.0000000000
Number of electron pairs (from Muller 2EDM)	=	2701.0000000000

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	1.0421372000E+00	2.7101251600E+00	2.1091157700E+00
H2	1.0	2.9803388500E+00	3.0591810500E+00	2.7331454800E+00
H3	1.0	-1.6077837000E-01	4.2692894000E+00	2.7331418400E+00
C4	6.0	9.9385181000E-01	2.5853810700E+00	-8.5970058000E-01
H5	1.0	1.6838121300E+00	4.3819912300E+00	-1.6163622300E+00
C6	6.0	2.7099647900E+00	4.3066769000E-01	-1.7874510900E+00
H7	1.0	4.6430010300E+00	7.3584458000E-01	-1.1154830300E+00
H8	1.0	2.7707157300E+00	4.4214706000E-01	-3.8572305100E+00
C9	6.0	1.8269697300E+00	-2.2631093200E+00	2.1035315200E+00
H10	1.0	1.1617815500E+00	-4.1187721100E+00	2.7214154400E+00
H11	1.0	3.7782295400E+00	-2.0012259500E+00	2.7290961400E+00
C12	6.0	1.7431093400E+00	-2.1502361600E+00	-8.6426017000E-01
H13	1.0	2.9527509100E+00	-3.6451146000E+00	-1.6248660100E+00
C14	6.0	-9.8156878000E-01	-2.5565229700E+00	-1.7934802100E+00
H15	1.0	-1.0017977800E+00	-2.6088209900E+00	-3.8633825600E+00
H16	1.0	-1.6838800600E+00	-4.3853124300E+00	-1.1273702900E+00
C17	6.0	-2.8746712400E+00	-4.5599606000E-01	2.1022297900E+00
H18	1.0	-4.1484793400E+00	1.0463235400E+00	2.7254961300E+00
H19	1.0	-3.6241537200E+00	-2.2786350800E+00	2.7217748000E+00

C20	6.0	-1.7234911300E+00	2.1332992500E+00	-1.7889072900E+00
H21	1.0	-2.9544253700E+00	3.6554130900E+00	-1.1183873000E+00
H22	1.0	-1.7601584600E+00	2.1815883900E+00	-3.8587010000E+00
C23	6.0	-2.7343297300E+00	-4.3087842000E-01	-8.6529415000E-01
H24	1.0	-4.6335246900E+00	-7.3019040000E-01	-1.6268079100E+00
B25	5.0	-3.0527700000E-03	-4.0176500000E-03	2.6619638800E+00

Some Atomic Properties:

 $q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

C1	-6.3235473940E-01	-2.9275241655E-04	3.8173341344E+01	-3.8353794364E+01	1.0541372671E+00
H2	-1.6959622100E-02	5.6400171638E-05	6.2226874793E-01	-6.2521033676E-01	1.5533155661E-01
H3	-1.7077220100E-02	5.7514393082E-05	6.2234428794E-01	-6.2528623386E-01	1.5533713075E-01
C4	4.1486895400E-02	7.3842787013E-05	3.7839101678E+01	-3.8017974680E+01	3.7059216053E-02
H5	-1.1986112200E-02	6.1369542684E-05	6.3129775564E-01	-6.3428202639E-01	1.5192954168E-01
C6	2.7472796300E-02	-4.9204407160E-05	3.7879721494E+01	-3.8058786514E+01	4.9394915895E-02
H7	-1.4891190900E-02	7.4762962274E-05	6.2616087334E-01	-6.2912086102E-01	1.5300067766E-01
H8	-1.7519366100E-02	7.6176124371E-05	6.2621075276E-01	-6.2917097623E-01	1.5368662862E-01
C9	-6.3211238100E-01	-1.3174887451E-04	3.8173484954E+01	-3.8353938652E+01	1.0545024590E+00

H10 -1.7038315900E-02 5.9542619383E-05 6.2232573489E-01 -6.2526759311E-01 1.5533243916E-01

H11 -1.6981940000E-02 5.5950290808E-05 6.2230250312E-01 -6.2524425151E-01 1.5532465576E-01

C12 4.1488706900E-02 -4.4512991905E-05 3.7839191210E+01 -3.8018064635E+01 3.7337799561E-02

H13 -1.2087496800E-02 5.9380331686E-05 6.3134935757E-01 -6.3433387225E-01 1.5193968823E-01

C14 2.6753564600E-02 -4.7050781017E-04 3.7879359930E+01 -3.8058423241E+01 4.9571653080E-02

H15 -1.7551645000E-02 7.5990262109E-05 6.2624533364E-01 -6.2920572058E-01 1.5371093558E-01

H16 -1.4835684800E-02 7.6839727415E-05 6.2611430807E-01 -6.2907407562E-01 1.5297829871E-01

C17 -6.3186133530E-01 1.3282993350E-04 3.8173632135E+01 -3.8354086529E+01 1.0545542591E+00

H18 -1.7034708100E-02 5.5481869795E-05 6.2228364219E-01 -6.2522530143E-01 1.5531032285E-01

H19 -1.6977144500E-02 5.6062875091E-05 6.2228965975E-01 -6.2523134743E-01 1.5534989391E-01

C20 2.7262218900E-02 -1.0065662551E-04 3.7879414200E+01 -3.8058477767E+01 4.9663682070E-02

H21 -1.4919308600E-02 6.9156492123E-05 6.2613665386E-01 -6.2909652705E-01 1.5299061069E-01

H22 -1.7496619100E-02 7.5672846203E-05 6.2620286511E-01 -6.2916305130E-01 1.5368500448E-01

C23 4.0821304000E-02 -6.2443193569E-04 3.7839143770E+01 -3.8018016971E+01 3.7728680002E-02

H24 -1.2011413900E-02 6.1292884151E-05 6.3132427697E-01 -6.3430867309E-01 1.5194558738E-01

B25 1.9263197138E+00 5.4192274935E-04 2.3945498758E+01 -2.4058693919E+01 1.8562841075E-01

Total -9.1043900001E-05 6.3738011810E-06 3.7500674623E+02 -3.7677947812E+02

Molecular charge q(Mol) from the wfn file: 0.0000000000E+00

Molecular energy E(Mol) from the wfn file: -3.7677948489E+02

Molecular virial ratio (-V(Mol))/T(Mol)) from the wfn file: 2.0047272000E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	63	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C4	57	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H5	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C6	54	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H7	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	15	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C9	64	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H10	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H11	21	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C12	70	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H13	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C14	62	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H15	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H16	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

C17	73	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H18	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H19	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C20	64	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H21	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H22	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C23	67	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H24	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
B25	74	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00

Total 904

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 1.04213808932369E+00 2.71012747477714E+00 2.10911371941745E+00

Type = (3,-3) NACP C1

Rho = 1.1963571275E+02 Rho at Nucleus = 1.1963571181E+02

GradRho = -6.7347794008E-12 3.8105796296E-11 -3.9419231768E-11

HessRho_EigVals = -1.8159700610E+05 -1.8159608519E+05 -1.8159492993E+05

HessRho_EigVec1 = 8.3376523118E-02 2.1566880283E-01 9.7290046915E-01

HessRho_EigVec2 = 9.3337526539E-01 -3.5890169914E-01 -4.2931894691E-04

HessRho_EigVec3 = 3.4908304076E-01 9.0811702872E-01 -2.3122390190E-01

DelSqRho = -5.4478802121E+05

Bond Ellipticity = NA

V = -1.3621260576E+05

G = 7.8002273196E+00

K = 1.3620480553E+05

L = 1.3619700530E+05

Vnuc = 1.8646658647E+06
Ven = -2.2308062977E+08
Vrep = 2.2294441716E+08
DelSqV = 4.6164957177E+09
DelSqVen = 1.0158476227E+12
DelSqVrep = -1.0112311269E+12
DelSqG = 2.0676018461E+08
DelSqK = -4.8232559023E+09
Stress_EigVals = -4.5404472406E+04 -4.5404195255E+04 -4.5403938096E+04
Stress_EigVec1 = 3.5347282516E-01 9.1977078662E-01 -1.7052466672E-01
Stress_EigVec2 = 9.3342651005E-01 -3.5876856597E-01 -2.5767859418E-04
Stress_EigVec3 = 6.1415895387E-02 1.5908116216E-01 9.8535337399E-01
-DivStress = -1.3356696949E+03 -3.4765542874E+03 3.0799049928E+03

CP# 2 Coords = 2.95615434370179E+00 3.05484563702525E+00 2.72509385532089E+00

Type = (3,-3) NACP H2

Rho = 4.3948424808E-01 Rho at Nucleus = 4.3662634684E-01

GradRho = 1.5352302762E-15 -1.7486012638E-15 -1.3496148643E-15

HessRho_EigVals = -8.9571533563E+00 -8.9530633293E+00 -8.3385468042E+00

HessRho_EigVec1 = -3.4233173288E-01 6.5649049789E-01 6.7218242378E-01

HessRho_EigVec2 = -9.0743486218E-02 -7.3516434384E-01 6.7178791836E-01

HessRho_EigVec3 = 9.3518693552E-01 1.6897814571E-01 3.1124232023E-01

DelSqRho = -2.6248763490E+01

Bond Ellipticity = NA

V = -6.5767533551E+00

G = 7.2812413152E-03

K = 6.5694721138E+00

L = 6.5621908725E+00

Vnuc = 5.2889487722E+01

Ven = -2.3244096743E+01

Vrep = 1.6667343388E+01

DelSqV = 1.7068172498E+03

DelSqVen = 1.3882836543E+03

DelSqVrep = 3.1853359543E+02

DelSqG = 1.3109906327E+02

DelSqK = -1.8379163130E+03

Stress_EigVals = -2.2450756535E+00 -2.2444411394E+00 -2.0872365622E+00

Stress_EigVec1 = -7.6262100321E-03 8.8963241188E-01 -4.5661363608E-01

Stress_EigVec2 = -3.5442569947E-01 4.2457807083E-01 8.3313617454E-01

Stress_EigVec3 = 9.3505308110E-01 1.6818927881E-01 3.1207066831E-01

-DivStress = 1.3363376032E+01 2.3980315050E+00 4.4509968413E+00

CP# 3 Coords = -1.45752071459471E-01 4.24984681418453E+00 2.72509066936420E+00

Type = (3,-3) NACP H3

Rho = 4.3952169673E-01 Rho at Nucleus = 4.3666314750E-01

GradRho = 6.3936703154E-14 -7.9096668451E-14 -3.4380484570E-14

HessRho_EigVals = -8.9577354110E+00 -8.9536479029E+00 -8.3390260366E+00

HessRho_EigVec1 = 6.9416909857E-01 2.5696939639E-01 6.7238083845E-01

HessRho_EigVec2 = -4.2615893821E-01 -6.0608592192E-01 6.7160138076E-01

HessRho_EigVec3 = -5.8010156178E-01 7.5274602927E-01 3.1121631296E-01

DelSqRho = -2.6250409350E+01

Bond Ellipticity = NA

V = -6.5771688603E+00

G = 7.2832613583E-03

K = 6.5698855990E+00

L = 6.5626023376E+00

Vnuc = 5.2884341513E+01

Ven = -2.3243815512E+01

Vrep = 1.6666646652E+01

DelSqV = 1.7069133290E+03

DelSqVen = 1.3882356129E+03

DelSqVrep = 3.1867771606E+02

DelSqG = 1.3110440806E+02

DelSqK = -1.8380177371E+03

Stress_EigVals = -2.2452239475E+00 -2.2445880156E+00 -2.0873568973E+00
Stress_EigVec1 = -6.0244873328E-01 -6.5454373408E-01 4.5675816790E-01
Stress_EigVec2 = 5.4775488558E-01 7.7180301179E-02 8.3307129733E-01
Stress_EigVec3 = -5.8053433067E-01 7.5207426580E-01 3.1203235349E-01
-DivStress = -8.3017702258E+00 1.0745639621E+01 4.4509860233E+00

CP# 4 Coords = 9.93851509504271E-01 2.58538029929687E+00 -8.59699406389520E-01

Type = (3,-3) NACP C4

Rho = 1.1961602833E+02 Rho at Nucleus = 1.1961602814E+02

GradRho = -2.8731794721E-10 -7.5063610883E-10 1.1079820394E-09

HessRho_EigVals = -1.8157253401E+05 -1.8157200631E+05 -1.8157158029E+05

HessRho_EigVec1 = 6.3864105042E-02 1.6160827925E-01 9.8478634239E-01

HessRho_EigVec2 = 9.3373887205E-01 -3.5795032427E-01 -1.8122321221E-03

HessRho_EigVec3 = 3.5221171888E-01 9.1964902513E-01 -1.7376010949E-01

DelSqRho = -5.4471612061E+05

Bond Ellipticity = NA

V = -1.3619413389E+05

G = 7.5518666098E+00

K = 1.3618658202E+05

L = 1.3617903015E+05

Vnuc = 4.1787484884E+06

Ven = -4.9984529757E+08

Vrep = 4.9970910344E+08

DelSqV = 4.6158900538E+09

DelSqVen = 2.2762314793E+12

DelSqVrep = -2.2716155892E+12

DelSqG = 2.0673900665E+08

DelSqK = -4.8226290604E+09

Stress_EigVals = -4.5398175134E+04 -4.5398052778E+04 -4.5397905973E+04

Stress_EigVec1 = 3.5242382028E-01 9.2078686680E-01 -1.6717953471E-01

Stress_EigVec2 = 9.3384436667E-01 -3.5767683826E-01 -1.4064877929E-03

Stress_EigVec3 = 6.1091322886E-02 1.5562398691E-01 9.8592546623E-01

-DivStress = 4.5062442134E+02 1.1557370886E+03 -1.7621410331E+03

CP# 5 Coords = 1.67512806478647E+00 4.35937391966587E+00 -1.60700291036328E+00

Type = (3,-3) NACP H5

Rho = 4.4622315571E-01 Rho at Nucleus = 4.4329474423E-01

GradRho = -1.6872880742E-09 -4.3944305330E-09 1.8213686098E-09

HessRho_EigVals = -9.1021802136E+00 -9.1019683998E+00 -8.4656807012E+00

HessRho_EigVec1 = 1.3203102899E-01 3.3929667798E-01 9.3136758141E-01

HessRho_EigVec2 = 9.3332911749E-01 -3.5901873456E-01 -1.5187771474E-03

HessRho_EigVec3 = 3.3386309444E-01 8.6947300852E-01 -3.6407708197E-01

DelSqRho = -2.6669829315E+01

Bond Ellipticity = NA

V = -6.6810300245E+00

G = 6.7863479030E-03

K = 6.6742436766E+00

L = 6.6674573287E+00

Vnuc = 5.3082526755E+01

Ven = -2.3686652602E+01

Vrep = 1.7005622577E+01

DelSqV = 1.7335888388E+03

DelSqVen = 1.4157019431E+03

DelSqVrep = 3.1788689569E+02

DelSqG = 1.3327791130E+02

DelSqK = -1.8668667501E+03

Stress_EigVals = -2.2809025307E+00 -2.2807973850E+00 -2.1193301088E+00

Stress_EigVec1 = 1.3010868609E-01 3.3939180978E-01 9.3160341845E-01

Stress_EigVec2 = 9.3356924919E-01 -3.5839701877E-01 1.8413890699E-04

Stress_EigVec3 = 3.3394638309E-01 8.6969234583E-01 -3.6347632225E-01

-DivStress = 4.8738986895E+00 1.2693867073E+01 -5.2529667079E+00

CP# 6 Coords = 2.70996441457362E+00 4.30667627810787E-01 -1.78745099255115E+00

Type = (3,-3) NACP C6

Rho = 1.1963065840E+02 Rho at Nucleus = 1.1963065838E+02
GradRho = -4.2077480389E-11 -8.5021018004E-12 2.5797475267E-11
HessRho_EigVals = -1.8158855362E+05 -1.8158841891E+05 -1.8158804996E+05
HessRho_EigVec1 = -1.5425032116E-01 9.8803101493E-01 -1.2457719645E-03
HessRho_EigVec2 = 8.0131539312E-01 1.2436265930E-01 -5.8517311090E-01
HessRho_EigVec3 = 5.7801425516E-01 9.1261396544E-02 8.1090744128E-01
DelSqRho = -5.4476502248E+05
Bond Ellipticity = NA
V = -1.3620668151E+05
G = 7.7129462010E+00
K = 1.3619896857E+05
L = 1.3619125562E+05
Vnuc = 1.5274127696E+07
Ven = -1.8272539528E+09
Vrep = 1.8271177461E+09
DelSqV = 4.6162992408E+09
DelSqVen = 8.3208154644E+12
DelSqVrep = -8.3161991652E+12
DelSqG = 2.0675124226E+08
DelSqK = -4.8230504831E+09
Stress_EigVals = -4.5402298581E+04 -4.5402213532E+04 -4.5402169401E+04
Stress_EigVec1 = 5.9294997563E-01 9.3537704684E-02 7.9978811206E-01
Stress_EigVec2 = 7.9021822205E-01 1.2335631440E-01 -6.0028191814E-01
Stress_EigVec3 = -1.5480790659E-01 9.8794428866E-01 -7.7107507525E-04
-DivStress = 5.6333112576E+02 9.3323275398E+01 -1.4611563780E+02

CP# 7 Coords = 4.61872103744212E+00 7.32010520642675E-01 -1.12380136749456E+00

Type = (3,-3) NACP H7

Rho = 4.4300922696E-01 Rho at Nucleus = 4.4010896485E-01
GradRho = 2.2447321779E-15 1.7347234760E-17 -1.0885389812E-15
HessRho_EigVals = -9.0281514786E+00 -9.0271047805E+00 -8.3989592661E+00
HessRho_EigVec1 = -1.5684232164E-01 9.8762009409E-01 2.6525253588E-03

HessRho_EigVec2 = -3.1521715985E-01 -5.2604052728E-02 9.4756052882E-01

HessRho_EigVec3 = 9.3596935221E-01 1.4778147173E-01 3.1956534283E-01

DelSqRho = -2.6454215525E+01

Bond Ellipticity = NA

V = -6.6269608191E+00

G = 6.7034689069E-03

K = 6.6202573502E+00

L = 6.6135538813E+00

Vnuc = 5.3186952037E+01

Ven = -2.3562310506E+01

Vrep = 1.6935349687E+01

DelSqV = 1.7196164758E+03

DelSqVen = 1.4070190923E+03

DelSqVrep = 3.1259738350E+02

DelSqG = 1.3208035795E+02

DelSqK = -1.8516968338E+03

Stress_EigVals = -2.2624047076E+00 -2.2620801145E+00 -2.1024759970E+00

Stress_EigVec1 = -1.5626025892E-01 9.8771550154E-01 9.0526284544E-04

Stress_EigVec2 = -3.1542470120E-01 -5.0769846978E-02 9.4759151564E-01

Stress_EigVec3 = 9.3599678918E-01 1.4778535332E-01 3.1948317638E-01

-DivStress = 1.3520148939E+01 2.1349639562E+00 4.6284932656E+00

CP# 8 Coords = 2.76975594176373E+00 4.41971016490789E-01 -3.83137980265685E+00

Type = (3,-3) NACP H8

Rho = 4.4237462517E-01 Rho at Nucleus = 4.3949655655E-01

GradRho = -1.8483478637E-15 -1.8735013541E-16 -4.1286418728E-16

HessRho_EigVals = -9.0133410227E+00 -9.0125359385E+00 -8.3883936344E+00

HessRho_EigVec1 = -1.5593114082E-01 9.8776749255E-01 9.2735023126E-04

HessRho_EigVec2 = 9.8708926519E-01 1.5578914106E-01 3.7209220400E-02

HessRho_EigVec3 = -3.6609587239E-02 -6.7174536444E-03 9.9930706689E-01

DelSqRho = -2.6414270596E+01

Bond Ellipticity = NA

V = -6.6170238931E+00
G = 6.7281220893E-03
K = 6.6102957710E+00
L = 6.6035676489E+00
Vnuc = 5.3335881297E+01
Ven = -2.3594440497E+01
Vrep = 1.6977416604E+01
DelSqV = 1.7172268677E+03
DelSqVen = 1.4088284010E+03
DelSqVrep = 3.0839846667E+02
DelSqG = 1.3187043259E+02
DelSqK = -1.8490973003E+03
Stress_EigVals = -2.2587445002E+00 -2.2584602982E+00 -2.0998190947E+00
Stress_EigVec1 = -1.5693667006E-01 9.8760826359E-01 8.9402160411E-04
Stress_EigVec2 = 9.8691895361E-01 1.5679318067E-01 3.7508365614E-02
Stress_EigVec3 = -3.6903395344E-02 -6.7687648648E-03 9.9929591375E-01
-DivStress = 5.3690381709E-01 9.8393924034E-02 -1.4371974975E+01

CP# 9 Coords = 1.82697128889478E+00 -2.26311124083658E+00 2.10352946373814E+00

Type = (3,-3) NACP C9

Rho = 1.1963545328E+02 Rho at Nucleus = 1.1963545234E+02

GradRho = 8.8649643182E-12 2.2462920413E-11 2.3397728199E-11

HessRho_EigVals = -1.8159653431E+05 -1.8159561577E+05 -1.8159446162E+05

HessRho_EigVec1 = 1.4529731528E-01 -1.8369055038E-01 9.7218643884E-01

HessRho_EigVec2 = 7.7751286355E-01 6.2886158409E-01 2.6182208691E-03

HessRho_EigVec3 = -6.1185164639E-01 7.5550704150E-01 2.3419366569E-01

DelSqRho = -5.4478661170E+05

Bond Ellipticity = NA

V = -1.3621225416E+05

G = 7.8006175967E+00

K = 1.3620445354E+05

L = 1.3619665293E+05

Vnuc = 1.8652063379E+06
Ven = -2.2314480569E+08
Vrep = 2.2300859344E+08
DelSqV = 4.6164837276E+09
DelSqVen = 1.0161394442E+12
DelSqVrep = -1.0115229605E+12
DelSqG = 2.0675956427E+08
DelSqK = -4.8232432919E+09
Stress_EigVals = -4.5404354784E+04 -4.5404077901E+04 -4.5403821476E+04
Stress_EigVec1 = -6.1976788256E-01 7.6541762726E-01 1.7327327439E-01
Stress_EigVec2 = 7.7747342644E-01 6.2890983106E-01 2.7378059383E-03
Stress_EigVec3 = 1.0687770080E-01 -1.3641217054E-01 9.8486997964E-01
-DivStress = -2.3412805091E+03 2.8848885780E+03 3.0884167633E+03

CP# 10 Coords = 1.17010124526345E+00 -4.09562568091147E+00 2.71344364500465E+00

Type = (3,-3) NACP H10

Rho = 4.3951122672E-01 Rho at Nucleus = 4.3665312247E-01

GradRho = 2.8354321009E-09 7.8917831796E-09 -2.7168875968E-09

HessRho_EigVals = -8.9576743587E+00 -8.9535844967E+00 -8.3390209103E+00

HessRho_EigVec1 = -7.3915807471E-01 3.3036437145E-02 -6.7272129029E-01

HessRho_EigVec2 = 5.9237174921E-01 -4.4343845510E-01 -6.7265001842E-01

HessRho_EigVec3 = 3.2053244974E-01 8.9569578003E-01 -3.0820126267E-01

DelSqRho = -2.6250279766E+01

Bond Ellipticity = NA

V = -6.5771315303E+00

G = 7.2807944519E-03

K = 6.5698507359E+00

L = 6.5625699414E+00

Vnuc = 5.2888281390E+01

Ven = -2.3244993433E+01

Vrep = 1.6667861903E+01

DelSqV = 1.7069133329E+03

DelSqVen = 1.3883322091E+03
DelSqVrep = 3.1858112381E+02
DelSqG = 1.3110611378E+02
DelSqK = -1.8380194467E+03
Stress_EigVals = -2.2452051797E+00 -2.2445711534E+00 -2.0873551972E+00
Stress_EigVec1 = 7.7443022936E-01 -4.3605711145E-01 -4.5837977203E-01
Stress_EigVec2 = 5.4508984186E-01 9.2109709195E-02 8.3330238556E-01
Stress_EigVec3 = 3.2114620371E-01 8.9519271502E-01 -3.0902284514E-01
-DivStress = -4.5952445557E+00 -1.2791731941E+01 4.4071264532E+00

CP# 11 Coords = 3.75388395108059E+00 -2.00451145827133E+00 2.72102573499249E+00

Type = (3,-3) NACP H11

Rho = 4.3951357783E-01 Rho at Nucleus = 4.3665499985E-01

GradRho = 5.3256010712E-16 1.3912482277E-15 -1.1136924716E-15

HessRho_EigVals = -8.9577174425E+00 -8.9536312846E+00 -8.3389997932E+00

HessRho_EigVec1 = 1.2380282832E-01 7.3275049910E-01 -6.6914091622E-01

HessRho_EigVec2 = -3.1274720175E-01 6.6877419298E-01 6.7448518635E-01

HessRho_EigVec3 = 9.4173353317E-01 1.2576877539E-01 3.1196180477E-01

DelSqRho = -2.6250348520E+01

Bond Ellipticity = NA

V = -6.5771540874E+00

G = 7.2834786674E-03

K = 6.5698706087E+00

L = 6.5625871301E+00

Vnuc = 5.2884033160E+01

Ven = -2.3243250624E+01

Vrep = 1.6666096537E+01

DelSqV = 1.7069130556E+03

DelSqVen = 1.3882243016E+03

DelSqVrep = 3.1868875395E+02

DelSqG = 1.3110623868E+02

DelSqK = -1.8380192942E+03

Stress_EigVals = -2.2452191081E+00 -2.2445850915E+00 -2.0873498877E+00
Stress_EigVec1 = -2.6631649439E-01 8.4771570368E-01 4.5875223221E-01
Stress_EigVec2 = -2.0713810421E-01 -5.1515428963E-01 8.3169096644E-01
Stress_EigVec3 = 9.4136567316E-01 1.2646795491E-01 3.1278830825E-01
-DivStress = 1.3453939727E+01 1.8131939768E+00 4.4616292577E+00

CP# 12 Coords = 1.74310881461494E+00 -2.15023552826595E+00 -8.64258999237984E-01

Type = (3,-3) NACP C12

Rho = 1.1961603716E+02 Rho at Nucleus = 1.1961603697E+02

GradRho = -4.9260218127E-10 5.6635718337E-10 1.0899607605E-09

HessRho_EigVals = -1.8157263417E+05 -1.8157210976E+05 -1.8157168289E+05

HessRho_EigVec1 = 1.1072736892E-01 -1.3733719132E-01 9.8431597856E-01

HessRho_EigVec2 = 7.7833419540E-01 6.2785020367E-01 4.4991589493E-05

HessRho_EigVec3 = -6.1800916663E-01 7.6612180339E-01 1.7641443343E-01

DelSqRho = -5.4471642681E+05

Bond Ellipticity = NA

V = -1.3619421146E+05

G = 7.5523781492E+00

K = 1.3618665908E+05

L = 1.3617910670E+05

Vnuc = 4.1948961254E+06

Ven = -5.0177685080E+08

Vrep = 5.0164065659E+08

DelSqV = 4.6158927762E+09

DelSqVen = 2.2850288353E+12

DelSqVrep = -2.2804129426E+12

DelSqG = 2.0673922634E+08

DelSqK = -4.8226320025E+09

Stress_EigVals = -4.5398200774E+04 -4.5398078268E+04 -4.5397932418E+04

Stress_EigVec1 = -6.1817719704E-01 7.6750955370E-01 1.6966448668E-01

Stress_EigVec2 = 7.7873405247E-01 6.2735388452E-01 -6.1572180808E-04

Stress_EigVec3 = 1.0691224715E-01 -1.3174288809E-01 9.8550169094E-01

-DivStress = 7.8790093111E+02 -9.4734897546E+02 -1.7578623592E+03

CP# 13 Coords = 2.93752851689034E+00 -3.62629309035133E+00 -1.61545972196414E+00

Type = (3,-3) NACP H13

Rho = 4.4621888771E-01 Rho at Nucleus = 4.4329101425E-01

GradRho = -5.7214649685E-14 7.1172234772E-14 3.4994576681E-14

HessRho_EigVals = -9.1018554232E+00 -9.1016358269E+00 -8.4654628422E+00

HessRho_EigVec1 = 2.0635875982E-01 -3.0351470748E-01 9.3021227931E-01

HessRho_EigVec2 = -7.8411991202E-01 -6.1996216643E-01 -2.8335062421E-02

HessRho_EigVec3 = -5.8529652811E-01 7.2355078228E-01 3.6592654953E-01

DelSqRho = -2.6668954092E+01

Bond Ellipticity = NA

V = -6.6808182543E+00

G = 6.7898656171E-03

K = 6.6740283887E+00

L = 6.6672385231E+00

Vnuc = 5.3086233803E+01

Ven = -2.3688080200E+01

Vrep = 1.7007261946E+01

DelSqV = 1.7335329648E+03

DelSqVen = 1.4157543322E+03

DelSqVrep = 3.1777863259E+02

DelSqG = 1.3327056722E+02

DelSqK = -1.8668035320E+03

Stress_EigVals = -2.2808243772E+00 -2.2807166513E+00 -2.1192772258E+00

Stress_EigVec1 = 2.3154919126E-01 -2.8257275129E-01 9.3088002033E-01

Stress_EigVec2 = -7.7694795621E-01 -6.2956114466E-01 2.1537105915E-03

Stress_EigVec3 = -5.8543731122E-01 7.2374401922E-01 3.6531869549E-01

-DivStress = 8.5432033421E+00 -1.0563114108E+01 -5.2791278258E+00

CP# 14 Coords = -9.81568644797060E-01 -2.55652261185732E+00 -1.79348010987510E+00

Type = (3,-3) NACP C14

Rho = 1.1963052355E+02 Rho at Nucleus = 1.1963052354E+02
GradRho = 1.4500345369E-11 -4.2541525858E-12 -8.4952045398E-12
HessRho_EigVals = -1.8158825962E+05 -1.8158812292E+05 -1.8158775325E+05
HessRho_EigVec1 = 9.3259594900E-01 -3.6091574026E-01 -2.1504287905E-03
HessRho_EigVec2 = 2.9357908705E-01 7.5510726390E-01 5.8619479668E-01
HessRho_EigVec3 = -2.0994312458E-01 -5.4731421363E-01 8.1016728890E-01
DelSqRho = -5.4476413578E+05
Bond Ellipticity = NA
V = -1.3620645826E+05
G = 7.7121593356E+00
K = 1.3619874610E+05
L = 1.3619103395E+05
Vnuc = 1.5163379596E+07
Ven = -1.8140030399E+09
Vrep = 1.8138668334E+09
DelSqV = 4.6162915692E+09
DelSqVen = 8.2604636242E+12
DelSqVrep = -8.2558473326E+12
DelSqG = 2.0675079989E+08
DelSqK = -4.8230423691E+09
Stress_EigVals = -4.5402224475E+04 -4.5402139227E+04 -4.5402094562E+04
Stress_EigVec1 = -2.1529369177E-01 -5.6179802081E-01 7.9876880892E-01
Stress_EigVec2 = 2.8929681923E-01 7.4454277105E-01 6.0163395221E-01
Stress_EigVec3 = 9.3271430603E-01 -3.6060927039E-01 -2.2310186066E-03
-DivStress = -2.0286274294E+02 -5.3738639205E+02 -1.5013186882E+02

CP# 15 Coords = -1.00147169409816E+00 -2.60797833813255E+00 -3.83752897600026E+00

Type = (3,-3) NACP H15

Rho = 4.4239143840E-01 Rho at Nucleus = 4.3951323335E-01
GradRho = -3.1398494915E-16 1.4675760607E-15 -8.2312628935E-16
HessRho_EigVals = -9.0136122100E+00 -9.0128045796E+00 -8.3886242603E+00
HessRho_EigVec1 = 9.3337875814E-01 -3.5889286505E-01 -7.2611950052E-05

HessRho_EigVec2 = 3.5867773516E-01 9.3282623235E-01 -3.4431127638E-02

HessRho_EigVec3 = 1.2424820377E-02 3.2111238866E-02 9.9940707031E-01

DelSqRho = -2.6415041050E+01

Bond Ellipticity = NA

V = -6.6172203544E+00

G = 6.7300459551E-03

K = 6.6104903084E+00

L = 6.6037602625E+00

Vnuc = 5.3337412000E+01

Ven = -2.3596014415E+01

Vrep = 1.6978794061E+01

DelSqV = 1.7172751866E+03

DelSqVen = 1.4089099275E+03

DelSqVrep = 3.0836525909E+02

DelSqG = 1.3187321476E+02

DelSqK = -1.8491484013E+03

Stress_EigVals = -2.2588138097E+00 -2.2585290782E+00 -2.0998774665E+00

Stress_EigVec1 = 9.3287329863E-01 -3.6020467486E-01 -3.0275191309E-05

Stress_EigVec2 = 3.5998635211E-01 9.3231079648E-01 -3.4733342250E-02

Stress_EigVec3 = 1.2539338140E-02 3.2390908902E-02 9.9939661497E-01

-DivStress = -1.8251029334E-01 -4.7161864294E-01 -1.4374001116E+01

CP# 16 Coords = -1.67505786913766E+00 -4.36234107746466E+00 -1.13561295314688E+00

Type = (3,-3) NACP H16

Rho = 4.4299537799E-01 Rho at Nucleus = 4.4009498071E-01

GradRho = 2.5732202454E-09 6.7002055085E-09 -2.4035547649E-09

HessRho_EigVals = -9.0280073034E+00 -9.0269578459E+00 -8.3988030154E+00

HessRho_EigVec1 = 9.3382868705E-01 -3.5771124871E-01 2.5779432724E-03

HessRho_EigVec2 = 1.1099075356E-01 2.9658452038E-01 9.4853501511E-01

HessRho_EigVec3 = 3.4006622277E-01 8.8548307991E-01 -3.1666177432E-01

DelSqRho = -2.6453768165E+01

Bond Ellipticity = NA

V = -6.6268442358E+00
G = 6.7010972946E-03
K = 6.6201431385E+00
L = 6.6134420412E+00
Vnuc = 5.3185619576E+01
Ven = -2.3560983647E+01
Vrep = 1.6934139412E+01
DelSqV = 1.7195885193E+03
DelSqVen = 1.4069600724E+03
DelSqVrep = 3.1262844688E+02
DelSqG = 1.3207994767E+02
DelSqK = -1.8516684669E+03
Stress_EigVals = -2.2623667607E+00 -2.2620421552E+00 -2.1024353198E+00
Stress_EigVec1 = 9.3348592514E-01 -3.5861390377E-01 -3.0917604566E-04
Stress_EigVec2 = 1.1379952758E-01 2.9540679025E-01 9.4856971056E-01
Stress_EigVec3 = 3.4007895420E-01 8.8551165791E-01 -3.1656817372E-01
-DivStress = -4.9125089643E+00 -1.2791250547E+01 4.5862642057E+00

CP# 17 Coords = -2.87467368588603E+00 -4.55996440896376E-01 2.10222773391424E+00

Type = (3,-3) NACP C17

Rho = 1.1963561233E+02 Rho at Nucleus = 1.1963561139E+02

GradRho = -8.9884766297E-12 5.8791860269E-13 1.4468315435E-11

HessRho_EigVals = -1.8159676892E+05 -1.8159585080E+05 -1.8159469481E+05

HessRho_EigVec1 = -2.3172864903E-01 -3.7052436015E-02 9.7207456000E-01

HessRho_EigVec2 = -1.5563155140E-01 9.8781502085E-01 5.5208080105E-04

HessRho_EigVec3 = 9.6025030769E-01 1.5115753891E-01 2.3467156837E-01

DelSqRho = -5.4478731453E+05

Bond Ellipticity = NA

V = -1.3621243000E+05

G = 7.8006852103E+00

K = 1.3620462932E+05

L = 1.3619682863E+05

Vnuc = 1.8645802720E+06
Ven = -2.2307020258E+08
Vrep = 2.2293399015E+08
DelSqV = 4.6164896495E+09
DelSqVen = 1.0157996585E+12
DelSqVrep = -1.0111831688E+12
DelSqG = 2.0675982212E+08
DelSqK = -4.8232494716E+09
Stress_EigVals = -4.5404413662E+04 -4.5404136290E+04 -4.5403880052E+04
Stress_EigVec1 = 9.7278753409E-01 1.5326513974E-01 1.7376481365E-01
Stress_EigVec2 = -1.5573537122E-01 9.8779863704E-01 5.8890857800E-04
Stress_EigVec3 = -1.7155438694E-01 -2.7634210682E-02 9.8478700373E-01
-DivStress = 3.6734397144E+03 5.7207427154E+02 3.0881530919E+03

CP# 18 Coords = -4.13260256857088E+00 1.02756877030852E+00 2.71745560141846E+00

Type = (3,-3) NACP H18

Rho = 4.3947761288E-01 Rho at Nucleus = 4.3661997422E-01

GradRho = 5.2885647250E-14 -6.3043320564E-14 -2.5695591488E-14

HessRho_EigVals = -8.9569763758E+00 -8.9528903648E+00 -8.3384399806E+00

HessRho_EigVec1 = -3.9784897684E-01 -6.2563483571E-01 6.7104190926E-01

HessRho_EigVec2 = 6.8069748060E-01 2.8909642044E-01 6.7310786624E-01

HessRho_EigVec3 = -6.1511554324E-01 7.2457181289E-01 3.1085134136E-01

DelSqRho = -2.6248306721E+01

Bond Ellipticity = NA

V = -6.5766370498E+00

G = 7.2801847582E-03

K = 6.5693568651E+00

L = 6.5620766803E+00

Vnuc = 5.2888115862E+01

Ven = -2.3243142909E+01

Vrep = 1.6666505859E+01

DelSqV = 1.7067885332E+03

DelSqVen = 1.3882234871E+03
DelSqVrep = 3.1856504615E+02
DelSqG = 1.3109638458E+02
DelSqK = -1.8378849178E+03
Stress_EigVals = -2.2450307444E+00 -2.2443966289E+00 -2.0872096766E+00
Stress_EigVec1 = 7.6540263324E-01 4.5158841279E-01 4.5850486853E-01
Stress_EigVec2 = -1.9159596347E-01 -5.2025167012E-01 8.3224346589E-01
Stress_EigVec3 = -6.1436942943E-01 7.2484902233E-01 3.1167948122E-01
-DivStress = -8.7748234575E+00 1.0361689438E+01 4.4447735777E+00

CP# 19 Coords = -3.61482010203074E+00 -2.25588525381025E+00 2.71378161018971E+00

Type = (3,-3) NACP H19

Rho = 4.3950671833E-01 Rho at Nucleus = 4.3664847698E-01

GradRho = 2.0468041437E-09 4.9870443890E-09 -1.7516807950E-09

HessRho_EigVals = -8.9576235578E+00 -8.9535315427E+00 -8.3389330096E+00

HessRho_EigVec1 = 5.7104885961E-01 -4.7139328375E-01 -6.7208003390E-01

HessRho_EigVec2 = 7.3668357912E-01 -6.6970138430E-02 6.7291329665E-01

HessRho_EigVec3 = 3.6221610149E-01 8.7937669550E-01 -3.0902447027E-01

DelSqRho = -2.6250088110E+01

Bond Ellipticity = NA

V = -6.5770866107E+00

G = 7.2822915780E-03

K = 6.5698043191E+00

L = 6.5625220275E+00

Vnuc = 5.2885243569E+01

Ven = -2.3243419849E+01

Vrep = 1.6666333239E+01

DelSqV = 1.7069006804E+03

DelSqVen = 1.3882423203E+03

DelSqVrep = 3.1865836007E+02

DelSqG = 1.3110561167E+02

DelSqK = -1.8380062921E+03

Stress_EigVals = -2.2451940473E+00 -2.2445592942E+00 -2.0873332691E+00
Stress_EigVec1 = 8.6703962886E-01 -1.9475063389E-01 4.5860055885E-01
Stress_EigVec2 = -3.4295601057E-01 4.3440000132E-01 8.3287322785E-01
Stress_EigVec3 = 3.6141867244E-01 8.7941391247E-01 -3.0985111547E-01
-DivStress = -5.1600544362E+00 -1.2570748545E+01 4.4189326370E+00

CP# 20 Coords = -1.72349088764551E+00 2.13329895745810E+00 -1.78890718848579E+00

Type = (3,-3) NACP C20

Rho = 1.1963055812E+02 Rho at Nucleus = 1.1963055811E+02

GradRho = 3.4446889785E-11 -3.1049107729E-11 1.5494494576E-11

HessRho_EigVals = -1.8158837677E+05 -1.8158823987E+05 -1.8158787212E+05

HessRho_EigVec1 = 7.7838979206E-01 6.2777441497E-01 2.9352221958E-03

HessRho_EigVec2 = -5.0754582347E-01 6.3205394918E-01 -5.8558094437E-01

HessRho_EigVec3 = -3.6946795355E-01 4.5432046975E-01 8.1060862447E-01

DelSqRho = -5.4476448876E+05

Bond Ellipticity = NA

V = -1.3620654710E+05

G = 7.7124552261E+00

K = 1.3619883465E+05

L = 1.3619112219E+05

Vnuc = 1.5258667432E+07

Ven = -1.8254029011E+09

Vrep = 1.8252666945E+09

DelSqV = 4.6162946495E+09

DelSqVen = 8.3123786220E+12

DelSqVrep = -8.3077623273E+12

DelSqG = 2.0675100948E+08

DelSqK = -4.8230456590E+09

Stress_EigVals = -4.5402253766E+04 -4.5402169015E+04 -4.5402124321E+04

Stress_EigVec1 = -3.7835531643E-01 4.6632039298E-01 7.9962025088E-01

Stress_EigVec2 = -5.0005869193E-01 6.2397294538E-01 -6.0049901587E-01

Stress_EigVec3 = 7.7896634019E-01 6.2705905186E-01 2.8959154592E-03

-DivStress = -3.6366165257E+02 4.3896297408E+02 -1.5221587232E+02

CP# 21 Coords = -2.93896907001566E+00 3.63629348326378E+00 -1.12668806482291E+00

Type = (3,-3) NACP H21

Rho = 4.4298081374E-01 Rho at Nucleus = 4.4008096521E-01

GradRho = 6.4658348120E-14 -7.6726819342E-14 -3.3134953115E-14

HessRho_EigVals = -9.0275281133E+00 -9.0264872539E+00 -8.3984473169E+00

HessRho_EigVec1 = -7.7789376256E-01 -6.2839466628E-01 -1.1989811768E-03

HessRho_EigVec2 = 1.9949929470E-01 -2.4876984579E-01 9.4779406795E-01

HessRho_EigVec3 = -5.9588700739E-01 7.3704389775E-01 3.1888080407E-01

DelSqRho = -2.6452462684E+01

Bond Ellipticity = NA

V = -6.6265211860E+00

G = 6.7027574566E-03

K = 6.6198184285E+00

L = 6.6131156710E+00

Vnuc = 5.3187996548E+01

Ven = -2.3561261992E+01

Vrep = 1.6934740806E+01

DelSqV = 1.7195050644E+03

DelSqVen = 1.4069534939E+03

DelSqVrep = 3.1255157048E+02

DelSqG = 1.3207128056E+02

DelSqK = -1.8515763450E+03

Stress_EigVals = -2.2622490157E+00 -2.2619244734E+00 -2.1023476969E+00

Stress_EigVec1 = -7.7834167575E-01 -6.2783233116E-01 -3.2862942187E-03

Stress_EigVec2 = 1.9772739995E-01 -2.5008951768E-01 9.4781807772E-01

Stress_EigVec3 = -5.9589270099E-01 7.3707652051E-01 3.1879474873E-01

-DivStress = -8.6061448519E+00 1.0645924214E+01 4.6183800960E+00

CP# 22 Coords = -1.75957068813543E+00 2.18082730975302E+00 -3.83284940905336E+00

Type = (3,-3) NACP H22

Rho = 4.4237839311E-01 Rho at Nucleus = 4.3950020566E-01
GradRho = -9.2287288922E-16 -1.3010426070E-16 -1.0217521274E-15
HessRho_EigVals = -9.0134816421E+00 -9.0126734772E+00 -8.3885053627E+00
HessRho_EigVec1 = 7.7399617601E-01 6.3318938360E-01 1.0601973049E-03
HessRho_EigVec2 = -6.3279450654E-01 7.7345212842E-01 3.6645839205E-02
HessRho_EigVec3 = 2.2383744476E-02 -2.9034626441E-02 9.9932775327E-01
DelSqRho = -2.6414660482E+01
Bond Ellipticity = NA
V = -6.6171214964E+00
G = 6.7281879446E-03
K = 6.6103933084E+00
L = 6.6036651205E+00
Vnuc = 5.3335631534E+01
Ven = -2.3594530973E+01
Vrep = 1.6977409477E+01
DelSqV = 1.7172530620E+03
DelSqVen = 1.4088425986E+03
DelSqVrep = 3.0841046345E+02
DelSqG = 1.3187322372E+02
DelSqK = -1.8491262857E+03
Stress_EigVals = -2.2587792297E+00 -2.2584956120E+00 -2.0998466547E+00
Stress_EigVec1 = 7.7567256423E-01 6.3113482526E-01 9.5155051277E-04
Stress_EigVec2 = -6.3073125781E-01 7.7512085708E-01 3.6955883665E-02
Stress_EigVec3 = 2.2586578530E-02 -2.9265837698E-02 9.9931644498E-01
-DivStress = -3.2890505961E-01 4.2573588624E-01 -1.4372701142E+01

CP# 23 Coords = -2.73432891564181E+00 -4.30878294858828E-01 -8.65292977345974E-01

Type = (3,-3) NACP C23

Rho = 1.1961607413E+02 Rho at Nucleus = 1.1961607394E+02
GradRho = 7.3870365380E-10 1.1614476048E-10 1.0958564889E-09
HessRho_EigVals = -1.8157264421E+05 -1.8157211983E+05 -1.8157169406E+05
HessRho_EigVec1 = -1.7544884975E-01 -2.8614985641E-02 9.8407260084E-01

HessRho_EigVec2 = -1.5696742723E-01 9.8760350886E-01 7.3216718709E-04

HessRho_EigVec3 = 9.7189450452E-01 1.5433888647E-01 1.7776552032E-01

DelSqRho = -5.4471645809E+05

Bond Ellipticity = NA

V = -1.3619421887E+05

G = 7.5521756391E+00

K = 1.3618666670E+05

L = 1.3617911452E+05

Vnuc = 4.1865591994E+06

Ven = -5.0077977553E+08

Vrep = 5.0064358131E+08

DelSqV = 4.6158929541E+09

DelSqVen = 2.2804876493E+12

DelSqVrep = -2.2758717563E+12

DelSqG = 2.0673918442E+08

DelSqK = -4.8226321385E+09

Stress_EigVals = -4.5398203138E+04 -4.5398080727E+04 -4.5397935010E+04

Stress_EigVec1 = 9.7312229999E-01 1.5437874221E-01 1.7088064027E-01

Stress_EigVec2 = -1.5678759087E-01 9.8763215839E-01 6.0914249049E-04

Stress_EigVec3 = -1.6867317693E-01 -2.7384734057E-02 9.8529154859E-01

-DivStress = -1.2212207820E+03 -1.8766147831E+02 -1.7606944682E+03

CP# 24 Coords = -4.60961555240471E+00 -7.26421518683924E-01 -1.61739384644612E+00

Type = (3,-3) NACP H24

Rho = 4.4622752172E-01 Rho at Nucleus = 4.4329940872E-01

GradRho = -2.1458529398E-15 5.1087606368E-16 7.6848249986E-16

HessRho_EigVals = -9.1022667301E+00 -9.1020483984E+00 -8.4658047257E+00

HessRho_EigVec1 = -3.6046816576E-01 -6.5385854859E-02 9.3047696987E-01

HessRho_EigVec2 = -1.5874126135E-01 9.8728875918E-01 7.8814935117E-03

HessRho_EigVec3 = 9.1916479122E-01 1.4486406035E-01 3.6626560117E-01

DelSqRho = -2.6670119854E+01

Bond Ellipticity = NA

V = -6.6811053784E+00
G = 6.7877074363E-03
K = 6.6743176710E+00
L = 6.6675299635E+00
Vnuc = 5.3085093403E+01
Ven = -2.3688029669E+01
Vrep = 1.7006924291E+01
DelSqV = 1.7336112672E+03
DelSqVen = 1.4157858035E+03
DelSqVrep = 3.1782546365E+02
DelSqG = 1.3327956421E+02
DelSqK = -1.8668908314E+03
Stress_EigVals = -2.2809262991E+00 -2.2808168752E+00 -2.1193622042E+00
Stress_EigVec1 = -3.5986547957E-01 -6.5271611919E-02 9.3071824592E-01
Stress_EigVec2 = -1.5872446145E-01 9.8729156983E-01 7.8677492276E-03
Stress_EigVec3 = 9.1940381876E-01 1.4489642099E-01 3.6565235570E-01
-DivStress = -1.3419038186E+01 -2.1152735258E+00 -5.2837363241E+00

CP# 25 Coords = -3.05277498700274E-03 -4.01765000430564E-03 2.66196720916929E+00

Type = (3,-3) NACP B25

Rho = 6.7285975620E+01 Rho at Nucleus = 6.7285975247E+01

GradRho = -5.8583645747E-12 1.2709885228E-14 3.8530683366E-09

HessRho_EigVals = -6.7253864874E+04 -6.7251385363E+04 -6.7251384474E+04

HessRho_EigVec1 = -3.3414523851E-04 -1.2870185389E-03 9.9999911596E-01

HessRho_EigVec2 = 7.0447127295E-01 7.0973157304E-01 1.1488344293E-03

HessRho_EigVec3 = 7.0973242419E-01 -7.0447103405E-01 -6.6951416263E-04

DelSqRho = -2.0175663471E+05

Bond Ellipticity = NA

V = -5.0442510146E+04

G = 1.6757342693E+00

K = 5.0440834412E+04

L = 5.0439158678E+04

Vnuc = 1.5018908139E+06
Ven = -1.0105618869E+08
Vrep = 1.0100574618E+08
DelSqV = 1.0749716153E+09
DelSqVen = 3.0301643776E+11
DelSqVrep = -3.0194146614E+11
DelSqG = 5.0418140326E+07
DelSqK = -1.1253897556E+09
Stress_EigVals = -1.6814414071E+04 -1.6814413812E+04 -1.6813682263E+04
Stress_EigVec1 = 7.8081703010E-01 -6.2475953804E-01 -5.3398450168E-04
Stress_EigVec2 = 6.2475966971E-01 7.8081614915E-01 1.2232418908E-03
Stress_EigVec3 = -3.4728831627E-04 -1.2887400811E-03 9.9999910927E-01
-DivStress = 1.7304364659E+00 6.0555344988E-03 -1.1635851741E+03

CP# 26 Coords = 1.31183210002199E+00 2.06644523830779E-01 5.47564083614068E-01

Type = (3,+1) RCP C1 C4 C6 C12 C9 B25

Rho = 2.1939096661E-02

GradRho = -1.7347234760E-18 -3.0357660830E-18 2.2659825405E-17

HessRho_EigVals = -1.8118672770E-02 6.0475792749E-02 6.8662349696E-02

HessRho_EigVec1 = 9.2910379520E-01 1.4634395471E-01 3.3963154251E-01

HessRho_EigVec2 = -1.5342156562E-01 9.8814213991E-01 -6.0773792328E-03

HessRho_EigVec3 = -3.3649362691E-01 -4.6460286876E-02 9.4053893104E-01

DelSqRho = 1.1101946967E-01

Bond Ellipticity = NA

V = -2.0042133618E-02

G = 2.3898500518E-02

K = -3.8563669004E-03

L = -2.7754867419E-02

Vnuc = 2.1088477509E+01

Ven = -4.6266214650E-01

Vrep = 4.4262001288E-01

DelSqV = -1.1160206861E-01

DelSqVen = -2.3412315893E+00

DelSqVrep = 2.2296295207E+00

DelSqG = 8.1880644542E-02

DelSqK = 2.9721424064E-02

Stress_EigVals = -7.7756308968E-03 -6.1900894529E-03 -6.0764132682E-03

Stress_EigVec1 = 8.2123171865E-01 1.2828881547E-01 5.5598601071E-01

Stress_EigVec2 = -5.4783264096E-01 -9.5195597270E-02 8.3115413478E-01

Stress_EigVec3 = -1.5955519979E-01 9.8715742315E-01 7.8968433675E-03

-DivStress = -1.4417703005E-03 -2.3067907168E-04 6.6856275393E-04

CP# 27 Coords = 2.26216073648365E+00 2.92903214601274E+00 2.49467425495932E+00

Type = (3,-1) BCP H2 C1

Rho = 2.6931042015E-01

GradRho = -7.9797279895E-17 -5.5511151231E-17 1.2229800506E-16

HessRho_EigVals = -6.7835236043E-01 -6.6199579591E-01 4.6467991052E-01

HessRho_EigVec1 = -3.5120288697E-01 5.5873306986E-01 7.5131477347E-01

HessRho_EigVec2 = 4.6277414866E-02 8.1180795443E-01 -5.8208783357E-01

HessRho_EigVec3 = 9.3515503156E-01 1.6966202215E-01 3.1096601933E-01

DelSqRho = -8.7566824582E-01

Bond Ellipticity = 2.4707958302E-02

V = -3.1120675623E-01

G = 4.6144847388E-02

K = 2.6506190884E-01

L = 2.1891706146E-01

Vnuc = 1.8215601678E+01

Ven = -4.9056513413E+00

Vrep = 4.5944445851E+00

DelSqV = -2.2743516049E+00

DelSqVen = 1.5950823968E+01

DelSqVrep = -1.8225175573E+01

DelSqG = 1.6459574957E+00

DelSqK = 6.2839410923E-01

Stress_EigVals = -2.1166428799E-01 -2.0797154968E-01 1.0842908144E-01
Stress_EigVec1 = -2.2452780640E-02 9.0232191921E-01 -4.3047767277E-01
Stress_EigVec2 = -3.5189928579E-01 3.9589769585E-01 8.4819331941E-01
Stress_EigVec3 = 9.3576854259E-01 1.7052908414E-01 3.0863743480E-01
-DivStress = -1.7090826862E-01 -2.9257651967E-02 -5.3793470220E-02
BPL = 2.0402554095E+00 = 7.4199018100E-01 + 1.2982652285E+00
GBL_I = 2.0400295003E+00
GBL_II = 2.0658844908E+00
GBL_III = 2.0400777398E+00 = 7.4199013060E-01 + 1.2980876092E+00
GBL_IV = 2.0659339564E+00 = 7.6784573002E-01 + 1.2980882264E+00

CP# 28 Coords = -8.36436175662787E-01 1.03192939797596E+00 5.47029239594010E-01

Type = (3,+1) RCP C1 C4 C20 C23 C17 B25
Rho = 2.1928556245E-02
GradRho = -2.9490299092E-17 -7.3725747729E-18 2.2551405188E-17
HessRho_EigVals = -1.8112158578E-02 6.0420306418E-02 6.8665429957E-02
HessRho_EigVec1 = -5.9196617012E-01 7.3121003209E-01 3.3898074046E-01
HessRho_EigVec2 = 7.7613078461E-01 6.3055376543E-01 -4.7910420232E-03
HessRho_EigVec3 = 2.1724884030E-01 -2.6025725327E-01 9.4078111350E-01
DelSqRho = 1.1097357780E-01
Bond Ellipticity = NA
V = -2.0029702361E-02
G = 2.3886548405E-02
K = -3.8568460439E-03
L = -2.7743394449E-02
Vnuc = 2.1087654133E+01
Ven = -4.6242180974E-01
Vrep = 4.4239210738E-01
DelSqV = -1.1154221661E-01
DelSqVen = -2.3401724265E+00
DelSqVrep = 2.2286302099E+00
DelSqG = 8.1844947351E-02

DelSqK = 2.9697269254E-02

Stress_EigVals = -7.7733075333E-03 -6.1839638099E-03 -6.0724310181E-03

Stress_EigVec1 = -5.2413514140E-01 6.4579342999E-01 5.5518753528E-01

Stress_EigVec2 = 3.4532269031E-01 -4.3475173772E-01 8.3171098713E-01

Stress_EigVec3 = 7.7848223686E-01 6.2764780915E-01 4.8615388930E-03

-DivStress = 9.1203177062E-04 -1.1404096752E-03 6.7287730087E-04

CP# 29 Coords = 2.84455563116234E-01 3.69093891967428E+00 2.49467278038937E+00

Type = (3,-1) BCP H3 C1

Rho = 2.6934374353E-01

GradRho = -3.2959746044E-15 2.9507646326E-15 9.6450625264E-16

HessRho_EigVals = -6.7845501200E-01 -6.6210931979E-01 4.6464973835E-01

HessRho_EigVec1 = 6.3546533976E-01 1.7889278109E-01 7.5111994704E-01

HessRho_EigVec2 = -5.1011928486E-01 -6.3298515685E-01 5.8232989483E-01

HessRho_EigVec3 = -5.7962239189E-01 7.5321123470E-01 3.1098347020E-01

DelSqRho = -8.7591459343E-01

Bond Ellipticity = 2.4687301204E-02

V = -3.1129646227E-01

G = 4.6158906957E-02

K = 2.6513755532E-01

L = 2.1897864836E-01

Vnuc = 1.8214380840E+01

Ven = -4.9059295216E+00

Vrep = 4.5946330594E+00

DelSqV = -2.2742548674E+00

DelSqVen = 1.5954241988E+01

DelSqVrep = -1.8228496856E+01

DelSqG = 1.6463539649E+00

DelSqK = 6.2790090251E-01

Stress_EigVals = -2.1170516572E-01 -2.0801125708E-01 1.0841996053E-01

Stress_EigVec1 = -6.2177808544E-01 -6.5399410873E-01 4.3091033664E-01

Stress_EigVec2 = 5.2687044629E-01 5.7807506494E-02 8.4797749087E-01

Stress_EigVec3 = -5.7948213545E-01 7.5428774214E-01 3.0862672722E-01

-DivStress = 1.0717369817E-01 -1.3647372019E-01 -5.3844229945E-02

BPL = 2.0401392809E+00 = 7.4198997298E-01 + 1.2981493079E+00

GBL_I = 2.0399133026E+00

GBL_II = 2.0657704451E+00

GBL_III = 2.0399612990E+00 = 7.4198992396E-01 + 1.2979713751E+00

GBL_IV = 2.0658196538E+00 = 7.6784765786E-01 + 1.2979719960E+00

CP# 30 Coords = -3.42405010158909E-04 8.38193821540059E-05 2.60316770065659E-02

Type = (3,+3) CCP C1 C4 C6 C9 C12 C14 C17 C20 C23 B25

Rho = 1.3956374331E-02

GradRho = 3.3779233215E-15 8.3586308143E-15 -3.4692084275E-14

HessRho_EigVals = 2.2035219994E-02 2.7799289135E-02 2.7825624306E-02

HessRho_EigVec1 = -5.6713319532E-03 -4.3053415918E-03 9.9997464969E-01

HessRho_EigVec2 = 9.5177428740E-01 -3.0677203670E-01 4.0771728772E-03

HessRho_EigVec3 = 3.0674670631E-01 9.5177328263E-01 5.8375194797E-03

DelSqRho = 7.7660133435E-02

Bond Ellipticity = NA

V = -1.3677441775E-02

G = 1.6546237567E-02

K = -2.8687957921E-03

L = -1.9415033359E-02

Vnuc = 2.1632251446E+01

Ven = -3.0190779880E-01

Vrep = 2.8823035703E-01

DelSqV = -7.1788005783E-02

DelSqVen = -1.6799635338E+00

DelSqVrep = 1.6081755281E+00

DelSqG = 7.3901585713E-02

DelSqK = -2.1135799304E-03

Stress_EigVals = -4.6537284003E-03 -4.5120812071E-03 -4.5116321672E-03

Stress_EigVec1 = -6.1626142367E-03 -3.6364376504E-03 9.9997439893E-01

Stress_EigVec2 = 9.8097900229E-01 -1.9404041424E-01 5.3399160050E-03

Stress_EigVec3 = 1.9401602833E-01 9.8098679602E-01 4.7630651975E-03

-DivStress = -1.6974077423E-06 -2.5667358249E-06 1.3310651938E-03

CP# 31 Coords = 1.01485932848644E+00 2.63971562268454E+00 6.32082105734683E-01

Type = (3,-1) BCP C1 C4

Rho = 2.1433878215E-01

GradRho = -1.2143064332E-17 4.5102810375E-17 -3.2959746044E-17

HessRho_EigVals = -3.7416081375E-01 -3.5419412766E-01 3.2845243920E-01

HessRho_EigVec1 = 9.3328881011E-01 -3.5912669571E-01 -1.1558183536E-04

HessRho_EigVec2 = 3.5880772451E-01 9.3247334178E-01 -4.1838782307E-02

HessRho_EigVec3 = 1.5133200623E-02 3.9006195700E-02 9.9912436810E-01

DelSqRho = -3.9990250221E-01

Bond Ellipticity = 5.6372154499E-02

V = -2.1056963362E-01

G = 5.5297004032E-02

K = 1.5527262958E-01

L = 9.9975625552E-02

Vnuc = 2.1472724591E+01

Ven = -4.6024376382E+00

Vrep = 4.3918680046E+00

DelSqV = -1.4752460950E+00

DelSqVen = 8.5869962932E+00

DelSqVrep = -1.0062242388E+01

DelSqG = 9.4764687717E-01

DelSqK = 5.2759921786E-01

Stress_EigVals = -1.3888924360E-01 -1.3820372694E-01 6.6523336923E-02

Stress_EigVec1 = 3.5737910156E-01 9.3227832531E-01 -5.6011623153E-02

Stress_EigVec2 = 9.3373957172E-01 -3.5795301334E-01 -2.2899858600E-04

Stress_EigVec3 = 2.0263019708E-02 5.2218429706E-02 9.9843009051E-01

-DivStress = -3.9577803198E-04 -1.0682113501E-03 5.6353433347E-03

BPL = 2.9719609383E+00 = 1.4790282529E+00 + 1.4929326854E+00

GBL_I = 2.9718251677E+00

GBL_II = 2.9718282398E+00

GBL_III = 2.9718790927E+00 = 1.4789605632E+00 + 1.4929185295E+00

GBL_IV = 2.9718821545E+00 = 1.4789624845E+00 + 1.4929196699E+00

CP# 32 Coords = 1.13007304145455E-03 1.86006053476798E-03 -1.29583459900684E+00

Type = (3,+1) RCP C4 C6 C12 C14 C23 C20

Rho = 1.9870317352E-02

GradRho = -5.2977174243E-14 -1.4037247859E-13 1.0702246381E-13

HessRho_EigVals = -1.5654578800E-02 6.7117165387E-02 6.7226639663E-02

HessRho_EigVec1 = -8.6637423041E-04 -1.1495253711E-03 9.9999896399E-01

HessRho_EigVec2 = 9.9764066742E-01 -6.8647518759E-02 7.8541891469E-04

HessRho_EigVec3 = 6.8646544781E-02 9.9764031432E-01 1.2062876997E-03

DelSqRho = 1.1868922625E-01

Bond Ellipticity = NA

V = -1.9411991878E-02

G = 2.4542149220E-02

K = -5.1301573422E-03

L = -2.9672306562E-02

Vnuc = 2.1258656196E+01

Ven = -4.2241624509E-01

Vrep = 4.0300425321E-01

DelSqV = -1.2053152578E-01

DelSqVen = -2.5231734550E+00

DelSqVrep = 2.4026419292E+00

DelSqG = 9.3622541507E-02

DelSqK = 2.6908984277E-02

Stress_EigVals = -7.0116765504E-03 -6.2006428665E-03 -6.1996724612E-03

Stress_EigVec1 = -1.3186690849E-03 -1.8008099710E-03 9.9999750909E-01

Stress_EigVec2 = 9.9041278404E-01 1.3813073474E-01 1.5547777969E-03

Stress_EigVec3 = -1.3813319053E-01 9.9041236725E-01 1.6013964874E-03

-DivStress = 2.5908083848E-08 -4.0902898236E-07 5.0269163394E-04

CP# 33 Coords = 1.43021108892679E+00 3.72157510455503E+00 -1.33778713412813E+00

Type = (3,-1) BCP H5 C4

Rho = 2.7484980128E-01

GradRho = 6.2970462178E-15 1.6119050539E-14 -6.8382799423E-15

HessRho_EigVals = -7.0151436460E-01 -7.0004041864E-01 4.8852909202E-01

HessRho_EigVec1 = 1.3486522886E-01 3.4353550127E-01 9.2940557854E-01

HessRho_EigVec2 = 9.3316496212E-01 -3.5943934619E-01 -2.5514482173E-03

HessRho_EigVec3 = 3.3318842046E-01 8.6763282313E-01 -3.6905116271E-01

DelSqRho = -9.1302569123E-01

Bond Ellipticity = 2.1055155111E-03

V = -3.1334506128E-01

G = 4.2544319234E-02

K = 2.7080074204E-01

L = 2.2825642281E-01

Vnuc = 1.8864788057E+01

Ven = -5.1849832486E+00

Vrep = 4.8716381874E+00

DelSqV = -2.4209147231E+00

DelSqVen = 1.7224036155E+01

DelSqVrep = -1.9644950878E+01

DelSqG = 1.6760731844E+00

DelSqK = 7.4484153866E-01

Stress_EigVals = -2.1353090626E-01 -2.1311409233E-01 1.1329993732E-01

Stress_EigVec1 = 9.3330579938E-01 -3.5907905505E-01 -1.5865261513E-03

Stress_EigVec2 = 1.3364635945E-01 3.4326133582E-01 9.2968290612E-01

Stress_EigVec3 = 3.3328506634E-01 8.6789048132E-01 -3.6835740389E-01

-DivStress = -5.6328300713E-02 -1.4666809241E-01 6.0554742377E-02

BPL = 2.0419985048E+00 = 7.3433652882E-01 + 1.3076619760E+00

GBL_I = 2.0419729760E+00

GBL_II = 2.0679434622E+00

GBL_III = 2.0419732476E+00 = 7.3433560919E-01 + 1.3076376384E+00

$$\text{GBL\_IV} = 2.0679436345\text{E}+00 = 7.6030719503\text{E}-01 + 1.3076364394\text{E}+00$$

$$\text{CP\# 34 Coords} = 1.84817889430715\text{E}+00 \ 1.50066844897684\text{E}+00 \ -1.31701360251168\text{E}+00$$

$$\text{Type} = (3,-1) \text{ BCP C4 C6}$$

$$\text{Rho} = 2.3831696246\text{E}-01$$

$$\text{GradRho} = 6.2450045135\text{E}-17 \ -6.9388939039\text{E}-17 \ -9.5409791179\text{E}-17$$

$$\text{HessRho\_EigVals} = -4.3410460249\text{E}-01 \ -4.3279136969\text{E}-01 \ 3.4508292625\text{E}-01$$

$$\text{HessRho\_EigVec1} = -4.8354771885\text{E}-02 \ -4.2971090034\text{E}-01 \ 9.0167087020\text{E}-01$$

$$\text{HessRho\_EigVec2} = 8.0592529566\text{E}-01 \ 5.1648279537\text{E}-01 \ 2.8936126192\text{E}-01$$

$$\text{HessRho\_EigVec3} = -5.9003917993\text{E}-01 \ 7.4067136047\text{E}-01 \ 3.2134047665\text{E}-01$$

$$\text{DelSqRho} = -5.2181304594\text{E}-01$$

$$\text{Bond Ellipticity} = 3.0343322339\text{E}-03$$

$$\text{V} = -2.4264618729\text{E}-01$$

$$\text{G} = 5.6096462901\text{E}-02$$

$$\text{K} = 1.8654972439\text{E}-01$$

$$\text{L} = 1.3045326148\text{E}-01$$

$$\text{Vnuc} = 2.1885693404\text{E}+01$$

$$\text{Ven} = -5.2157319734\text{E}+00$$

$$\text{Vrep} = 4.9730857861\text{E}+00$$

$$\text{DelSqV} = -1.6175637460\text{E}+00$$

$$\text{DelSqVen} = 1.1420240338\text{E}+01$$

$$\text{DelSqVrep} = -1.3037804084\text{E}+01$$

$$\text{DelSqG} = 1.0803234759\text{E}+00$$

$$\text{DelSqK} = 5.3724027009\text{E}-01$$

$$\text{Stress\_EigVals} = -1.5750395694\text{E}-01 \ -1.5729768393\text{E}-01 \ 7.2155453581\text{E}-02$$

$$\text{Stress\_EigVec1} = 7.6772934540\text{E}-01 \ 3.9171845378\text{E}-01 \ 5.0709792465\text{E}-01$$

$$\text{Stress\_EigVec2} = -2.5027678125\text{E}-01 \ -5.4520835804\text{E}-01 \ 8.0006835901\text{E}-01$$

$$\text{Stress\_EigVec3} = -5.8987556738\text{E}-01 \ 7.4115079389\text{E}-01 \ 3.2053442206\text{E}-01$$

$$-\text{DivStress} = -8.5086880095\text{E}-04 \ 9.5969257235\text{E}-04 \ -9.0944689252\text{E}-04$$

$$\text{BPL} = 2.9068229242\text{E}+00 = 1.4545954137\text{E}+00 + 1.4522275105\text{E}+00$$

$$\text{GBL\_I} = 2.9066395038\text{E}+00$$

$$\text{GBL\_II} = 2.9066397298\text{E}+00$$

$$\text{GBL\_III} = 2.9067150033\text{E}+00 = 1.4545141294\text{E}+00 + 1.4522008739\text{E}+00$$

$$\text{GBL\_IV} = 2.9067152411\text{E}+00 = 1.4545141587\text{E}+00 + 1.4522010824\text{E}+00$$

CP# 35 Coords = 3.92797255087223E+00 6.22956379221319E-01 -1.35887238537086E+00

Type = (3,-1) BCP H7 C6

Rho = 2.7241559759E-01

GradRho = -2.0816681712E-17 4.5102810375E-17 -4.5102810375E-17

HessRho_EigVals = -6.8848719193E-01 -6.8758936459E-01 4.7720320957E-01

HessRho_EigVec1 = -1.5635638956E-01 9.8769988139E-01 1.2742645222E-03

HessRho_EigVec2 = -3.1315436350E-01 -5.0796933512E-02 9.4834277356E-01

HessRho_EigVec3 = 9.3674277369E-01 1.4788041065E-01 3.1724495281E-01

DelSqRho = -8.9887334695E-01

Bond Ellipticity = 1.3057609459E-03

V = -3.1187910250E-01

G = 4.3580382880E-02

K = 2.6829871962E-01

L = 2.2471833674E-01

Vnuc = 1.8716834587E+01

Ven = -5.0987576789E+00

Vrep = 4.7868785764E+00

DelSqV = -2.3495728077E+00

DelSqVen = 1.6824063749E+01

DelSqVrep = -1.9173636557E+01

DelSqG = 1.6657894925E+00

DelSqK = 6.8378331521E-01

Stress_EigVals = -2.1143064533E-01 -2.1133512193E-01 1.1088666476E-01

Stress_EigVec1 = -1.5743080957E-01 9.8751973210E-01 4.5076507401E-03

Stress_EigVec2 = -3.1410614465E-01 -5.4401406111E-02 9.4782794689E-01

Stress_EigVec3 = 9.3624402273E-01 1.4780144021E-01 3.1875047322E-01

-DivStress = -1.6164045081E-01 -2.5527058427E-02 -5.8971443139E-02

$$\text{BPL} = 2.0433037154\text{E}+00 = 7.3775667179\text{E}-01 + 1.3055470436\text{E}+00$$

$$\text{GBL\_I} = 2.0431813941\text{E}+00$$

GBL_II = 2.0691310043E+00

GBL_III = 2.0432060088E+00 = 7.3775650516E-01 + 1.3054495036E+00

GBL_IV = 2.0691558281E+00 = 7.6370665189E-01 + 1.3054491762E+00

CP# 36 Coords = 2.74273164129101E+00 4.37017081163367E-01 -3.09220224981741E+00

Type = (3,-1) BCP C6 H8

Rho = 2.7149165510E-01

GradRho = 9.7144514655E-17 1.5612511284E-17 5.7245874707E-17

HessRho_EigVals = -6.8384796523E-01 -6.8312594830E-01 4.7379522161E-01

HessRho_EigVec1 = -1.5491086706E-01 9.8792799159E-01 9.5220450635E-04

HessRho_EigVec2 = 9.8723178817E-01 1.5476536565E-01 3.7697188632E-02

HessRho_EigVec3 = -3.7094739575E-02 -6.7797507341E-03 9.9928875470E-01

DelSqRho = -8.9317869192E-01

Bond Ellipticity = 1.0569309156E-03

V = -3.1107698436E-01

G = 4.3891155692E-02

K = 2.6718582867E-01

L = 2.2329467298E-01

Vnuc = 1.8744865304E+01

Ven = -5.0890745060E+00

Vrep = 4.7779975216E+00

DelSqV = -2.3139542641E+00

DelSqVen = 1.6742514272E+01

DelSqVrep = -1.9056468536E+01

DelSqG = 1.6569432437E+00

DelSqK = 6.5701102042E-01

Stress_EigVals = -2.1057742448E-01 -2.1053026267E-01 1.1003070279E-01

Stress_EigVec1 = -1.6678744957E-01 9.8599273640E-01 5.2003656310E-04

Stress_EigVec2 = 9.8535135628E-01 1.6665988666E-01 3.6155039039E-02

Stress_EigVec3 = -3.5561936642E-02 -6.5426254831E-03 9.9934605754E-01

-DivStress = -2.7423129358E-03 -5.8819657023E-04 1.7651736572E-01

BPL = 2.0449609594E+00 = 1.3052729686E+00 + 7.3968799075E-01

GBL_I = 2.0448344124E+00

GBL_II = 2.0707026103E+00

GBL_III = 2.0448660721E+00 = 1.3051780913E+00 + 7.3968798078E-01

GBL_IV = 2.0707350786E+00 = 1.3051779842E+00 + 7.6555709440E-01

CP# 37 Coords = 3.49143227210913E-01 9.11202071825024E-01 2.55128407030356E+00

Type = (3,-1) BCP C1 B25

Rho = 1.8237954789E-01

GradRho = -1.1018963519E-14 -3.3240771247E-14 -1.2653073034E-14

HessRho_EigVals = -3.8058115989E-01 -2.9630762730E-01 4.6195125964E-01

HessRho_EigVec1 = 5.9701636939E-02 1.5512838112E-01 9.8608868765E-01

HessRho_EigVec2 = 9.3322092444E-01 -3.5930308324E-01 2.3617369755E-05

HessRho_EigVec3 = 3.5430836955E-01 9.2023718668E-01 -1.6622003347E-01

DelSqRho = -2.1493752755E-01

Bond Ellipticity = 2.8441229595E-01

V = -3.2237596136E-01

G = 1.3432078974E-01

K = 1.8805517162E-01

L = 5.3734381886E-02

Vnuc = 2.1856391335E+01

Ven = -3.9861587703E+00

Vrep = 3.6637828089E+00

DelSqV = -3.4711720855E+00

DelSqVen = 4.6977587147E+00

DelSqVrep = -8.1689308001E+00

DelSqG = 5.5276695043E+00

DelSqK = -2.0564974188E+00

Stress_EigVals = -1.4437136439E-01 -1.1998246527E-01 -5.8022131705E-02

Stress_EigVec1 = 9.3309522584E-01 -3.5962928366E-01 -2.7900276069E-04

Stress_EigVec2 = 9.7760296483E-02 2.5290241572E-01 9.6254002127E-01

Stress_EigVec3 = 3.4608701787E-01 8.9816877393E-01 -2.7113950211E-01

-DivStress = -1.8458116061E-01 -4.7960794060E-01 5.6997550566E-02

BPL = 2.9651767923E+00 = 1.9781164415E+00 + 9.8706035086E-01

GBL_I = 2.9605159487E+00

GBL_II = 2.9605125062E+00

GBL_III = 2.9647234278E+00 = 1.9778496160E+00 + 9.8687381180E-01

GBL_IV = 2.9647201772E+00 = 1.9778467406E+00 + 9.8687343664E-01

CP# 38 Coords = 2.22077704655990E+00 -8.53859906630978E-01 -1.31920830160314E+00

Type = (3,-1) BCP C6 C12

Rho = 2.3832844261E-01

GradRho = -2.7755575616E-17 1.0581813203E-16 -8.8470897275E-17

HessRho_EigVals = -4.3413109281E-01 -4.3282120922E-01 3.4505733758E-01

HessRho_EigVec1 = 1.8019670049E-01 -3.9262620086E-01 -9.0187239426E-01

HessRho_EigVec2 = 9.2574277696E-01 -2.4220457356E-01 2.9040877304E-01

HessRho_EigVec3 = 3.3245971191E-01 8.8723255742E-01 -3.1982640449E-01

DelSqRho = -5.2189496444E-01

Bond Ellipticity = 3.0263849334E-03

V = -2.4266589156E-01

G = 5.6096075224E-02

K = 1.8656981633E-01

L = 1.3047374111E-01

Vnuc = 2.1886023085E+01

Ven = -5.2160617968E+00

Vrep = 4.9733959053E+00

DelSqV = -1.6175834847E+00

DelSqVen = 1.1422205240E+01

DelSqVrep = -1.3039788724E+01

DelSqG = 1.0804109258E+00

DelSqK = 5.3717255887E-01

Stress_EigVals = -1.5751495539E-01 -1.5730598098E-01 7.2155044812E-02

Stress_EigVec1 = 8.5472847682E-01 -1.4018250118E-01 4.9978805235E-01

Stress_EigVec2 = -3.9890071175E-01 4.3870554317E-01 8.0524261472E-01

Stress_EigVec3 = 3.3214071277E-01 8.8762960335E-01 -3.1905522119E-01

-DivStress = -4.7581542187E-04 -1.0638497619E-03 -9.8550849518E-04

BPL = 2.9067561889E+00 = 1.4521171422E+00 + 1.4546390467E+00

GBL_I = 2.9065708849E+00

GBL_II = 2.9065711102E+00

GBL_III = 2.9066472107E+00 = 1.4520903847E+00 + 1.4545568259E+00

GBL_IV = 2.9066474479E+00 = 1.4520905976E+00 + 1.4545568503E+00

CP# 39 Coords = 6.13833810570059E-01 -7.66078836258980E-01 2.54929494356806E+00

Type = (3,-1) BCP B25 C9

Rho = 1.8240847772E-01

GradRho = -1.7277845821E-14 2.3918367287E-14 -1.2757156442E-14

HessRho_EigVals = -3.8064040456E-01 -2.9640691184E-01 4.6176825509E-01

HessRho_EigVec1 = 1.0494255350E-01 -1.3140275904E-01 9.8575878154E-01

HessRho_EigVec2 = 7.7724514287E-01 6.2919688102E-01 1.1281828535E-03

HessRho_EigVec3 = -6.2038459712E-01 7.6605783061E-01 1.6816168357E-01

DelSqRho = -2.1527906132E-01

Bond Ellipticity = 2.8418194500E-01

V = -3.2239298094E-01

G = 1.3428660781E-01

K = 1.8810637314E-01

L = 5.3819765330E-02

Vnuc = 2.1856302064E+01

Ven = -3.9867747880E+00

Vrep = 3.6643818071E+00

DelSqV = -3.4702522005E+00

DelSqVen = 4.7052041922E+00

DelSqVrep = -8.1754563926E+00

DelSqG = 5.5264433391E+00

DelSqK = -2.0561911386E+00

Stress_EigVals = -1.4437506341E-01 -1.1999616495E-01 -5.8021752576E-02

Stress_EigVec1 = 7.7697647196E-01 6.2952902368E-01 8.7770347711E-04

Stress_EigVec2 = 1.7108140049E-01 -2.1249319685E-01 9.6206953787E-01

Stress_EigVec3 = -6.0583720291E-01 7.4735523658E-01 2.7280292142E-01

-DivStress = -3.2330243646E-01 3.9936829739E-01 5.8011256189E-02

BPL = 2.9651137907E+00 = 9.8709115479E-01 + 1.9780226359E+00

GBL_I = 2.9604635857E+00

GBL_II = 2.9604601373E+00

GBL_III = 2.9646600827E+00 = 9.8690493487E-01 + 1.9777551478E+00

GBL_IV = 2.9646568259E+00 = 9.8690455168E-01 + 1.9777522742E+00

CP# 40 Coords = 1.77970634437346E+00 -2.19992255298109E+00 6.27047241747387E-01

Type = (3,-1) BCP C9 C12

Rho = 2.1448929695E-01

GradRho = 2.2551405188E-17 0.0000000000E+00 1.0581813203E-16

HessRho_EigVals = -3.7452989816E-01 -3.5451873571E-01 3.2850603327E-01

HessRho_EigVec1 = 7.7691889320E-01 6.2959743740E-01 2.0248954970E-03

HessRho_EigVec2 = -6.2905432445E-01 7.7610670831E-01 4.4147867597E-02

HessRho_EigVec3 = 2.6223849327E-02 -3.5573081699E-02 9.9902295548E-01

DelSqRho = -4.0054260061E-01

Bond Ellipticity = 5.6445994054E-02

V = -2.1085022595E-01

G = 5.5357287899E-02

K = 1.5549293805E-01

L = 1.0013565015E-01

Vnuc = 2.1474296627E+01

Ven = -4.6060067861E+00

Vrep = 4.3951565602E+00

DelSqV = -1.4766741110E+00

DelSqVen = 8.6013706173E+00

DelSqVrep = -1.0078044728E+01

DelSqG = 9.4874263069E-01

DelSqK = 5.2793148036E-01

Stress_EigVals = -1.3904091315E-01 -1.3835049693E-01 6.6541184128E-02

Stress_EigVec1 = -6.2925493321E-01 7.7500511463E-01 5.8354959783E-02

Stress_EigVec2 = 7.7640348932E-01 6.3023268617E-01 2.0935774135E-03

Stress_EigVec3 = 3.5154669852E-02 -4.6624388310E-02 9.9829370207E-01

-DivStress = -7.4626887208E-04 8.4229129467E-04 5.6822433820E-03

BPL = 2.9712530587E+00 = 1.4786562268E+00 + 1.4925968318E+00

GBL_I = 2.9711180054E+00

GBL_II = 2.9711210730E+00

GBL_III = 2.9711718622E+00 = 1.4785893741E+00 + 1.4925824882E+00

GBL_IV = 2.9711749195E+00 = 1.4785912955E+00 + 1.4925836240E+00

CP# 41 Coords = -4.77425398904755E-01 -1.24095967866376E+00 5.44941653170318E-01

Type = (3,+1) RCP C9 C12 C14 C23 C17 B25

Rho = 2.1937169359E-02

GradRho = -1.0408340856E-17 7.8062556419E-18 6.5052130349E-17

HessRho_EigVals = -1.8117834785E-02 6.0385991810E-02 6.8740297097E-02

HessRho_EigVec1 = 3.3777668179E-01 8.7880940769E-01 -3.3704738270E-01

HessRho_EigVec2 = 9.3258983571E-01 -3.6088211934E-01 -6.3477762287E-03

HessRho_EigVec3 = -1.2721285926E-01 -3.1218283247E-01 -9.4146628593E-01

DelSqRho = 1.1100845412E-01

Bond Ellipticity = NA

V = -2.0041012230E-02

G = 2.3896562880E-02

K = -3.8555506502E-03

L = -2.7752113531E-02

Vnuc = 2.1087745999E+01

Ven = -4.6260545538E-01

Vrep = 4.4256444315E-01

DelSqV = -1.1158582466E-01

DelSqVen = -2.3409180842E+00

DelSqVrep = 2.2293322596E+00

DelSqG = 8.1853886008E-02

DelSqK = 2.9731938649E-02

Stress_EigVals = -7.7776625056E-03 -6.1873547682E-03 -6.0759949564E-03

Stress_EigVec1 = 2.9930639982E-01 7.7683159013E-01 -5.5402920465E-01
Stress_EigVec2 = 1.8602961108E-01 5.2199498709E-01 8.3241469067E-01
Stress_EigVec3 = 9.3584649533E-01 -3.5221288169E-01 1.1722761727E-02
-DivStress = 5.2128171373E-04 1.3621235202E-03 6.7882682575E-04

CP# 42 Coords = 1.40760374820777E+00 -3.43071753684029E+00 2.48524718568518E+00

Type = (3,-1) BCP C9 H10

Rho = 2.6932552464E-01

GradRho = 3.4694469520E-17 -6.4184768611E-17 1.2490009027E-16

HessRho_EigVals = -6.7838435392E-01 -6.6204632371E-01 4.6463582363E-01

HessRho_EigVec1 = 6.5981010222E-01 2.2601248210E-02 7.5109241282E-01

HessRho_EigVec2 = 6.7993428324E-01 -4.4349315326E-01 -5.8395478720E-01

HessRho_EigVec3 = 3.1990623546E-01 8.9599274919E-01 -3.0798862629E-01

DelSqRho = -8.7579485400E-01

Bond Ellipticity = 2.4678077076E-02

V = -3.1125247256E-01

G = 4.6151879530E-02

K = 2.6510059303E-01

L = 2.1894871350E-01

Vnuc = 1.8214950950E+01

Ven = -4.9057512209E+00

Vrep = 4.5944987484E+00

DelSqV = -2.2739266017E+00

DelSqVen = 1.5952560308E+01

DelSqVrep = -1.8226486910E+01

DelSqG = 1.6461613607E+00

DelSqK = 6.2776524091E-01

Stress_EigVals = -2.1167850746E-01 -2.0798980595E-01 1.0841584086E-01

Stress_EigVec1 = 7.9278188035E-01 -4.2964992881E-01 -4.3231681539E-01

Stress_EigVec2 = 5.1908931186E-01 1.0420377220E-01 8.4834418733E-01

Stress_EigVec3 = 3.1944197674E-01 8.9696293822E-01 -3.0563754835E-01

-DivStress = 6.0007433866E-02 1.6296527506E-01 -5.3298849841E-02

BPL = 2.0402206875E+00 = 1.2982072272E+00 + 7.4201346035E-01

GBL_I = 2.0399957675E+00

GBL_II = 2.0658509732E+00

GBL_III = 2.0400434626E+00 = 1.2980300520E+00 + 7.4201341056E-01

GBL_IV = 2.0658998616E+00 = 1.2980306715E+00 + 7.6786919011E-01

CP# 43 Coords = 3.05492877267019E+00 -2.09745498352072E+00 2.49007123239917E+00

Type = (3,-1) BCP H11 C9

Rho = 2.6934114453E-01

GradRho = -3.8163916471E-17 -6.9388939039E-17 -2.6020852140E-17

HessRho_EigVals = -6.7844718683E-01 -6.6210123444E-01 4.6467617492E-01

HessRho_EigVec1 = -1.6232103073E-01 -6.4286640214E-01 7.4858177375E-01

HessRho_EigVec2 = -2.9405448275E-01 7.5568820810E-01 5.8520705166E-01

HessRho_EigVec3 = 9.4190437102E-01 1.2513241446E-01 3.1170183621E-01

DelSqRho = -8.7587224635E-01

Bond Ellipticity = 2.4687995642E-02

V = -3.1128925766E-01

G = 4.6160598034E-02

K = 2.6512865962E-01

L = 2.1896806159E-01

Vnuc = 1.8214274844E+01

Ven = -4.9058536333E+00

Vrep = 4.5945643756E+00

DelSqV = -2.2747311074E+00

DelSqVen = 1.5953377823E+01

DelSqVrep = -1.8228108931E+01

DelSqG = 1.6463953893E+00

DelSqK = 6.2833571811E-01

Stress_EigVals = -2.1170377635E-01 -2.0801321254E-01 1.0842773124E-01

Stress_EigVec1 = -2.5632693372E-01 8.6392252720E-01 4.3351397907E-01

Stress_EigVec2 = -2.1330635318E-01 -4.8799895779E-01 8.4637900310E-01

Stress_EigVec3 = 9.4276025730E-01 1.2447844871E-01 3.0936744021E-01

-DivStress = -1.7169078524E-01 -2.4579210322E-02 -5.3976595706E-02

BPL = 2.0401187419E+00 = 7.4196825706E-01 + 1.2981504849E+00

GBL_I = 2.0398940904E+00

GBL_II = 2.0657513983E+00

GBL_III = 2.0399420591E+00 = 7.4196820861E-01 + 1.2979738505E+00

GBL_IV = 2.0658005766E+00 = 7.6782610881E-01 + 1.2979744678E+00

CP# 44 Coords = 2.50812737800124E+00 -3.09553030347579E+00 -1.34485849472121E+00

Type = (3,-1) BCP C12 H13

Rho = 2.7483591136E-01

GradRho = 4.8572257327E-17 4.3368086899E-17 -3.5561831258E-17

HessRho_EigVals = -7.0140855507E-01 -6.9994542218E-01 4.8845588498E-01

HessRho_EigVec1 = 2.2274500581E-01 -2.9685905997E-01 9.2857921627E-01

HessRho_EigVec2 = -7.8049564804E-01 -6.2503432354E-01 -1.2595149531E-02

HessRho_EigVec3 = -5.8413286655E-01 7.2194653051E-01 3.7092047842E-01

DelSqRho = -9.1289809226E-01

Bond Ellipticity = 2.0903528264E-03

V = -3.1334697947E-01

G = 4.2561228201E-02

K = 2.7078575127E-01

L = 2.2822452307E-01

Vnuc = 1.8865795443E+01

Ven = -5.1849980841E+00

Vrep = 4.8716511046E+00

DelSqV = -2.4200815177E+00

DelSqVen = 1.7222548669E+01

DelSqVrep = -1.9642630187E+01

DelSqG = 1.6759227907E+00

DelSqK = 7.4415872704E-01

Stress_EigVals = -2.1351677832E-01 -2.1310674116E-01 1.1327654002E-01

Stress_EigVec1 = -7.7843101856E-01 -6.2771695118E-01 -4.0716763772E-03

Stress_EigVec2 = 2.2945314567E-01 -2.9057008632E-01 9.2893502404E-01

Stress_EigVec3 = -5.8429136849E-01 7.2217757798E-01 3.7022039729E-01

-DivStress = -9.8826134817E-02 1.2209098245E-01 6.0926978552E-02

BPL = 2.0420061752E+00 = 1.3076214926E+00 + 7.3438468261E-01

GBL_I = 2.0419811159E+00

GBL_II = 2.0679495937E+00

GBL_III = 2.0419813563E+00 = 1.3075976023E+00 + 7.3438375404E-01

GBL_IV = 2.0679497421E+00 = 1.3075964079E+00 + 7.6035333418E-01

CP# 45 Coords = 3.76319255247096E-01 -2.34640699474649E+00 -1.32219629655703E+00

Type = (3,-1) BCP C12 C14

Rho = 2.3815569931E-01

GradRho = -3.6429192996E-17 0.0000000000E+00 -2.0816681712E-17

HessRho_EigVals = -4.3366727597E-01 -4.3238867791E-01 3.4505967462E-01

HessRho_EigVec1 = -3.4790460130E-01 2.5269916064E-01 9.0283194594E-01

HessRho_EigVec2 = 4.4845763824E-02 -9.5740211102E-01 2.8525436942E-01

HessRho_EigVec3 = 9.3645675066E-01 1.3972949588E-01 3.2175211284E-01

DelSqRho = -5.2099627926E-01

Bond Ellipticity = 2.9570572321E-03

V = -2.4233796267E-01

G = 5.6044446429E-02

K = 1.8629351624E-01

L = 1.3024906982E-01

Vnuc = 2.1885268529E+01

Ven = -5.2121014312E+00

Vrep = 4.9697634686E+00

DelSqV = -1.6164378230E+00

DelSqVen = 1.1402143474E+01

DelSqVrep = -1.3018581297E+01

DelSqG = 1.0791330867E+00

DelSqK = 5.3730473630E-01

Stress_EigVals = -1.5734484765E-01 -1.5713751543E-01 7.2144400406E-02

Stress_EigVec1 = 4.7109820571E-02 8.5869558108E-01 -5.1031614107E-01

Stress_EigVec2 = -3.4671477601E-01 4.9317760773E-01 7.9785005567E-01

Stress_EigVec3 = 9.3678681081E-01 1.3934757358E-01 3.2095595466E-01

-DivStress = 1.4058655050E-03 2.6442368075E-04 -8.7709972777E-04

BPL = 2.9074851947E+00 = 1.4548337670E+00 + 1.4526514276E+00

GBL_I = 2.9072991460E+00

GBL_II = 2.9072993847E+00

GBL_III = 2.9073760686E+00 = 1.4547520449E+00 + 1.4526240237E+00

GBL_IV = 2.9073763192E+00 = 1.4547520848E+00 + 1.4526242344E+00

CP# 46 Coords = -9.92305000510734E-01 -2.58427421679405E+00 -3.09829413407022E+00

Type = (3,-1) BCP C14 H15

Rho = 2.7150737138E-01

GradRho = -1.3877787808E-17 -1.4745149546E-16 4.0766001685E-17

HessRho_EigVals = -6.8390057179E-01 -6.8317483458E-01 4.7382305801E-01

HessRho_EigVec1 = 9.3593070884E-01 -3.5218405923E-01 -3.1091872044E-04

HessRho_EigVec2 = 3.5195898839E-01 9.3536341984E-01 -3.4930549824E-02

HessRho_EigVec3 = 1.2592804826E-02 3.2583143618E-02 9.9938969377E-01

DelSqRho = -8.9325234836E-01

Bond Ellipticity = 1.0623008531E-03

V = -3.1111300507E-01

G = 4.3899958991E-02

K = 2.6721304608E-01

L = 2.2331308709E-01

Vnuc = 1.8746593522E+01

Ven = -5.0898383295E+00

Vrep = 4.7787253244E+00

DelSqV = -2.3142529995E+00

DelSqVen = 1.6745438687E+01

DelSqVrep = -1.9059691686E+01

DelSqG = 1.6570722309E+00

DelSqK = 6.5718076853E-01

Stress_EigVals = -2.1059717451E-01 -2.1055158055E-01 1.1003574998E-01

Stress_EigVec1 = 9.2549239275E-01 -3.7876565825E-01 6.3804348842E-04

Stress_EigVec2 = 3.7857442164E-01 9.2496889409E-01 -3.3375923289E-02

Stress_EigVec3 = 1.2051483174E-02 3.1130710049E-02 9.9944266501E-01

-DivStress = 8.2683886664E-04 2.1583544267E-03 1.7654823880E-01

BPL = 2.0449197267E+00 = 1.3052481237E+00 + 7.3967160297E-01

GBL_I = 2.0447932879E+00

GBL_II = 2.0706617382E+00

GBL_III = 2.0448248630E+00 = 1.3051532702E+00 + 7.3967159278E-01

GBL_IV = 2.0706941181E+00 = 1.3051531613E+00 + 7.6554095673E-01

CP# 47 Coords = -1.42409669720953E+00 -3.70886901499135E+00 -1.36855549722348E+00

Type = (3,-1) BCP C14 H16

Rho = 2.7240894992E-01

GradRho = -9.3178936789E-14 -2.4255597530E-13 1.1271192313E-13

HessRho_EigVals = -6.8849603074E-01 -6.8757040337E-01 4.7720686622E-01

HessRho_EigVec1 = 9.3381944204E-01 -3.5773587800E-01 2.5082382072E-03

HessRho_EigVec2 = 1.1024250290E-01 2.9442852570E-01 9.4929364994E-01

HessRho_EigVec3 = 3.4033489421E-01 8.8619235206E-01 -3.1438078016E-01

DelSqRho = -8.9885956789E-01

Bond Ellipticity = 1.3462292226E-03

V = -3.1185106792E-01

G = 4.3568087976E-02

K = 2.6828297995E-01

L = 2.2471489197E-01

Vnuc = 1.8716819393E+01

Ven = -5.0986291168E+00

Vrep = 4.7867780488E+00

DelSqV = -2.3496516149E+00

DelSqVen = 1.6823792192E+01

DelSqVrep = -1.9173443807E+01

DelSqG = 1.6656780628E+00

DelSqK = 6.8397355206E-01

Stress_EigVals = -2.1141681462E-01 -2.1132720152E-01 1.1089294822E-01
Stress_EigVec1 = 9.3346948260E-01 -3.5865653621E-01 -4.6269441938E-04
Stress_EigVec2 = 1.1369528954E-01 2.9468883298E-01 9.4880549790E-01
Stress_EigVec3 = 3.4015894254E-01 8.8573358339E-01 -3.1586059118E-01
-DivStress = 5.8703466198E-02 1.5287395783E-01 -5.8491974184E-02
BPL = 2.0433306757E+00 = 1.3055843028E+00 + 7.3774637291E-01
GBL_I = 2.0432074851E+00
GBL_II = 2.0691579081E+00
GBL_III = 2.0432324192E+00 = 1.3054862069E+00 + 7.3774621230E-01
GBL_IV = 2.0691830646E+00 = 1.3054858775E+00 + 7.6369718703E-01

CP# 48 Coords = -1.84996456188415E+00 -1.49166541925620E+00 -1.32267403751322E+00

Type = (3,-1) BCP C23 C14
Rho = 2.3816789450E-01
GradRho = 3.8163916471E-17 3.4694469520E-17 -8.6736173799E-18
HessRho_EigVals = -4.3370690994E-01 -4.3240606160E-01 3.4504484925E-01
HessRho_EigVec1 = 4.2758355014E-01 -4.4674160076E-02 9.0287126827E-01
HessRho_EigVec2 = -6.7401539361E-01 -6.8132142929E-01 2.8548968310E-01
HessRho_EigVec3 = -6.0239153116E-01 7.3061982549E-01 3.2143290711E-01
DelSqRho = -5.2106812228E-01
Bond Ellipticity = 3.0083952518E-03
V = -2.4236231878E-01
G = 5.6047644106E-02
K = 1.8631467468E-01
L = 1.3026703057E-01
Vnuc = 2.1884968848E+01
Ven = -5.2122969517E+00
Vrep = 4.9699346329E+00
DelSqV = -1.6164689258E+00
DelSqVen = 1.1403559624E+01
DelSqVrep = -1.3020028550E+01
DelSqG = 1.0792142873E+00

DelSqK = 5.3725463845E-01

Stress_EigVals = -1.5735800678E-01 -1.5714793092E-01 7.2143618923E-02

Stress_EigVec1 = -5.4012856207E-01 -6.6954445772E-01 5.0987386242E-01

Stress_EigVec2 = 5.8716197315E-01 1.3422644233E-01 7.9826316429E-01

Stress_EigVec3 = -6.0291123204E-01 7.3054327820E-01 3.2063150961E-01

-DivStress = -7.3853704796E-04 1.0263101248E-03 -9.6458204686E-04

BPL = 2.9074290678E+00 = 1.4549242982E+00 + 1.4525047696E+00

GBL_I = 2.9072433132E+00

GBL_II = 2.9072435506E+00

GBL_III = 2.9073200504E+00 = 1.4548426264E+00 + 1.4524774240E+00

GBL_IV = 2.9073202997E+00 = 1.4548426616E+00 + 1.4524776382E+00

CP# 49 Coords = -9.71550041201060E-01 -1.56518293906528E-01 2.54928011015459E+00

Type = (3,-1) BCP B25 C17

Rho = 1.8235930611E-01

GradRho = 2.0400348077E-14 1.6783449630E-15 -1.2266446539E-14

HessRho_EigVals = -3.8054076557E-01 -2.9625828653E-01 4.6205625650E-01

HessRho_EigVec1 = -1.6619053604E-01 -2.7386264618E-02 9.8571329414E-01

HessRho_EigVec2 = -1.5572296711E-01 9.8780005198E-01 1.1894637534E-03

HessRho_EigVec3 = 9.7372021815E-01 1.5330052127E-01 1.6842769053E-01

DelSqRho = -2.1474279559E-01

Bond Ellipticity = 2.8448986195E-01

V = -3.2232165233E-01

G = 1.3431797671E-01

K = 1.8800367561E-01

L = 5.3685698899E-02

Vnuc = 2.1854974952E+01

Ven = -3.9854580672E+00

Vrep = 3.6631364149E+00

DelSqV = -3.4714090274E+00

DelSqVen = 4.6931984187E+00

DelSqVrep = -8.1646074461E+00

DelSqG = 5.5271051064E+00

DelSqK = -2.0556960791E+00

Stress_EigVals = -1.4435398557E-01 -1.1998594525E-01 -5.7981721511E-02

Stress_EigVec1 = -1.5565026690E-01 9.8781156942E-01 1.1391791738E-03

Stress_EigVec2 = -2.7007865055E-01 -4.3665747742E-02 9.6184761007E-01

Stress_EigVec3 = 9.5017394036E-01 1.4940416925E-01 2.7358340096E-01

-DivStress = 5.0748238647E-01 7.9912624863E-02 5.8058643813E-02

BPL = 2.9650736805E+00 = 9.8707265284E-01 + 1.9780010276E+00

GBL_I = 2.9603715584E+00

GBL_II = 2.9603681142E+00

GBL_III = 2.9646165677E+00 = 9.8688488860E-01 + 1.9777316791E+00

GBL_IV = 2.9646133164E+00 = 9.8688451336E-01 + 1.9777288031E+00

CP# 50 Coords = -2.79592282127874E+00 -4.42072476996424E-01 6.25873461367989E-01

Type = (3,-1) BCP C17 C23

Rho = 2.1453120459E-01

GradRho = -1.5612511284E-17 -2.2551405188E-17 -2.4286128664E-17

HessRho_EigVals = -3.7465029566E-01 -3.5458286235E-01 3.2851173360E-01

HessRho_EigVec1 = -1.5595649028E-01 9.8776343625E-01 9.8343286887E-04

HessRho_EigVec2 = 9.8677835250E-01 1.5575633767E-01 4.4815692633E-02

HessRho_EigVec3 = -4.4114126652E-02 -7.9597283988E-03 9.9899478805E-01

DelSqRho = -4.0072142441E-01

Bond Ellipticity = 5.6594481670E-02

V = -2.1092287975E-01

G = 5.5371261825E-02

K = 1.5555161793E-01

L = 1.0018035610E-01

Vnuc = 2.1473814902E+01

Ven = -4.6068033780E+00

Vrep = 4.3958804982E+00

DelSqV = -1.4769619723E+00

DelSqVen = 8.6050176949E+00

DelSqVrep = -1.0081979667E+01

DelSqG = 9.4897494309E-01

DelSqK = 5.2798702919E-01

Stress_EigVals = -1.3907918674E-01 -1.3838908767E-01 6.6545394663E-02

Stress_EigVec1 = 9.8581114667E-01 1.5712242530E-01 5.9067136042E-02

Stress_EigVec2 = -1.5744903022E-01 9.8752671630E-01 8.8740225407E-04

Stress_EigVec3 = -5.8190944103E-02 -1.0174874321E-02 9.9825361805E-01

-DivStress = 1.1017372793E-03 1.6190497705E-04 5.6606347347E-03

BPL = 2.9710813701E+00 = 1.4785868525E+00 + 1.4924945176E+00

GBL_I = 2.9709437470E+00

GBL_II = 2.9709468137E+00

GBL_III = 2.9709986609E+00 = 1.4785186889E+00 + 1.4924799720E+00

GBL_IV = 2.9710017172E+00 = 1.4785206081E+00 + 1.4924811091E+00

CP# 51 Coords = -3.67574654661849E+00 4.90039058172203E-01 2.48729756602746E+00

Type = (3,-1) BCP H18 C17

Rho = 2.6929455550E-01

GradRho = -4.2327252814E-16 4.9786563761E-16 1.6653345369E-16

HessRho_EigVals = -6.7827353994E-01 -6.6191991027E-01 4.6459352086E-01

HessRho_EigVec1 = -3.0968811300E-01 -5.8482112403E-01 7.4971829747E-01

HessRho_EigVec2 = 7.2459921143E-01 3.6538836667E-01 5.8433494188E-01

HessRho_EigVec3 = -6.1566976169E-01 7.2420687265E-01 3.1060449151E-01

DelSqRho = -8.7559992935E-01

Bond Ellipticity = 2.4706357093E-02

V = -3.1119021858E-01

G = 4.6145118123E-02

K = 2.6504510046E-01

L = 2.1889998234E-01

Vnuc = 1.8213093044E+01

Ven = -4.9046867956E+00

Vrep = 4.5934965770E+00

DelSqV = -2.2733972957E+00

DelSqVen = 1.5947382983E+01

DelSqVrep = -1.8220780278E+01

DelSqG = 1.6458321230E+00

DelSqK = 6.2756517263E-01

Stress_EigVals = -2.1164464496E-01 -2.0795291106E-01 1.0840733743E-01

Stress_EigVec1 = 7.6881070357E-01 4.7018277786E-01 4.3342618459E-01

Stress_EigVec2 = -1.6898843734E-01 -5.0430805140E-01 8.4682719450E-01

Stress_EigVec3 = -6.1674387725E-01 7.2429382484E-01 3.0826197491E-01

-DivStress = 1.1104632307E-01 -1.3328739197E-01 -5.3748063868E-02

BPL = 2.0402891232E+00 = 7.4204340173E-01 + 1.2982457214E+00

GBL_I = 2.0400627781E+00

GBL_II = 2.0659167909E+00

GBL_III = 2.0401110203E+00 = 7.4204335284E-01 + 1.2980676675E+00

GBL_IV = 2.0659662478E+00 = 7.6789795842E-01 + 1.2980682894E+00

CP# 52 Coords = -3.34563036573071E+00 -1.60341441922311E+00 2.48498900439059E+00

Type = (3,-1) BCP C17 H19

Rho = 2.6933145653E-01

GradRho = -6.2450045135E-17 2.0903417886E-16 1.9949319974E-17

HessRho_EigVals = -6.7843623371E-01 -6.6206511289E-01 4.6468239958E-01

HessRho_EigVec1 = 4.7474510695E-01 -4.5957385585E-01 -7.5060572502E-01

HessRho_EigVec2 = 8.0184316260E-01 -1.2575949323E-01 5.8415074464E-01

HessRho_EigVec3 = 3.6285620570E-01 8.7919077616E-01 -3.0880244996E-01

DelSqRho = -8.7581894702E-01

Bond Ellipticity = 2.4727357620E-02

V = -3.1126199058E-01

G = 4.6153626915E-02

K = 2.6510836367E-01

L = 2.1895473675E-01

Vnuc = 1.8213165937E+01

Ven = -4.9053785098E+00

Vrep = 4.5941165192E+00

DelSqV = -2.2745913561E+00

DelSqVen = 1.5951435813E+01

DelSqVrep = -1.8226027169E+01

DelSqG = 1.6462683003E+00

DelSqK = 6.2832305579E-01

Stress_EigVals = -2.1169230574E-01 -2.0799828929E-01 1.0842860444E-01

Stress_EigVec1 = 8.7623064464E-01 -2.1160295755E-01 4.3294808667E-01

Stress_EigVec2 = -3.1597301144E-01 4.2605806456E-01 8.4772376495E-01

Stress_EigVec3 = 3.6384187971E-01 8.7960145178E-01 -3.0646430884E-01

-DivStress = 6.4629495404E-02 1.6109941526E-01 -5.3423829646E-02

BPL = 2.0401796569E+00 = 1.2982042993E+00 + 7.4197535767E-01

GBL_I = 2.0399545576E+00

GBL_II = 2.0658104958E+00

GBL_III = 2.0400024282E+00 = 1.2980271189E+00 + 7.4197530928E-01

GBL_IV = 2.0658595625E+00 = 1.2980277368E+00 + 7.6783182574E-01

CP# 53 Coords = -3.66999384239135E-01 2.35129139443767E+00 -1.31771754292456E+00

Type = (3,-1) BCP C4 C20

Rho = 2.3817837920E-01

GradRho = 4.1633363423E-17 -4.1633363423E-17 -6.9388939039E-18

HessRho_EigVals = -4.3373940394E-01 -4.3243092660E-01 3.4505389543E-01

HessRho_EigVec1 = 2.4995510307E-01 3.5962146261E-01 -8.9899657957E-01

HessRho_EigVec2 = -2.5535173384E-01 9.2008234998E-01 2.9705885155E-01

HessRho_EigVec3 = 9.3397962423E-01 1.5530895945E-01 3.2180924263E-01

DelSqRho = -5.2111643510E-01

Bond Ellipticity = 3.0258643941E-03

V = -2.4237956092E-01

G = 5.6050226074E-02

K = 1.8632933485E-01

L = 1.3027910878E-01

Vnuc = 2.1884370241E+01

Ven = -5.2123838337E+00

Vrep = 4.9700042728E+00
DelSqV = -1.6165596688E+00
DelSqVen = 1.1404305004E+01
DelSqVrep = -1.3020864673E+01
DelSqG = 1.0792527992E+00
DelSqK = 5.3730686966E-01
Stress_EigVals = -1.5736814084E-01 -1.5715809471E-01 7.2146674622E-02
Stress_EigVec1 = -3.0703313027E-01 8.0937894811E-01 5.0063597082E-01
Stress_EigVec2 = -1.8185805569E-01 -5.6624764878E-01 8.0392241406E-01
Stress_EigVec3 = 9.3416181922E-01 1.5578613102E-01 3.2104886993E-01
-DivStress = 1.2376348783E-03 1.6033597135E-04 -9.3202140184E-04
BPL = 2.9073763793E+00 = 1.4548995364E+00 + 1.4524768429E+00
GBL_I = 2.9071901117E+00
GBL_II = 2.9071903507E+00
GBL_III = 2.9072668140E+00 = 1.4548173025E+00 + 1.4524495115E+00
GBL_IV = 2.9072670650E+00 = 1.4548173382E+00 + 1.4524497269E+00

CP# 54 Coords = -2.22070700076219E+00 8.51685234941600E-01 -1.32036920946902E+00

Type = (3,-1) BCP C20 C23
Rho = 2.3826579509E-01
GradRho = -5.2041704279E-17 9.7144514655E-17 -3.0791341699E-17
HessRho_EigVals = -4.3397765550E-01 -4.3267167481E-01 3.4506596158E-01
HessRho_EigVec1 = 3.9237262284E-01 1.7323062316E-01 9.0334648726E-01
HessRho_EigVec2 = -8.5168288121E-01 4.3934309848E-01 2.8568148639E-01
HessRho_EigVec3 = 3.4739026280E-01 8.8145833311E-01 -3.1992376012E-01
DelSqRho = -5.2158336872E-01
Bond Ellipticity = 3.0184104224E-03
V = -2.4254362983E-01
G = 5.6073893822E-02
K = 1.8646973600E-01
L = 1.3039584218E-01
Vnuc = 2.1885334699E+01

Ven = -5.2145266730E+00

Vrep = 4.9719830432E+00

DelSqV = -1.6171111158E+00

DelSqVen = 1.1415026598E+01

DelSqVrep = -1.3032137714E+01

DelSqG = 1.0799433809E+00

DelSqK = 5.3716773487E-01

Stress_EigVals = -1.5745223063E-01 -1.5724346638E-01 7.2152067187E-02

Stress_EigVec1 = 7.2675137663E-01 -4.6861169184E-01 -5.0223054351E-01

Stress_EigVec2 = 5.9229205755E-01 5.7215263332E-02 8.0368932567E-01

Stress_EigVec3 = 3.4788296182E-01 8.8154948580E-01 -3.1913625455E-01

-DivStress = -4.1260803468E-04 -1.2740900171E-03 -9.4014817988E-04

BPL = 2.9070506356E+00 = 1.4523649546E+00 + 1.4546856810E+00

GBL_I = 2.9068645842E+00

GBL_II = 2.9068648113E+00

GBL_III = 2.9069413221E+00 = 1.4523379203E+00 + 1.4546034018E+00

GBL_IV = 2.9069415610E+00 = 1.4523381282E+00 + 1.4546034328E+00

CP# 55 Coords = -2.49915705508513E+00 3.09234318049073E+00 -1.36126222882653E+00

Type = (3,-1) BCP H21 C20

Rho = 2.7238735570E-01

GradRho = -7.9797279895E-17 4.1633363423E-17 -3.8163916471E-17

HessRho_EigVals = -6.8837649005E-01 -6.8746973242E-01 4.7714119607E-01

HessRho_EigVec1 = -7.7526600623E-01 -6.3154153321E-01 1.0858702374E-02

HessRho_EigVec2 = 2.0792639960E-01 -2.3893702628E-01 9.4851236672E-01

HessRho_EigVec3 = -5.9643040829E-01 7.3760720530E-01 3.1655391130E-01

DelSqRho = -8.9870502639E-01

Bond Ellipticity = 1.3189782600E-03

V = -3.1182667811E-01

G = 4.3575210754E-02

K = 2.6825146735E-01

L = 2.2467625660E-01

Vnuc = 1.8716300329E+01
Ven = -5.0980835553E+00
Vrep = 4.7862568772E+00
DelSqV = -2.3487729377E+00
DelSqVen = 1.6820433181E+01
DelSqVrep = -1.9169206119E+01
DelSqG = 1.6654231230E+00
DelSqK = 6.8334981463E-01
Stress_EigVals = -2.1139594217E-01 -2.1130377206E-01 1.1087303613E-01
Stress_EigVec1 = -7.8151193582E-01 -6.2359316981E-01 -1.9252343684E-02
Stress_EigVec2 = 1.8413243463E-01 -2.6002635385E-01 9.4788266248E-01
Stress_EigVec3 = -5.9609927083E-01 7.3723663357E-01 3.1803742774E-01
-DivStress = 1.0294697097E-01 -1.2724853605E-01 -5.8857493562E-02
BPL = 2.0433820685E+00 = 7.3779524721E-01 + 1.3055868213E+00
GBL_I = 2.0432606109E+00
GBL_II = 2.0692091973E+00
GBL_III = 2.0432850395E+00 = 7.3779507913E-01 + 1.3054899603E+00
GBL_IV = 2.0692338279E+00 = 7.6374419318E-01 + 1.3054896347E+00

CP# 56 Coords = -1.74306641324567E+00 2.15939177024629E+00 -3.09367588723076E+00

Type = (3,-1) BCP C20 H22
Rho = 2.7149770621E-01
GradRho = 3.4694469520E-17 6.2450045135E-17 -5.7245874707E-17
HessRho_EigVals = -6.8388772207E-01 -6.8314627758E-01 4.7382660674E-01
HessRho_EigVec1 = 7.7309671854E-01 6.3428710863E-01 1.1522165427E-03
HessRho_EigVec2 = -6.3388357816E-01 7.7253745757E-01 3.7114498368E-02
HessRho_EigVec3 = 2.2651117419E-02 -2.9423468043E-02 9.9931035540E-01
DelSqRho = -8.9320739291E-01
Bond Ellipticity = 1.0853378134E-03
V = -3.1108391380E-01
G = 4.3891032785E-02
K = 2.6719288101E-01

L = 2.2330184823E-01
Vnuc = 1.8745039072E+01
Ven = -5.0892351110E+00
Vrep = 4.7781511972E+00
DelSqV = -2.3143167095E+00
DelSqVen = 1.6743207480E+01
DelSqVrep = -1.9057524189E+01
DelSqG = 1.6569951935E+00
DelSqK = 6.5732151601E-01
Stress_EigVals = -2.1058287526E-01 -2.1054017031E-01 1.1003913178E-01
Stress_EigVec1 = 7.6140990318E-01 6.4826833558E-01 1.7676054501E-03
Stress_EigVec2 = -6.4790735548E-01 7.6088898071E-01 3.5553027312E-02
Stress_EigVec3 = 2.1702950331E-02 -2.8215671656E-02 9.9936622808E-01
-DivStress = 1.5572472527E-03 -2.1944106302E-03 1.7650000806E-01
BPL = 2.0449395728E+00 = 1.3052711449E+00 + 7.3966842786E-01
GBL_I = 2.0448130715E+00
GBL_II = 2.0706816115E+00
GBL_III = 2.0448448021E+00 = 1.3051763840E+00 + 7.3966841815E-01
GBL_IV = 2.0707141566E+00 = 1.3051762730E+00 + 7.6553788356E-01

CP# 57 Coords = -3.93535847008417E+00 -6.20165567406906E-01 -1.34653011667797E+00

Type = (3,-1) BCP C23 H24
Rho = 2.7484473646E-01
GradRho = -2.0036056148E-15 -3.3653635434E-16 -1.0720591082E-15
HessRho_EigVals = -7.0146601755E-01 -7.0001331458E-01 4.8850965586E-01
HessRho_EigVec1 = -3.6671956785E-01 -5.8236396829E-02 9.2850701701E-01
HessRho_EigVec2 = -1.5581957046E-01 9.8778544803E-01 4.1246838742E-04
HessRho_EigVec3 = 9.1718974047E-01 1.4452830433E-01 3.7131462297E-01
DelSqRho = -9.1296967627E-01
Bond Ellipticity = 2.0752504777E-03
V = -3.1334728422E-01
G = 4.2552432578E-02

K = 2.7079485165E-01
L = 2.2824241907E-01
Vnuc = 1.8865274955E+01
Ven = -5.1850215231E+00
Vrep = 4.8716742389E+00
DelSqV = -2.4206156137E+00
DelSqVen = 1.7223423968E+01
DelSqVrep = -1.9644039582E+01
DelSqG = 1.6760342247E+00
DelSqK = 7.4458138892E-01
Stress_EigVals = -2.1352309559E-01 -2.1311503126E-01 1.1329084263E-01
Stress_EigVec1 = -1.5463412728E-01 9.8796849397E-01 -2.5576557467E-03
Stress_EigVec2 = -3.6651931191E-01 -5.4962157542E-02 9.2878563471E-01
Stress_EigVec3 = 9.1747037046E-01 1.4455938628E-01 3.7060855786E-01
-DivStress = 1.5506646613E-01 2.4459539854E-02 6.0992056859E-02
BPL = 2.0420091758E+00 = 1.3076512961E+00 + 7.3435787969E-01
GBL_I = 2.0419846925E+00
GBL_II = 2.0679536659E+00
GBL_III = 2.0419848763E+00 = 1.3076279465E+00 + 7.3435692980E-01
GBL_IV = 2.0679537679E+00 = 1.3076267488E+00 + 7.6032701902E-01

Number of NACPs = 25

Number of NNACPs = 0

Number of BCPs = 27

Number of RCPs = 4

Number of CCPs = 1

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H3	C1	H2	109.93486180	109.12521515	109.11985595	109.44966829	109.44959104
C4	C1	H2	107.74867196	108.90368130	108.91068369	108.78382903	108.78367962
C4	C1	H3	107.74059856	108.89763731	108.90459520	108.77598224	108.77583263
H5	C4	C1	109.11686367	108.88753673	108.88324745	109.20893999	109.20893886
C6	C4	C1	108.55598530	109.90030554	109.90024915	109.45386389	109.45379919
C6	C4	H5	110.66857256	109.28252898	109.28476999	109.69571744	109.69578464
H7	C6	C4	109.61850321	109.78911649	109.79065781	109.80393183	109.80393804
H8	C6	C4	109.41821643	109.40286083	109.40557832	109.58202263	109.58201615
H8	C6	H7	109.28247663	107.24968149	107.24075826	107.70112478	107.70115089
B25	C1	H2	114.96692251	115.45262429	115.44960790	114.60026178	114.60040736
B25	C1	H3	114.98606771	115.46809152	115.46506574	114.60444159	114.60458701
B25	C1	C4	100.57664249	98.18288923	98.18286241	99.99166443	99.99172259
C12	C6	C4	109.47478824	111.12906639	111.12910292	110.32895858	110.32893469
C12	C6	H7	109.61967230	109.78878600	109.79036370	109.80107933	109.80108528
C12	C6	H8	109.41319028	109.39730499	109.40006422	109.57964035	109.57963360
C9	B25	C1	119.06040236	116.49524169	116.49529947	118.70023724	118.70031154
C9	C12	C6	108.60869369	109.97508764	109.97503143	109.51932567	109.51926141
C12	C9	B25	100.53421805	98.16255477	98.16252788	99.96882908	99.96888717
H10	C9	B25	114.98547801	115.46988530	115.46686255	114.60901707	114.60916245
H10	C9	C12	107.74512907	108.88571582	108.89261764	108.76998114	108.76983162
H11	C9	B25	114.98783061	115.47258730	115.46961673	114.61860082	114.61874634
H11	C9	C12	107.76960205	108.91815341	108.92510943	108.79404042	108.79389095
H11	C9	H10	109.92979774	109.11927541	109.11395557	109.44359086	109.44351369
H13	C12	C6	110.67831952	109.29561208	109.29798709	109.70757940	109.70764665
H13	C12	C9	109.11087489	108.87435359	108.87000621	109.19708452	109.19708341

C14	C12	C6	109.19331838	109.53128755	109.53129719	109.28481535	109.28481179
C14	C12	C9	108.55720646	109.90137988	109.90132336	109.45497589	109.45491086
C14	C12	H13	110.63976222	109.24402791	109.24611564	109.66360521	109.66367145
H15	C14	C12	109.41871941	109.39865617	109.40140338	109.57966015	109.57965363
H16	C14	C12	109.62837632	109.79728259	109.79888504	109.81263136	109.81263756
H16	C14	H15	109.27287187	107.23647874	107.22750269	107.68896427	107.68899060
C23	C14	C12	109.48095008	111.14955549	111.14959174	110.34509145	110.34506736
C23	C14	H15	109.39491260	109.37087046	109.37358627	109.55589247	109.55588574
C23	C14	H16	109.63091278	109.80252201	109.80410076	109.81369802	109.81370400
C17	B25	C1	119.08702195	116.55914914	116.55920692	118.73323269	118.73330625
C17	B25	C9	119.11156262	116.58026335	116.58032127	118.75515766	118.75523204
C17	C23	C14	108.58892582	109.94986853	109.94981195	109.49511317	109.49504829
C23	C17	B25	100.27097007	98.14888425	98.14885748	99.96415230	99.96421058
H18	C17	B25	115.09107056	115.47249599	115.46948526	114.60954903	114.60969444
H18	C17	C23	107.77253341	108.91744586	108.92441185	108.79729449	108.79714489
H19	C17	B25	115.08653518	115.46588468	115.46289217	114.60358636	114.60373197
H19	C17	C23	107.76981093	108.90753057	108.91444204	108.78982989	108.78968053
H19	C17	H18	109.92785279	109.11740157	109.11207371	109.44220183	109.44212448
C20	C4	C1	108.57968172	109.93870703	109.93865047	109.48790411	109.48783903
C20	C4	H5	110.66182000	109.26711557	109.26927798	109.68518472	109.68525151
C20	C4	C6	109.20438772	109.54580968	109.54581923	109.29567467	109.29567106
C20	C23	C14	109.17969152	109.50356708	109.50357665	109.26310918	109.26310551
C20	C23	C17	108.58820471	109.95331559	109.95325932	109.49731626	109.49725160
C23	C20	C4	109.47411574	111.14009332	111.14012977	110.33587849	110.33585449
H21	C20	C4	109.60414745	109.75799863	109.75943252	109.77808587	109.77809156
H21	C20	C23	109.64077004	109.81773885	109.81938715	109.82670051	109.82670666
H22	C20	C4	109.42649522	109.41243009	109.41521649	109.59175547	109.59174879
H22	C20	C23	109.41278810	109.38825167	109.39096184	109.57349016	109.57348393
H22	C20	H21	109.26852185	107.23955188	107.23064467	107.69044219	107.69046842
H24	C23	C14	110.66518807	109.28470029	109.28697495	109.69865172	109.69871848
H24	C23	C17	109.11118492	108.86187378	108.85741160	109.19038506	109.19038406
H24	C23	C20	110.65523220	109.26857223	109.27087750	109.68292494	109.68299194

Total time for electron density critical point search, analysis and connectivity = 200 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.8173341344E+01	3.8173341344E+01	-1.8910612458E+02	-9.1810247021E+01		
H2	-6.2226874793E-01	6.2226874793E-01	-1.5159200352E+01	-1.2917423978E+00		
H3	-6.2234428794E-01	6.2234428794E-01	-1.5158817106E+01	-1.2918748083E+00		
C4	-3.7839101678E+01	3.7839101678E+01	-1.8484363354E+02	-8.9808991488E+01		
H5	-6.3129775564E-01	6.3129775564E-01	-1.5407568136E+01	-1.2969878756E+00		
C6	-3.7879721494E+01	3.7879721494E+01	-1.8047941599E+02	-8.9916445272E+01		
H7	-6.2616087334E-01	6.2616087334E-01	-1.5567245751E+01	-1.2951095116E+00		
H8	-6.2621075276E-01	6.2621075276E-01	-1.5636033324E+01	-1.2962187770E+00		
C9	-3.8173484954E+01	3.8173484954E+01	-1.8910052313E+02	-9.1810098400E+01		

H10	-6.2232573489E-01	6.2232573489E-01	-1.5159373467E+01	-1.2918369035E+00
H11	-6.2230250312E-01	6.2230250312E-01	-1.5157413996E+01	-1.2917912935E+00
C12	-3.7839191210E+01	3.7839191210E+01	-1.8484823257E+02	-8.9809200846E+01
H13	-6.3134935757E-01	6.3134935757E-01	-1.5409828487E+01	-1.2970747355E+00
C14	-3.7879359930E+01	3.7879359930E+01	-1.8049459502E+02	-8.9917313978E+01
H15	-6.2624533364E-01	6.2624533364E-01	-1.5638455999E+01	-1.2962694904E+00
H16	-6.2611430807E-01	6.2611430807E-01	-1.5566352049E+01	-1.2950417941E+00
C17	-3.8173632135E+01	3.8173632135E+01	-1.8908802155E+02	-9.1809850726E+01
H18	-6.2228364219E-01	6.2228364219E-01	-1.5157404332E+01	-1.2917866205E+00
H19	-6.2228965975E-01	6.2228965975E-01	-1.5156432576E+01	-1.2917751993E+00
C20	-3.7879414200E+01	3.7879414200E+01	-1.8048089409E+02	-8.9916253268E+01
H21	-6.2613665386E-01	6.2613665386E-01	-1.5567209684E+01	-1.2950930804E+00
H22	-6.2620286511E-01	6.2620286511E-01	-1.5636011392E+01	-1.2962038418E+00
C23	-3.7839143770E+01	3.7839143770E+01	-1.8485520379E+02	-8.9810420301E+01
H24	-6.3132427697E-01	6.3132427697E-01	-1.5408338482E+01	-1.2970174272E+00
B25	-2.3945498758E+01	2.3945498758E+01	-1.0236304511E+02	-5.2634401860E+01

Total	-3.7500674623E+02	3.7500674623E+02	-1.9964453745E+03	-8.8665904692E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
C1	-3.8173341344E+01					
H2	-6.2226874793E-01					
H3	-6.2234428794E-01					
C4	-3.7839101678E+01					
H5	-6.3129775564E-01					
C6	-3.7879721494E+01					
H7	-6.2616087334E-01					
H8	-6.2621075276E-01					
C9	-3.8173484954E+01					
H10	-6.2232573489E-01					
H11	-6.2230250312E-01					
C12	-3.7839191210E+01					
H13	-6.3134935757E-01					
C14	-3.7879359930E+01					
H15	-6.2624533364E-01					
H16	-6.2611430807E-01					
C17	-3.8173632135E+01					
H18	-6.2228364219E-01					
H19	-6.2228965975E-01					
C20	-3.7879414200E+01					
H21	-6.2613665386E-01					
H22	-6.2620286511E-01					
C23	-3.7839143770E+01					
H24	-6.3132427697E-01					
B25	-2.3945498758E+01					
Total	-3.7500674623E+02					

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	$E\_IQA(A)$ $VeeX(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$

C1 4.3815445024E+01			3.8173341344E+01	-8.8230607785E+01	-9.4553062291E+01	
H2 7.0712126688E+00			6.2226874793E-01	-7.6384757027E+00	-7.5796001760E+00	
H3 7.0702243105E+00			6.2234428794E-01	-7.6375109735E+00	-7.5794085529E+00	
C4 4.8124463164E+01			3.7839101678E+01	-9.2407641201E+01	-9.2421816768E+01	
H5 7.2496090685E+00			6.3129775564E-01	-7.8159869051E+00	-7.7037840680E+00	
C6 4.5775917284E+01			3.7879721494E+01	-9.0110719680E+01	-9.0239707995E+01	
H7 7.2889208281E+00			6.2616087334E-01	-7.8538243901E+00	-7.7836228753E+00	
H8 7.3031291720E+00			6.2621075276E-01	-7.8670906677E+00	-7.8180166618E+00	

C9 4.3814595918E+01	3.8173484954E+01 -8.8229732020E+01 -9.4550261564E+01
H10 7.0707411768E+00	6.2232573489E-01 -7.6380215551E+00 -7.5796867337E+00
H11 7.0701935144E+00	6.2230250312E-01 -7.6374495728E+00 -7.5787069981E+00
C12 4.8127099620E+01	3.7839191210E+01 -9.2410287818E+01 -9.2424116286E+01
H13 7.2499818491E+00	6.3134935757E-01 -7.8163704505E+00 -7.7049142435E+00
C14 4.5777956373E+01	3.7879359930E+01 -9.0112650991E+01 -9.0247297509E+01
H15 7.3040823620E+00	6.2624533364E-01 -7.8680552309E+00 -7.8192279994E+00
H16 7.2888629441E+00	6.2611430807E-01 -7.8537565969E+00 -7.7831760246E+00
C17 4.3811065171E+01	3.8173632135E+01 -8.8226306161E+01 -9.4544010775E+01
H18 7.0697825941E+00	6.2228364219E-01 -7.6370552001E+00 -7.5787021661E+00
H19 7.0697691200E+00	6.2228965975E-01 -7.6370431218E+00 -7.5782162882E+00
C20 4.5775384050E+01	3.7879414200E+01 -9.0110046425E+01 -9.0240447044E+01
H21 7.2886808646E+00	6.2613665386E-01 -7.8535805047E+00 -7.7836048419E+00
H22 7.3032671363E+00	6.2620286511E-01 -7.8672215953E+00 -7.8180056958E+00
C23 4.8125648043E+01	3.7839143770E+01 -9.2408855170E+01 -9.2427601894E+01
H24 7.2497997873E+00	6.3132427697E-01 -7.8161828806E+00 -7.7041692408E+00
B25 4.0834217580E+01	2.3945498758E+01 -6.9538356166E+01 -5.1181522556E+01

Total 5.6193004962E+02	3.7500674623E+02 -9.9822282876E+02 -9.9822268725E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)
C1	3.8173341344E+01	-9.1810247021E+01				
H2	6.2226874793E-01	-1.2917423978E+00				
H3	6.2234428794E-01	-1.2918748083E+00				
C4	3.7839101678E+01	-8.9808991488E+01				
H5	6.3129775564E-01	-1.2969878756E+00				
C6	3.7879721494E+01	-8.9916445272E+01				
H7	6.2616087334E-01	-1.2951095116E+00				
H8	6.2621075276E-01	-1.2962187770E+00				
C9	3.8173484954E+01	-9.1810098400E+01				
H10	6.2232573489E-01	-1.2918369035E+00				
H11	6.2230250312E-01	-1.2917912935E+00				
C12	3.7839191210E+01	-8.9809200846E+01				
H13	6.3134935757E-01	-1.2970747355E+00				
C14	3.7879359930E+01	-8.9917313978E+01				
H15	6.2624533364E-01	-1.2962694904E+00				
H16	6.2611430807E-01	-1.2950417941E+00				
C17	3.8173632135E+01	-9.1809850726E+01				
H18	6.2228364219E-01	-1.2917866205E+00				

H19	6.2228965975E-01 -1.2917751993E+00
C20	3.7879414200E+01 -8.9916253268E+01
H21	6.2613665386E-01 -1.2950930804E+00
H22	6.2620286511E-01 -1.2962038418E+00
C23	3.7839143770E+01 -8.9810420301E+01
H24	6.3132427697E-01 -1.2970174272E+00
B25	2.3945498758E+01 -5.2634401860E+01

Total	3.7500674623E+02 -8.8665904692E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$	$VeeX(A,A')$

C1	-4.2325484274E+01	-4.8647938780E+01		4.3815445024E+01			

H2	-6.9926045038E+00 -6.9337289771E+00	7.0712126688E+00
H3	-6.9915735693E+00 -6.9334711488E+00	7.0702243105E+00
C4	-4.7503145457E+01 -4.7517321024E+01	4.8124463164E+01
H5	-7.1674929673E+00 -7.0552901302E+00	7.2496090685E+00
C6	-4.5152497044E+01 -4.5281485359E+01	4.5775917284E+01
H7	-7.2062696343E+00 -7.1360681195E+00	7.2889208281E+00
H8	-7.2189812792E+00 -7.1699072733E+00	7.3031291720E+00
C9	-4.2324682820E+01 -4.8645212364E+01	4.3814595918E+01
H10	-6.9921031033E+00 -6.9337682819E+00	7.0707411768E+00
H11	-6.9915539261E+00 -6.9328113513E+00	7.0701935144E+00
C12	-4.7505687395E+01 -4.7519515864E+01	4.8127099620E+01
H13	-7.1678330828E+00 -7.0563768757E+00	7.2499818491E+00
C14	-4.5153994002E+01 -4.5288640520E+01	4.5777956373E+01
H15	-7.2199204857E+00 -7.1710932542E+00	7.3040823620E+00
H16	-7.2062356999E+00 -7.1356551275E+00	7.2888629441E+00
C17	-4.2321380798E+01 -4.8639085412E+01	4.3811065171E+01
H18	-6.9911618899E+00 -6.9328088559E+00	7.0697825941E+00
H19	-6.9911555222E+00 -6.9323286885E+00	7.0697691200E+00
C20	-4.5151919791E+01 -4.5282320410E+01	4.5775384050E+01
H21	-7.2060339645E+00 -7.1360583017E+00	7.2886808646E+00
H22	-7.2191196744E+00 -7.1699037749E+00	7.3032671363E+00
C23	-4.7503645020E+01 -4.7522391744E+01	4.8125648043E+01
H24	-7.1676741670E+00 -7.0556605272E+00	7.2497997873E+00
B25	-4.3221155236E+01 -2.4864321627E+01	4.0834217580E+01

Total	-5.5489330531E+02 -5.5489316379E+02	5.6193004962E+02

Atomic Electron Populations, Localization and Delocalization Data:

 $N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1 3.0026473470E+01	6.6323547392E+00		4.6408925030E+00	6.9973526530E+01	1.9914622362E+00
H2 5.5616903965E+01	1.0169596222E+00		4.5135816576E-01	4.4383096035E+01	5.6560145644E-01
H3 5.5610336675E+01	1.0170772206E+00		4.5147715398E-01	4.4389663325E+01	5.6560006662E-01
C4 3.5599109165E+01	5.9585131042E+00		3.8373355196E+00	6.4400890835E+01	2.1211775846E+00
H5 5.5364654404E+01	1.0119861124E+00		4.5170349865E-01	4.4635345596E+01	5.6028261375E-01
C6 3.4868341154E+01	5.9725272034E+00		3.8900060426E+00	6.5131658846E+01	2.0825211608E+00
H7 5.5433183509E+01	1.0148911912E+00		4.5230469476E-01	4.4566816491E+01	5.6258649644E-01
H8 5.5345727092E+01	1.0175193662E+00		4.5436587468E-01	4.4654272908E+01	5.6315349152E-01
C9 3.0027885030E+01	6.6321123814E+00		4.6406293005E+00	6.9972114970E+01	1.9914830809E+00
H10 5.5612176745E+01	1.0170383162E+00		4.5144117023E-01	4.4387823255E+01	5.6559714597E-01
H11 5.5614355502E+01	1.0169819400E+00		4.5139398850E-01	4.4385644498E+01	5.6558795150E-01
C12 3.5601146932E+01	5.9585112934E+00		3.8372129329E+00	6.4398853068E+01	2.1212983605E+00

H13	1.0120874970E+00 5.5361889775E+01	4.5177673249E-01	4.4638110225E+01	5.6031076451E-01
C14	5.9732464354E+00 3.4865506570E+01	3.8906438070E+00	6.5134493430E+01	2.0826026284E+00
H15	1.0175516450E+00 5.5346936251E+01	4.5436798472E-01	4.4653063749E+01	5.6318366028E-01
H16	1.0148356842E+00 5.5435318018E+01	4.5225829530E-01	4.4564681982E+01	5.6257738890E-01
C17	6.6318613348E+00 3.0027288098E+01	4.6404932255E+00	6.9972711902E+01	1.9913681093E+00
H18	1.0170347084E+00 5.5611408005E+01	4.5144738716E-01	4.4388591995E+01	5.6558732124E-01
H19	1.0169771446E+00 5.5614055132E+01	4.5139491472E-01	4.4385944868E+01	5.6558222988E-01
C20	5.9727377810E+00 3.4866543517E+01	3.8902505634E+00	6.5133456483E+01	2.0824872176E+00
H21	1.0149193086E+00 5.5432027142E+01	4.5232896199E-01	4.4567972858E+01	5.6259034661E-01
H22	1.0174966194E+00 5.5347450608E+01	4.5433818054E-01	4.4652549392E+01	5.6315843886E-01
C23	5.9591786960E+00 3.5605747349E+01	3.8373685854E+00	6.4394252651E+01	2.1218101106E+00
H24	1.0120114140E+00 5.5364273643E+01	4.5171864546E-01	4.4635726357E+01	5.6029276854E-01
B25	3.0736802858E+00 2.9604476482E+01	2.1637333285E+00	7.0395523518E+01	9.0994695733E-01

Total	7.4000091045E+01 3.7767317841E+01	4.6052241457E+01	6.2232682159E+01	2.7947849587E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1 2.6186141411E-01	6.6323547392E+00		4.6408925030E+00	1.9914622362E+00	1.7296008221E+00
H2 7.7849790800E-02	1.0169596222E+00		4.5135816576E-01	5.6560145644E-01	4.8775166564E-01
H3 7.7738167270E-02	1.0170772206E+00		4.5147715398E-01	5.6560006662E-01	4.8786189935E-01
C4 2.0713857909E-01	5.9585131042E+00		3.8373355196E+00	2.1211775846E+00	1.9140390055E+00
H5 9.5155847023E-02	1.0119861124E+00		4.5170349865E-01	5.6028261375E-01	4.6512676672E-01
C6 1.8142870537E-01	5.9725272034E+00		3.8900060426E+00	2.0825211608E+00	1.9010924554E+00
H7 9.3763672894E-02	1.0148911912E+00		4.5230469476E-01	5.6258649644E-01	4.6882282354E-01
H8 9.4026573581E-02	1.0175193662E+00		4.5436587468E-01	5.6315349152E-01	4.6912691794E-01
C9 2.6178090420E-01	6.6321123814E+00		4.6406293005E+00	1.9914830809E+00	1.7297021767E+00
H10 7.7866323650E-02	1.0170383162E+00		4.5144117023E-01	5.6559714597E-01	4.8773082232E-01
H11 7.7786428596E-02	1.0169819400E+00		4.5139398850E-01	5.6558795150E-01	4.8780152291E-01
C12 2.0707919942E-01	5.9585112934E+00		3.8372129329E+00	2.1212983605E+00	1.9142191611E+00

H13	1.0120874970E+00	4.5177673249E-01	5.6031076451E-01	4.6512104644E-01
9.5189718069E-02				
C14	5.9732464354E+00	3.8906438070E+00	2.0826026284E+00	1.9012197296E+00
1.8138289884E-01				
H15	1.0175516450E+00	4.5436798472E-01	5.6318366028E-01	4.6924585852E-01
9.3937801763E-02				
H16	1.0148356842E+00	4.5225829530E-01	5.6257738890E-01	4.6888162291E-01
9.3695765990E-02				
C17	6.6318613348E+00	4.6404932255E+00	1.9913681093E+00	1.7296719631E+00
2.6169614617E-01				
H18	1.0170347084E+00	4.5144738716E-01	5.6558732124E-01	4.8775354074E-01
7.7833780497E-02				
H19	1.0169771446E+00	4.5139491472E-01	5.6558222988E-01	4.8775033720E-01
7.7831892672E-02				
C20	5.9727377810E+00	3.8902505634E+00	2.0824872176E+00	1.9012188418E+00
1.8126837583E-01				
H21	1.0149193086E+00	4.5232896199E-01	5.6259034661E-01	4.6885850017E-01
9.3731846439E-02				
H22	1.0174966194E+00	4.5433818054E-01	5.6315843886E-01	4.6917448886E-01
9.3983950000E-02				
C23	5.9591786960E+00	3.8373685854E+00	2.1218101106E+00	1.9144056675E+00
2.0740444305E-01				
H24	1.0120114140E+00	4.5171864546E-01	5.6029276854E-01	4.6511661749E-01
9.5176151054E-02				
B25	3.0736802858E+00	2.1637333285E+00	9.0994695733E-01	8.0444658507E-01
1.0550037226E-01				

Total	7.4000091045E+01	4.6052241457E+01	2.7947849587E+01	2.4575740839E+01
3.3721087486E+00				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.9673618442E+01	2.2240732954E+02	2.4208094798E+02
H2	2.9142435371E-01	3.6827601857E+01	3.7119026210E+01
H3	2.9148445934E-01	3.6831834093E+01	3.7123318552E+01
C4	1.5833271447E+01	2.0165245686E+02	2.1748572830E+02
H5	2.8620619652E-01	3.6651286906E+01	3.6937493103E+01
C6	1.5890537576E+01	2.0210670535E+02	2.1799724292E+02
H7	2.8884971761E-01	3.6754678761E+01	3.7043528479E+01
H8	2.9048989296E-01	3.6848966973E+01	3.7139456866E+01
C9	1.9672142670E+01	2.2239995925E+02	2.4207210192E+02
H10	2.9146288320E-01	3.6830435658E+01	3.7121898541E+01
H11	2.9142913889E-01	3.6828411671E+01	3.7119840810E+01
C12	1.5833321950E+01	2.0165234026E+02	2.1748566221E+02
H13	2.8627218455E-01	3.6654921456E+01	3.6941193641E+01
C14	1.5894514586E+01	2.0212898031E+02	2.1802349489E+02
H15	2.9052168276E-01	3.6850113360E+01	3.7140635042E+01
H16	2.8881658531E-01	3.6752685888E+01	3.7041502473E+01
C17	1.9670545769E+01	2.2239239295E+02	2.4206293872E+02
H18	2.9145610546E-01	3.6830310751E+01	3.7121766857E+01
H19	2.9142379896E-01	3.6828241979E+01	3.7119665778E+01
C20	1.5891673019E+01	2.0211325599E+02	2.1800492901E+02
H21	2.8886612049E-01	3.6755688643E+01	3.7044554764E+01
H22	2.9048059498E-01	3.6848146013E+01	3.7138626608E+01
C23	1.5837221073E+01	2.0167280133E+02	2.1751002240E+02
H24	2.8622422830E-01	3.6652192383E+01	3.6938416611E+01
B25	3.6418885854E+00	1.0854744185E+02	1.1218933043E+02

Total 1.6218414306E+02 2.5388191801E+03 2.7010033231E+03

Diatomic Electron Pair Contributions and Delocalization Data:

 $2 * D2(A,B) = 2 * D2(B,A) = \text{Average Number of Electron Pairs Formed Between Atoms A and B}$
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) = \text{Electron Delocalization Index. Average Number of Electrons Delocalized}$

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)

C1	H2	6.2570853042E+00	9.7550333129E-01	7.3541251158E+00	4.7961753348E+01 (Bonded)
C1	H3	6.2577550248E+00	9.7572379869E-01	7.3557871756E+00	4.7967046107E+01 (Bonded)
H2	H3	1.0152924786E+00	3.8067974746E-02	1.8716561560E+00	1.8714397479E+00
C1	C4	3.9033108370E+01	9.7172851111E-01	7.3256674991E+00	8.1541191076E+00 (Bonded)
H2	C4	6.0398371113E+00	3.9460248028E-02	1.9401088876E+00	3.3112495801E-01
H3	C4	6.0405593076E+00	3.9417278596E-02	1.9377721670E+00	3.3076438624E-01
C1	H5	6.6875922023E+00	4.8517372565E-02	3.6576279823E-01	2.3971362833E+00
H2	H5	1.0270976767E+00	4.1026757095E-03	2.0171281238E-01	2.0270415074E-01
H3	H5	1.0272077065E+00	4.1206320031E-03	2.0257222951E-01	2.0359133157E-01
C4	H5	5.5648057453E+00	9.3025353345E-01	7.8060878375E+00	4.5961773687E+01 (Bonded)
C1	C6	3.9586943901E+01	4.9950402963E-02	3.7656612867E-01	4.1816806572E-01
H2	C6	6.0697428516E+00	8.1523133990E-03	4.0081794896E-01	6.8248440914E-02
H3	C6	6.0693571912E+00	1.0328353520E-02	5.0774677238E-01	8.6465520949E-02
C4	C6	3.5105835661E+01	9.6309189070E-01	8.0816461579E+00	8.0626831650E+00 (Bonded)
H5	C6	6.0237512097E+00	4.0726752243E-02	2.0122189299E+00	3.4095074711E-01

C1	H7	6.7265674448E+00	9.1019138800E-03	6.8617513975E-02	4.4841821266E-01
H2	H7	1.0284245759E+00	7.3575728628E-03	3.6174360821E-01	3.6248087118E-01
H3	H7	1.0318382493E+00	7.6892539516E-04	3.7800738212E-02	3.7882159281E-02
C4	H7	6.0274620258E+00	3.9560872565E-02	3.3196933424E-01	1.9490203929E+00
H5	H7	1.0252997411E+00	3.5120999962E-03	1.7352510836E-01	1.7302840081E-01
C6	H7	5.5926424244E+00	9.3764564709E-01	7.8496557249E+00	4.6194392819E+01 (Bonded)
C1	H8	6.7426430950E+00	1.1812591310E-02	8.9052770654E-02	5.8046026946E-01
H2	H8	1.0343976533E+00	7.5691386137E-04	3.7214548387E-02	3.7194076423E-02
H3	H8	1.0338072091E+00	2.1771195120E-03	1.0702823089E-01	1.0698172361E-01
C4	H8	6.0429563555E+00	3.9892243605E-02	3.3474998634E-01	1.9602695010E+00
H5	H8	1.0278075497E+00	3.8158360255E-03	1.8853203511E-01	1.8750680096E-01
C6	H8	5.6080351767E+00	9.3825383588E-01	7.8547472781E+00	4.6104962080E+01 (Bonded)
H7	H8	1.0141415739E+00	3.7059735377E-02	1.8257984550E+00	1.8210825567E+00
C1	C9	4.3921190442E+01	1.3066308383E-01	9.8504293699E-01	9.8507893349E-01
H2	C9	6.7394234298E+00	1.0334143860E-02	5.0809017558E-01	7.7909897071E-02
H3	C9	6.7404356124E+00	9.8696302669E-03	4.8519571902E-01	7.4407893740E-02
C4	C9	3.9511065768E+01	1.2925530443E-02	1.0846271727E-01	9.7446557748E-02
H5	C9	6.7108630772E+00	1.4850973673E-03	7.3375382781E-02	1.1196262080E-02
C6	C9	3.9585519934E+01	4.9903360319E-02	4.1777424045E-01	3.7622523149E-01
H7	C9	6.7263301222E+00	9.0846254791E-03	4.4756647599E-01	6.8489682900E-02
H8	C9	6.7423990962E+00	1.1807381355E-02	5.8020425692E-01	8.9016746674E-02
C1	H10	6.7404199425E+00	9.8779078596E-03	7.4467577866E-02	4.8562122499E-01
H2	H10	1.0340111528E+00	5.5149810704E-04	2.7115044443E-02	2.7112946398E-02
H3	H10	1.0335109201E+00	1.7911676101E-03	8.8054651790E-02	8.8058020113E-02
C4	H10	6.0596901251E+00	6.9201899223E-04	5.8069771781E-03	3.4021284214E-02
H5	H10	1.0291307718E+00	1.9575984975E-04	9.6720620646E-03	9.6240154690E-03
C6	H10	6.0691214234E+00	1.0335174082E-02	8.6522620409E-02	5.0810150991E-01
H7	H10	1.0317999328E+00	7.6659093858E-04	3.7767149091E-02	3.7687416805E-02
H8	H10	1.0337700347E+00	2.1722963248E-03	1.0674471646E-01	1.0679520576E-01
C9	H10	6.2573815869E+00	9.7546164464E-01	7.3540795794E+00	4.7955992862E+01 (Bonded)
C1	H11	6.7398237416E+00	1.0322495752E-02	7.7819237345E-02	5.0750634530E-01

H2	H11	1.0319423556E+00	4.5744278308E-03	2.2490705289E-01	2.2490211728E-01
H3	H11	1.0340740994E+00	5.5013097707E-04	2.7044700537E-02	2.7047234343E-02
C4	H11	6.0591639540E+00	1.0725244163E-03	8.9999333516E-03	5.2730750374E-02
H5	H11	1.0290130217E+00	3.1715624417E-04	1.5669989948E-02	1.5593012604E-02
C6	H11	6.0698968215E+00	8.1109610797E-03	6.7902253129E-02	3.9877606281E-01
H7	H11	1.0284719456E+00	7.3081338833E-03	3.6004519237E-01	3.5930499824E-01
H8	H11	1.0344221457E+00	7.5334673924E-04	3.7018791203E-02	3.7038353859E-02
C9	H11	6.2569369930E+00	9.7560304581E-01	7.3551456135E+00	4.7965603293E+01
(Bonded)					
H10	H11	1.0152746801E+00	3.8069839549E-02	1.8716030135E+00	1.8717067654E+00
C1	C12	3.9512465544E+01	1.2990141723E-02	9.7930088438E-02	1.0900492660E-01
H2	C12	6.0590274682E+00	1.0758512184E-03	5.2895473668E-02	9.0278524734E-03
H3	C12	6.0599170115E+00	6.9818735275E-04	3.4323222397E-02	5.8587398628E-03
C4	C12	3.5482371898E+01	4.2991450811E-02	3.6075653489E-01	3.6075664452E-01
H5	C12	6.0245332433E+00	1.0794872377E-02	5.3335081602E-01	9.0583636126E-02
C6	C12	3.5105774023E+01	9.6319353716E-01	8.0635341151E+00	8.0825015657E+00
(Bonded)					
H7	C12	6.0274578820E+00	3.9565484668E-02	1.9492476145E+00	3.3200813693E-01
H8	C12	6.0429408974E+00	3.9919474650E-02	1.9616076104E+00	3.3497859351E-01
C9	C12	3.9031567178E+01	9.7189869073E-01	7.3272181986E+00	8.1555496237E+00
(Bonded)					
H10	C12	6.0402962165E+00	3.9476152777E-02	1.9407406854E+00	3.3125852108E-01
H11	C12	6.0399714073E+00	3.9453934755E-02	1.9397559191E+00	3.3107208170E-01
C1	H13	6.7117791942E+00	1.4882260857E-03	1.1219439733E-02	7.3522600079E-02
H2	H13	1.0290932858E+00	3.1766552333E-04	1.5618394103E-02	1.5693580064E-02
H3	H13	1.0292739392E+00	1.9439854202E-04	9.5567248031E-03	9.6038407051E-03
C4	H13	6.0251373023E+00	1.0798622295E-02	9.0615075491E-02	5.3348264488E-01
H5	H13	1.0231307140E+00	2.1755550894E-03	1.0748937474E-01	1.0747860713E-01
C6	H13	6.0243551026E+00	4.0730010980E-02	3.4097802817E-01	2.0121783492E+00
H7	H13	1.0254046142E+00	3.5081424487E-03	1.7283342683E-01	1.7331221160E-01
H8	H13	1.0279075878E+00	3.8220813577E-03	1.8781369105E-01	1.8882168632E-01
C9	H13	6.6880083757E+00	4.8539288446E-02	3.6594138982E-01	2.3979788600E+00
H10	H13	1.0272700977E+00	4.1233321357E-03	2.0271272331E-01	2.0370433129E-01

H11	H13	1.0272181473E+00	4.1131177183E-03	2.0222176799E-01	2.0319971003E-01
C12	H13	5.5654137343E+00	9.3024209289E-01	7.8059942080E+00	4.5956604327E+01
(Bonded)					
C1	C14	3.9615853891E+01	1.6708266360E-03	1.2596028874E-02	1.3985917491E-02
H2	C14	6.0743586273E+00	3.8362189309E-04	1.8861215564E-02	3.2111674718E-03
H3	C14	6.0750615593E+00	3.8264638986E-04	1.8811078555E-02	3.2030018684E-03
C4	C14	3.5587454524E+01	8.4252711669E-03	7.0699443129E-02	7.0525059179E-02
H5	C14	6.0445178894E+00	6.4909839804E-04	3.2070519056E-02	5.4333803657E-03
C6	C14	3.5652560642E+01	4.5632371405E-02	3.8201894986E-01	3.8197295138E-01
H7	C14	6.0567574646E+00	1.0875451060E-02	5.3579394296E-01	9.1034675848E-02
H8	C14	6.0739157531E+00	7.9563480451E-03	3.9096789257E-01	6.6599864338E-02
C9	C14	3.9590232231E+01	5.0018820072E-02	3.7709569135E-01	4.1869041076E-01
H10	C14	6.0709290679E+00	8.1828580357E-03	4.0228858173E-01	6.8495901887E-02
H11	C14	6.0695076881E+00	1.0352119801E-02	5.0896281407E-01	8.6654049124E-02
C12	C14	3.5110104343E+01	9.6310400148E-01	8.0817502397E+00	8.0618137213E+00
(Bonded)					
H13	C14	6.0250515758E+00	4.0792915982E-02	2.0152860352E+00	3.4146352761E-01
C1	H15	6.7483534642E+00	8.2002182221E-04	6.1819810192E-03	4.0293867453E-02
H2	H15	1.0347742150E+00	6.9442942831E-05	3.4142428724E-03	3.4122564281E-03
H3	H15	1.0348938578E+00	6.9482316382E-05	3.4157837269E-03	3.4141911481E-03
C4	H15	6.0626989703E+00	7.9168128930E-04	6.6432789142E-03	3.8901282957E-02
H5	H15	1.0297071418E+00	8.1983157534E-05	4.0506068478E-03	4.0284519187E-03
C6	H15	6.0733712166E+00	7.9673280456E-03	6.6699805411E-02	3.9149502066E-01
H7	H15	1.0323504092E+00	7.0758381995E-04	3.4860082839E-02	3.4768938924E-02
H8	H15	1.0320446679E+00	6.6676740344E-03	3.2764359362E-01	3.2763320010E-01
C9	H15	6.7426183830E+00	1.1796961117E-02	8.8938187704E-02	5.7967382663E-01
H10	H15	1.0345106197E+00	7.5678394294E-04	3.7205281792E-02	3.7186512678E-02
H11	H15	1.0337423304E+00	2.1786312147E-03	1.0711258130E-01	1.0705261130E-01
C12	H15	6.0431448074E+00	3.9896321857E-02	3.3478431015E-01	1.9604077126E+00
H13	H15	1.0279429965E+00	3.8166018956E-03	1.8855098531E-01	1.8753848585E-01
C14	H15	5.6088408778E+00	9.3849171703E-01	7.8557927183E+00	4.6115188435E+01
(Bonded)					
C1	H16	6.7305580978E+00	3.8432365046E-04	2.8973393732E-03	1.8935264913E-02

H2	H16	1.0320146903E+00	6.4447396907E-05	3.1686310597E-03	3.1752626514E-03
H3	H16	1.0321340442E+00	6.4425608101E-05	3.1671935423E-03	3.1741891374E-03
C4	H16	6.0466013001E+00	6.2084572689E-04	5.2097370270E-03	3.0588485237E-02
H5	H16	1.0268688648E+00	2.6150797784E-04	1.2920531944E-02	1.2884252195E-02
C6	H16	6.0557045309E+00	1.0858399873E-02	9.0902891720E-02	5.3498315256E-01
H7	H16	1.0287408968E+00	2.4137991883E-03	1.1891911218E-01	1.1892561653E-01
H8	H16	1.0322614804E+00	7.0696355313E-04	3.4739562539E-02	3.4831429567E-02
C9	H16	6.7259647370E+00	9.0791385756E-03	6.8448316716E-02	4.4732062131E-01
H10	H16	1.0284517217E+00	7.3501074671E-03	3.6134860162E-01	3.6213288425E-01
H11	H16	1.0316851894E+00	7.6874693605E-04	3.7795505791E-02	3.7875438754E-02
C12	H16	6.0271312133E+00	3.9557343961E-02	3.3193982535E-01	1.9489531447E+00
H13	H16	1.0253442397E+00	3.5165355879E-03	1.7372685654E-01	1.7325640213E-01
C14	H16	5.5929820103E+00	9.3776324582E-01	7.8496949352E+00	4.6202713425E+01 (Bonded)
H15	H16	1.0141139400E+00	3.7067559776E-02	1.8214092601E+00	1.8262838188E+00
C1	C17	4.3919585229E+01	1.3054345011E-01	9.8414104221E-01	9.8421426140E-01
H2	C17	6.7394032744E+00	9.8638463004E-03	4.8496745028E-01	7.4367103008E-02
H3	C17	6.7399688129E+00	1.0292561886E-02	5.0598723860E-01	7.7599344786E-02
C4	C17	3.9509540609E+01	1.2984119790E-02	1.0895436129E-01	9.7891972817E-02
H5	C17	6.7106092597E+00	1.4846208781E-03	7.3351840502E-02	1.1193093486E-02
C6	C17	3.9608135617E+01	1.6732281115E-03	1.4007706072E-02	1.2615071599E-02
H7	C17	6.7304254687E+00	3.8436240198E-04	1.8936138441E-02	2.8978470943E-03
H8	C17	6.7476372279E+00	8.2022847868E-04	4.0305300613E-02	6.1839990108E-03
C9	C17	4.3918024584E+01	1.3045017173E-01	9.8347377294E-01	9.8351100197E-01
H10	C17	6.7397115574E+00	1.0291055647E-02	5.0593254369E-01	7.7587988706E-02
H11	C17	6.7395571464E+00	9.8521192574E-03	4.8438024659E-01	7.4278688592E-02
C12	C17	3.9509565719E+01	1.2909881366E-02	1.0833143322E-01	9.7332262497E-02
H13	C17	6.7112822133E+00	1.4834509078E-03	7.3286692712E-02	1.1184272657E-02
C14	C17	3.9588800551E+01	4.9883053869E-02	4.1755395837E-01	3.7608637568E-01
H15	C17	6.7423653462E+00	1.1792128816E-02	5.7943637919E-01	8.8905121964E-02
H16	C17	6.7257201596E+00	9.0587513373E-03	4.4631616124E-01	6.8297201042E-02
C1	H18	6.7401815638E+00	1.0306808731E-02	7.7700976019E-02	5.0670879989E-01

H2	H18	1.0340087608E+00	5.4894411610E-04	2.6989474514E-02	2.6987481920E-02
H3	H18	1.0321297738E+00	4.5461213711E-03	2.2348948925E-01	2.2349883114E-01
C4	H18	6.0594710074E+00	1.0872600758E-03	9.1235855052E-03	5.3452456775E-02
H5	H18	1.0290666424E+00	3.1671673680E-04	1.5648274859E-02	1.5570596273E-02
C6	H18	6.0740762355E+00	3.8245450130E-04	3.2017811579E-03	1.8802431134E-02
H7	H18	1.0321474062E+00	6.4321021418E-05	3.1688629272E-03	3.1621841854E-03
H8	H18	1.0348178156E+00	6.9392513650E-05	3.4098866299E-03	3.4115115776E-03
C9	H18	6.7401551098E+00	9.8667441174E-03	7.4386134839E-02	4.8507410986E-01
H10	H18	1.0340889122E+00	5.4871034770E-04	2.6975893580E-02	2.6975989274E-02
H11	H18	1.0334130270E+00	1.7858075752E-03	8.7799375042E-02	8.7794819610E-02
C12	H18	6.0596649327E+00	6.9572621826E-04	5.8380876028E-03	3.4203661513E-02
H13	H18	1.0292301105E+00	1.9600382448E-04	9.6831462233E-03	9.6360440241E-03
C14	H18	6.0698251183E+00	1.0347656618E-02	8.6616689348E-02	5.0871698539E-01
H15	H18	1.0337976232E+00	2.1754347181E-03	1.0689554328E-01	1.0694987595E-01
H16	H18	1.0317396966E+00	7.6683515287E-04	3.7781246995E-02	3.7699556689E-02
C17	H18	6.2570796180E+00	9.7550708148E-01	7.3547005300E+00	4.7958396770E+01
(Bonded)					
C1	H19	6.7400176194E+00	9.8711304549E-03	7.4416484364E-02	4.8531722209E-01
H2	H19	1.0333308205E+00	1.7877445120E-03	8.7896533596E-02	8.7895019149E-02
H3	H19	1.0340699732E+00	5.4862880961E-04	2.6970853269E-02	2.6973507346E-02
C4	H19	6.0593209961E+00	7.0129341156E-04	5.8848021251E-03	3.4479310341E-02
H5	H19	1.0290689813E+00	1.9553141289E-04	9.6607755036E-03	9.6133631877E-03
C6	H19	6.0737324730E+00	3.8237670224E-04	3.2011298502E-03	1.8799670389E-02
H7	H19	1.0320889388E+00	6.4413881869E-05	3.1734378241E-03	3.1669286872E-03
H8	H19	1.0347592439E+00	6.9391481601E-05	3.4098359159E-03	3.4116539378E-03
C9	H19	6.7395598450E+00	1.0293734556E-02	7.7605248252E-02	5.0609468514E-01
H10	H19	1.0320328966E+00	4.5436522373E-03	2.2337664987E-01	2.2339008607E-01
H11	H19	1.0339733592E+00	5.4806048762E-04	2.6945438560E-02	2.6945565617E-02
C12	H19	6.0591293064E+00	1.0809897371E-03	9.0709716228E-03	5.3147199171E-02
H13	H19	1.0291114521E+00	3.1680129929E-04	1.5650884940E-02	1.5575635154E-02
C14	H19	6.0705967355E+00	8.1167368290E-03	6.7942423913E-02	3.9906190970E-01
H15	H19	1.0344498223E+00	7.5388823454E-04	3.7044224647E-02	3.7065151294E-02

H16	H19	1.0284082946E+00	7.3128035456E-03	3.6029495511E-01	3.5953627790E-01
C17	H19	6.2567010664E+00	9.7550067441E-01	7.3546522248E+00	4.7960796346E+01
(Bonded)					
H18	H19	1.0152647547E+00	3.8072598009E-02	1.8717452656E+00	1.8718512117E+00
C1	C20	3.9588338793E+01	4.9953868801E-02	3.7659225694E-01	4.1818233641E-01
H2	C20	6.0688648321E+00	1.0336650244E-02	5.0821340486E-01	8.6531927427E-02
H3	C20	6.0706734925E+00	8.1240983361E-03	3.9938453893E-01	6.8009835974E-02
C4	C20	3.5107134298E+01	9.6300407568E-01	8.0809092708E+00	8.0616637712E+00
(Bonded)					
H5	C20	6.0239565188E+00	4.0742337196E-02	2.0129889480E+00	3.4106919381E-01
C6	C20	3.5649545569E+01	4.5586613255E-02	3.8163587793E-01	3.8162242280E-01
H7	C20	6.0562433254E+00	1.0871271793E-02	5.3558804564E-01	9.1007442410E-02
H8	C20	6.0734026675E+00	7.9473878675E-03	3.9052759739E-01	6.6530527196E-02
C9	C20	3.9611035491E+01	1.6653949468E-03	1.2555539254E-02	1.3941637888E-02
H10	C20	6.0743120282E+00	3.8229532032E-04	1.8794538722E-02	3.2003357115E-03
H11	C20	6.0739750559E+00	3.8279951459E-04	1.8820369347E-02	3.2045565085E-03
C12	C20	3.5584422878E+01	8.4052851003E-03	7.0531754380E-02	7.0363754517E-02
H13	C20	6.0446092694E+00	6.4792318323E-04	3.2009247479E-02	5.4240049286E-03
C14	C20	3.5653800177E+01	4.5668965634E-02	3.8227926914E-01	3.8231182507E-01
H15	C20	6.0735735973E+00	7.9911138877E-03	3.9266379879E-01	6.6896573906E-02
H16	C20	6.0559144908E+00	1.0865883450E-02	5.3535186137E-01	9.0962334601E-02
C17	C20	3.9585426286E+01	4.9884934173E-02	3.7610055198E-01	4.1760525912E-01
H18	C20	6.0704180104E+00	8.1272340833E-03	3.9955539453E-01	6.8036086476E-02
H19	C20	6.0689669710E+00	1.0341685853E-02	5.0845222567E-01	8.6574082371E-02
C1	H21	6.7267574286E+00	9.0949154129E-03	6.8564753926E-02	4.4806101016E-01
H2	H21	1.0317481147E+00	7.6768379510E-04	3.7744064678E-02	3.7819942364E-02
H3	H21	1.0285935446E+00	7.3155298516E-03	3.5963492759E-01	3.6039958003E-01
C4	H21	6.0276395630E+00	3.9540874034E-02	3.3180151946E-01	1.9479811695E+00
H5	H21	1.0253240871E+00	3.5203167600E-03	1.7393108052E-01	1.7342840609E-01
C6	H21	6.0562007055E+00	1.0864948762E-02	9.0957716828E-02	5.3526170358E-01
H7	H21	1.0288264851E+00	2.4123619021E-03	1.1884830231E-01	1.1884500973E-01
H8	H21	1.0323466345E+00	7.0683418377E-04	3.4733205443E-02	3.4822186246E-02
C9	H21	6.7308668183E+00	3.8418887093E-04	2.8964291378E-03	1.8927064825E-02

H10	H21	1.0321795917E+00	6.4465995762E-05	3.1693002483E-03	3.1759172978E-03
H11	H21	1.0321224305E+00	6.4353772449E-05	3.1639584696E-03	3.1703886163E-03
C12	H21	6.0470978927E+00	6.2053899854E-04	5.2071647429E-03	3.0570853923E-02
H13	H21	1.0270560793E+00	2.6212677372E-04	1.2949807921E-02	1.2913675575E-02
C14	H21	6.0569260588E+00	1.0874166929E-02	9.1023926827E-02	5.3571583657E-01
H15	H21	1.0323781611E+00	7.0930174521E-04	3.4853353572E-02	3.4943750661E-02
H16	H21	1.0287676926E+00	2.4172767629E-03	1.1909695336E-01	1.1908714035E-01
C17	H21	6.7262690177E+00	9.0702058403E-03	6.8383560681E-02	4.4684369306E-01
H18	H21	1.0285438813E+00	7.3285635722E-03	3.6029073107E-01	3.6104168628E-01
H19	H21	1.0317659837E+00	7.6751345967E-04	3.7735039757E-02	3.7811550789E-02
C20	H21	5.5929883990E+00	9.3771700035E-01	7.8499762984E+00	4.6196628264E+01
(Bonded)					
C1	H22	6.7424945640E+00	1.1807923498E-02	8.9017580954E-02	5.8024386878E-01
H2	H22	1.0336654388E+00	2.1750776617E-03	1.0694021740E-01	1.0688377830E-01
H3	H22	1.0344958367E+00	7.5359376512E-04	3.7047027987E-02	3.7031757686E-02
C4	H22	6.0428177023E+00	3.9898475784E-02	3.3480228277E-01	1.9606195747E+00
H5	H22	1.0277871138E+00	3.8106689204E-03	1.8827673985E-01	1.8725708016E-01
C6	H22	6.0730530801E+00	7.9463172396E-03	6.6523909971E-02	3.9048371700E-01
H7	H22	1.0322952335E+00	7.0624521555E-04	3.4794134666E-02	3.4705039903E-02
H8	H22	1.0319959058E+00	6.6532190641E-03	3.2693328919E-01	3.2694059800E-01
C9	H22	6.7477419527E+00	8.1994977186E-04	6.1816637347E-03	4.0292505951E-02
H10	H22	1.0347984118E+00	6.9273396672E-05	3.4056434044E-03	3.4041094266E-03
H11	H22	1.0347408999E+00	6.9572006309E-05	3.4205133627E-03	3.4187831675E-03
C12	H22	6.0623689593E+00	7.9227669328E-04	6.6482771809E-03	3.8932644993E-02
H13	H22	1.0297546326E+00	8.1948307082E-05	4.0484793718E-03	4.0269572163E-03
C14	H22	6.0737706763E+00	7.9747571710E-03	6.6753960826E-02	3.9188126127E-01
H15	H22	1.0320141350E+00	6.6824477622E-03	3.2835914497E-01	3.2837690243E-01
H16	H22	1.0322378618E+00	7.0803233130E-04	3.4884087263E-02	3.4792859151E-02
C17	H22	6.7419987280E+00	1.1795520911E-02	8.8930696194E-02	5.7963440302E-01
H18	H22	1.0344520084E+00	7.5473834970E-04	3.7104847232E-02	3.7088002815E-02
H19	H22	1.0336837042E+00	2.1742048665E-03	1.0689546358E-01	1.0684088896E-01
C20	H22	5.6080660119E+00	9.3834897773E-01	7.8552668151E+00	4.6110668077E+01
(Bonded)					

H21	H22	1.0141418943E+00	3.7070142271E-02	1.8262605686E+00	1.8216346651E+00
C1	C23	3.9516895956E+01	1.2982220882E-02	9.7870374795E-02	1.0892625934E-01
H2	C23	6.0598957260E+00	6.9677859825E-04	3.4257928389E-02	5.8462636698E-03
H3	C23	6.0604043862E+00	1.0810380333E-03	5.3144343979E-02	9.0703609377E-03
C4	C23	3.5486337900E+01	4.3012900472E-02	3.6093652662E-01	3.6089621294E-01
H5	C23	6.0252111346E+00	1.0789894096E-02	5.3310485016E-01	9.0531721289E-02
C6	C23	3.5587142350E+01	8.4290428605E-03	7.0565127403E-02	7.0723192662E-02
H7	C23	6.0476065778E+00	6.2277501647E-04	3.0681861360E-02	5.2253426877E-03
H8	C23	6.0631825963E+00	7.9426701778E-04	3.9029577429E-02	6.6642322566E-03
C9	C23	3.9515447898E+01	1.2989829392E-02	9.7931312414E-02	1.0899009792E-01
H10	C23	6.0601759944E+00	1.0741449960E-03	5.2807498936E-02	9.0125254737E-03
H11	C23	6.0600274507E+00	6.9932074608E-04	3.4382161500E-02	5.8675933527E-03
C12	C23	3.5486348328E+01	4.2970462387E-02	3.6058052315E-01	3.6054013967E-01
H13	C23	6.0258133087E+00	1.0793883841E-02	5.3324855178E-01	9.0565196914E-02
C14	C23	3.5114102656E+01	9.6308049479E-01	8.0616169549E+00	8.0806478872E+00
(Bonded)					
H15	C23	6.0437973996E+00	3.9949370645E-02	1.9630144004E+00	3.3519191724E-01
H16	C23	6.0278098674E+00	3.9554643552E-02	1.9488200981E+00	3.3187999194E-01
C17	C23	3.9034381793E+01	9.7212997554E-01	7.3292393075E+00	8.1565768131E+00
(Bonded)					
H18	C23	6.0408726461E+00	3.9637842511E-02	1.9486966464E+00	3.3257806598E-01
H19	C23	6.0406086021E+00	3.9479864643E-02	1.9410399168E+00	3.3125256564E-01
C20	C23	3.5110927926E+01	9.6336762975E-01	8.0647072170E+00	8.0830570695E+00
(Bonded)					
H21	C23	6.0282187000E+00	3.9733644002E-02	1.9574779820E+00	3.3338188053E-01
H22	C23	6.0434593963E+00	3.9969562572E-02	1.9641127946E+00	3.3536133594E-01
C1	H24	6.7112745897E+00	1.4882161975E-03	1.1219365188E-02	7.3527638961E-02
H2	H24	1.0290771930E+00	1.9510441468E-04	9.5925349653E-03	9.6394374602E-03
H3	H24	1.0291352335E+00	3.1704523608E-04	1.5586094628E-02	1.5664113650E-02
C4	H24	6.0246841983E+00	1.0798147221E-02	9.0611088975E-02	5.3349928032E-01
H5	H24	1.0230549969E+00	2.1729992914E-03	1.0736309840E-01	1.0736041419E-01
C6	H24	6.0439414154E+00	6.4856971887E-04	5.4296087467E-03	3.2043597033E-02
H7	H24	1.0269500084E+00	2.6292203406E-04	1.2953212933E-02	1.2990072564E-02

H8	H24	1.0297003518E+00	8.1721427858E-05	4.0157185491E-03	4.0375744150E-03
C9	H24	6.7110294288E+00	1.4880002234E-03	1.1218146933E-02	7.3516968424E-02
H10	H24	1.0290958150E+00	3.1713893505E-04	1.5591297299E-02	1.5668742993E-02
H11	H24	1.0290998854E+00	1.9489145192E-04	9.5818541242E-03	9.6289157032E-03
C12	H24	6.0246853078E+00	1.0792263082E-02	9.0561740598E-02	5.3320856528E-01
H13	H24	1.0231581076E+00	2.1719826410E-03	1.0730211802E-01	1.0731018499E-01
C14	H24	6.0246329221E+00	4.0721298342E-02	3.4086404087E-01	2.0118991633E+00
H15	H24	1.0278642096E+00	3.8193389616E-03	1.8767297858E-01	1.8870038958E-01
H16	H24	1.0252715054E+00	3.5075806575E-03	1.7281520113E-01	1.7329748504E-01
C17	H24	6.6872465689E+00	4.8545595895E-02	3.6600279653E-01	2.3984707694E+00
H18	H24	1.0271934638E+00	4.1145390633E-03	2.0228115271E-01	2.0328521034E-01
H19	H24	1.0271310854E+00	4.1227854257E-03	2.0269803739E-01	2.0369263472E-01
C20	H24	6.0241060498E+00	4.0745514893E-02	3.4109579549E-01	2.0130956198E+00
H21	H24	1.0253567317E+00	3.5063858145E-03	1.7274209806E-01	1.7323845196E-01
H22	H24	1.0278066022E+00	3.8231806758E-03	1.8787191048E-01	1.8889019545E-01
C23	H24	5.5656402409E+00	9.3023323498E-01	7.8050456483E+00	4.5959621705E+01
(Bonded)					
C1	B25	2.0117615009E+01	5.3624600308E-01	4.0426516989E+00	8.7231909831E+00
(Bonded)					
H2	B25	3.1187523840E+00	1.4112716495E-02	6.9386808419E-01	2.2957359229E-01
H3	B25	3.1191769684E+00	1.3986467455E-02	6.8758139360E-01	2.2751988096E-01
C4	B25	1.8299810748E+01	2.9507025847E-02	2.4760393517E-01	4.7999504020E-01
H5	B25	3.1072776666E+00	6.4881932277E-03	3.2056730563E-01	1.0554437392E-01
C6	B25	1.8355575623E+01	4.1269972499E-03	3.4549840539E-02	6.7134458794E-02
H7	B25	3.1191744337E+00	5.5322586967E-04	2.7255427699E-02	8.9994049191E-03
H8	B25	3.1267715999E+00	1.5152328779E-03	7.4457200926E-02	2.4648511508E-02
C9	B25	2.0116772594E+01	5.3644097231E-01	4.0442693177E+00	8.7263625756E+00
(Bonded)					
H10	B25	3.1190357210E+00	1.4029802889E-02	6.8973816745E-01	2.2822482471E-01
H11	B25	3.1188155340E+00	1.4123611971E-02	6.9438853411E-01	2.2975083056E-01
C12	B25	1.8299792791E+01	2.9531807589E-02	2.4781196288E-01	4.8039816836E-01
H13	B25	3.1075842841E+00	6.4982058990E-03	3.2102984763E-01	1.0570725148E-01
C14	B25	1.8357782380E+01	4.1348611144E-03	3.4611506148E-02	6.7262381412E-02

H15	B25	3.1268731584E+00	1.5105452964E-03	7.4224502700E-02	2.4572257945E-02
H16	B25	3.1190044083E+00	5.5205512465E-04	2.7199236943E-02	8.9803602411E-03
C17	B25	2.0116118346E+01	5.3620619475E-01	4.0426523391E+00	8.7225434153E+00
(Bonded)					
H18	B25	3.1190554463E+00	1.3968173731E-02	6.8671076883E-01	2.2722229432E-01
H19	B25	3.1188547724E+00	1.4015656209E-02	6.8908412954E-01	2.2799469863E-01
C20	B25	1.8356226647E+01	4.1194457326E-03	3.4485405886E-02	6.7011617174E-02
H21	B25	3.1192627619E+00	5.4941718955E-04	2.7067037985E-02	8.9374485708E-03
H22	B25	3.1267033611E+00	1.5118775956E-03	7.4293986178E-02	2.4593930646E-02
C23	B25	1.8301835993E+01	2.9548168310E-02	2.4792148228E-01	4.8066431057E-01
H24	B25	3.1073471260E+00	6.5048123510E-03	3.2138038470E-01	1.0581471959E-01

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	H2	4.8756863371E+01	3.8274718385E+01	3.0525183419E+01
C1	H3	4.8734514490E+01	3.8280765349E+01	3.0514334577E+01
C1	C4	5.1575896305E+01	4.3159801291E+01	3.6669251245E+01
C1	B25	4.8177593436E+01	4.0185635313E+01	3.4151284110E+01

C1	Total	1.9724486760E+02	1.5990092034E+02	1.3186005335E+02

H2	C1	4.8756863371E+01	3.8274718385E+01	3.0525183419E+01

H2	Total	4.8756863371E+01	3.8274718385E+01	3.0525183419E+01
H3	C1	4.8734514490E+01	3.8280765349E+01	3.0514334577E+01
H3	Total	4.8734514490E+01	3.8280765349E+01	3.0514334577E+01
C4	C1	5.1575896305E+01	4.3159801291E+01	3.6669251245E+01
C4	H5	4.5531394246E+01	3.5467728059E+01	2.8199281581E+01
C4	C6	5.0329398672E+01	4.2070755640E+01	3.5711237986E+01
C4	C20	5.0311864982E+01	4.2061269944E+01	3.5695387952E+01
C4	Total	1.9774855421E+02	1.6275955493E+02	1.3627515876E+02
H5	C4	4.5531394246E+01	3.5467728059E+01	2.8199281581E+01
H5	Total	4.5531394246E+01	3.5467728059E+01	2.8199281581E+01
C6	C4	5.0329398672E+01	4.2070755641E+01	3.5711237986E+01
C6	H7	4.9473190906E+01	3.9046595571E+01	3.1231044631E+01
C6	H8	4.9171399459E+01	3.8764981171E+01	3.0992208725E+01
C6	C12	5.0307239442E+01	4.2058201576E+01	3.5694704788E+01
C6	Total	1.9928122848E+02	1.6194053396E+02	1.3362919613E+02
H7	C6	4.9473190906E+01	3.9046595571E+01	3.1231044631E+01
H7	Total	4.9473190906E+01	3.9046595571E+01	3.1231044631E+01
H8	C6	4.9171399459E+01	3.8764981171E+01	3.0992208725E+01
H8	Total	4.9171399459E+01	3.8764981171E+01	3.0992208725E+01

C9	B25	4.8172070911E+01	4.0175390479E+01	3.4148261280E+01
C9	C12	5.1579499089E+01	4.3155416501E+01	3.6668092521E+01
C9	H10	4.8737945507E+01	3.8274026993E+01	3.0521054421E+01
C9	H11	4.8734468553E+01	3.8279398448E+01	3.0511501603E+01

C9	Total	1.9722398406E+02	1.5988423242E+02	1.3184890982E+02
H10	C9	4.8737945507E+01	3.8274026993E+01	3.0521054421E+01

H10	Total	4.8737945507E+01	3.8274026993E+01	3.0521054421E+01
H11	C9	4.8734468553E+01	3.8279398448E+01	3.0511501603E+01

H11	Total	4.8734468553E+01	3.8279398448E+01	3.0511501603E+01
C12	C6	5.0307239442E+01	4.2058201576E+01	3.5694704788E+01
C12	C9	5.1579499089E+01	4.3155416501E+01	3.6668092521E+01
C12	H13	4.5541264190E+01	3.5477891731E+01	2.8186819765E+01
C12	C14	5.0338859071E+01	4.2072912183E+01	3.5712752918E+01

C12	Total	1.9776686179E+02	1.6276442199E+02	1.3626236999E+02
H13	C12	4.5541264190E+01	3.5477891731E+01	2.8186819765E+01

H13	Total	4.5541264190E+01	3.5477891731E+01	2.8186819765E+01
C14	C12	5.0338859071E+01	4.2072912183E+01	3.5712752918E+01
C14	H15	4.9166250848E+01	3.8785404335E+01	3.0996807347E+01
C14	H16	4.9463744441E+01	3.9036473851E+01	3.1228858271E+01
C14	C23	5.0322589623E+01	4.2062115724E+01	3.5703615413E+01

C14	Total	1.9929144398E+02	1.6195690609E+02	1.3364203395E+02
H15	C14	4.9166250848E+01	3.8785404335E+01	3.0996807347E+01

H15	Total	4.9166250848E+01	3.8785404335E+01	3.0996807347E+01
H16	C14	4.9463744441E+01	3.9036473851E+01	3.1228858271E+01

H16	Total	4.9463744441E+01	3.9036473851E+01	3.1228858271E+01
C17	B25	4.8155691664E+01	4.0168331345E+01	3.4131888531E+01
C17	C23	5.1576127951E+01	4.3156910741E+01	3.6663885404E+01
C17	H18	4.8736631342E+01	3.8283569911E+01	3.0515640538E+01
C17	H19	4.8727184446E+01	3.8265867338E+01	3.0515862188E+01

C17	Total	1.9719563540E+02	1.5987467933E+02	1.3182727666E+02
H18	C17	4.8736631342E+01	3.8283569911E+01	3.0515640538E+01

H18	Total	4.8736631342E+01	3.8283569911E+01	3.0515640538E+01
H19	C17	4.8727184446E+01	3.8265867338E+01	3.0515862188E+01

H19	Total	4.8727184446E+01	3.8265867338E+01	3.0515862188E+01
C20	C4	5.0311864982E+01	4.2061269944E+01	3.5695387952E+01
C20	C23	5.0339321420E+01	4.2072541885E+01	3.5712158850E+01
C20	H21	4.9468432447E+01	3.9041874265E+01	3.1216519748E+01
C20	H22	4.9167271250E+01	3.8765443053E+01	3.0989498374E+01

C20	Total	1.9928689010E+02	1.6194112915E+02	1.3361356492E+02

H21	C20	4.9468432447E+01	3.9041874265E+01	3.1216519748E+01

H21	Total	4.9468432447E+01	3.9041874265E+01	3.1216519748E+01
H22	C20	4.9167271250E+01	3.8765443053E+01	3.0989498374E+01

H22	Total	4.9167271250E+01	3.8765443053E+01	3.0989498374E+01
C23	C14	5.0322589623E+01	4.2062115724E+01	3.5703615413E+01
C23	C17	5.1576127951E+01	4.3156910741E+01	3.6663885404E+01
C23	C20	5.0339321420E+01	4.2072541885E+01	3.5712158850E+01
C23	H24	4.5533809532E+01	3.5475930954E+01	2.8202652888E+01

C23	Total	1.9777184853E+02	1.6276749930E+02	1.3628231256E+02
H24	C23	4.5533809532E+01	3.5475930954E+01	2.8202652888E+01

H24	Total	4.5533809532E+01	3.5475930954E+01	2.8202652888E+01
B25	C1	4.8177593436E+01	4.0185635313E+01	3.4151284110E+01
B25	C9	4.8172070911E+01	4.0175390479E+01	3.4148261280E+01
B25	C17	4.8155691664E+01	4.0168331345E+01	3.4131888531E+01

B25	Total	1.4450535601E+02	1.2052935714E+02	1.0243143392E+02

Total	Total	2.6522610352E+03	2.1438399041E+03	1.7620195781E+03

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$DelSqRho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $DelSqRho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$DelSqRho\_IAS(A B)$	$V\_IAS(A B)$

C1	H2	9.9252916265E-01	5.5213263497E-01	3.7052600664E-01	-1.8160662833E-01	7.2642651333E-01	-9.2265864161E-01

C1	H3	9.9250209795E-01	5.5210897208E-01	3.7064189273E-01	-1.8146707934E-01	7.2586831738E-01	-9.2275086481E-01

C1	C4	1.1665257972E+00	8.0247716582E-01	2.7283100463E-01	-5.2964616119E-01	2.1185846447E+00	-1.0753081705E+00

C1	B25	1.0323954184E+00	7.6894512658E-01	4.4956855667E-01	-3.1937656991E-01	1.2775062796E+00	-1.2185136833E+00

C1	Total	4.1839524762E+00	2.6756638994E+00	1.4635674607E+00	-1.2120964388E+00	4.8483857550E+00	-4.1392313602E+00

H2	C1	9.9252916265E-01	5.5213263497E-01	3.7052600664E-01	-1.8160662833E-01	7.2642651333E-01	-9.2265864161E-01

H2	Total	9.9252916265E-01	5.5213263497E-01	3.7052600664E-01	-1.8160662833E-01	7.2642651333E-01	-9.2265864161E-01

H3	C1	9.9250209795E-01	5.5210897208E-01	3.7064189273E-01	-1.8146707934E-01	7.2586831738E-01	-9.2275086481E-01

H3	Total	9.9250209795E-01	5.5210897208E-01	3.7064189273E-01	-1.8146707934E-01	7.2586831738E-01	-9.2275086481E-01

C4 C1 1.1665257972E+00 8.0247716582E-01 2.7283100463E-01 -5.2964616119E-01
2.1185846447E+00 -1.0753081705E+00

C4 H5 9.8119858803E-01 5.5874927162E-01 3.7405992555E-01 -1.8468934608E-01
7.3875738430E-01 -9.3280919717E-01

C4 C6 1.1973201475E+00 8.2662906707E-01 3.1831087010E-01 -5.0831819696E-01
2.0332727879E+00 -1.1449399372E+00

C4 C20 1.1967125876E+00 8.2599778889E-01 3.1799480253E-01 -5.0800298635E-01
2.0320119454E+00 -1.1439925914E+00

C4 Total 4.5417571203E+00 3.0138532934E+00 1.2831966028E+00 -1.7306566906E+00
6.9226267623E+00 -4.2970498963E+00

H5 C4 9.8119858803E-01 5.5874927162E-01 3.7405992555E-01 -1.8468934608E-01
7.3875738430E-01 -9.3280919717E-01

H5 Total 9.8119858803E-01 5.5874927162E-01 3.7405992555E-01 -1.8468934608E-01
7.3875738430E-01 -9.3280919717E-01

C6 C4 1.1973201475E+00 8.2662906707E-01 3.1831087010E-01 -5.0831819696E-01
2.0332727879E+00 -1.1449399372E+00

C6 H7 9.9466839251E-01 5.6292503337E-01 3.7015020084E-01 -1.9277483253E-01
7.7109933010E-01 -9.3307523421E-01

C6 H8 9.9349301050E-01 5.6129791844E-01 3.6980424493E-01 -1.9149367351E-01
7.6597469402E-01 -9.3110216337E-01

C6 C12 1.1971510178E+00 8.2643580474E-01 3.1835950844E-01 -5.0807629631E-01
2.0323051852E+00 -1.1447953132E+00

C6 Total 4.3826325683E+00 2.7772878236E+00 1.3766248243E+00 -1.4006629993E+00
5.6026519972E+00 -4.1539126480E+00

H7 C6 9.9466839251E-01 5.6292503337E-01 3.7015020084E-01 -1.9277483253E-01
7.7109933010E-01 -9.3307523421E-01

H7 Total 9.9466839251E-01 5.6292503337E-01 3.7015020084E-01 -1.9277483253E-01
7.7109933010E-01 -9.3307523421E-01

H8 C6 9.9349301050E-01 5.6129791844E-01 3.6980424493E-01 -1.9149367351E-01
7.6597469402E-01 -9.3110216337E-01

H8 Total 9.9349301050E-01 5.6129791844E-01 3.6980424493E-01 -1.9149367351E-01
7.6597469402E-01 -9.3110216337E-01

C9 B25 1.0324089651E+00 7.6885568536E-01 4.4964975607E-01 -3.1920592929E-01
1.2768237171E+00 -1.2185054414E+00

C9 C12 1.1671185143E+00 8.0303702151E-01 2.7323383889E-01 -5.2980318261E-01
2.1192127305E+00 -1.0762708604E+00

C9 H10 9.9252761192E-01 5.5216313412E-01 3.7057585901E-01 -1.8158727511E-01
7.2634910042E-01 -9.2273899313E-01

C9 H11 9.9248655446E-01 5.5209410096E-01 3.7062273801E-01 -1.8147136295E-01
7.2588545180E-01 -9.2271683896E-01

C9 Total 4.1845416458E+00 2.6761499419E+00 1.4640821920E+00 -1.2120677500E+00
4.8482709998E+00 -4.1402321339E+00

H10 C9 9.9252761192E-01 5.5216313412E-01 3.7057585901E-01 -1.8158727511E-01
7.2634910042E-01 -9.2273899313E-01

H10 Total 9.9252761192E-01 5.5216313412E-01 3.7057585901E-01 -1.8158727511E-01
7.2634910042E-01 -9.2273899313E-01

H11 C9 9.9248655446E-01 5.5209410096E-01 3.7062273801E-01 -1.8147136295E-01
7.2588545180E-01 -9.2271683896E-01

H11 Total 9.9248655446E-01 5.5209410096E-01 3.7062273801E-01 -1.8147136295E-01
7.2588545180E-01 -9.2271683896E-01

C12 C6 1.1971510178E+00 8.2643580474E-01 3.1835950844E-01 -5.0807629631E-01
2.0323051852E+00 -1.1447953132E+00

C12 C9 1.1671185143E+00 8.0303702151E-01 2.7323383889E-01 -5.2980318261E-01
2.1192127305E+00 -1.0762708604E+00

C12 H13 9.8125688155E-01 5.5883405264E-01 3.7406197721E-01 -1.8477207543E-01
7.3908830171E-01 -9.3289602985E-01

C12	C14	1.1968553359E+00	8.2618773517E-01	3.1790874773E-01	-5.0827898744E-01
		2.0331159498E+00	-1.1440964829E+00		

C12	Total	4.5423817495E+00	3.0144946141E+00	1.2835640723E+00	-1.7309305418E+00
		6.9237221672E+00	-4.2980586864E+00		

H13	C12	9.8125688155E-01	5.5883405264E-01	3.7406197721E-01	-1.8477207543E-01
		7.3908830171E-01	-9.3289602985E-01		

H13	Total	9.8125688155E-01	5.5883405264E-01	3.7406197721E-01	-1.8477207543E-01
		7.3908830171E-01	-9.3289602985E-01		

C14	C12	1.1968553359E+00	8.2618773517E-01	3.1790874773E-01	-5.0827898744E-01
		2.0331159498E+00	-1.1440964829E+00		

C14	H15	9.9363598701E-01	5.6142604272E-01	3.6984470848E-01	-1.9158133424E-01
		7.6632533696E-01	-9.3127075120E-01		

C14	H16	9.9463412259E-01	5.6283684822E-01	3.7014170408E-01	-1.9269514415E-01
		7.7078057658E-01	-9.3297855230E-01		

C14	C23	1.1967667873E+00	8.2608625921E-01	3.1795327197E-01	-5.0813298724E-01
		2.0325319489E+00	-1.1440395312E+00		

C14	Total	4.3818922328E+00	2.7765368853E+00	1.3758484323E+00	-1.4006884531E+00
		5.6027538122E+00	-4.1523853176E+00		

H15	C14	9.9363598701E-01	5.6142604272E-01	3.6984470848E-01	-1.9158133424E-01
		7.6632533696E-01	-9.3127075120E-01		

H15	Total	9.9363598701E-01	5.6142604272E-01	3.6984470848E-01	-1.9158133424E-01
		7.6632533696E-01	-9.3127075120E-01		

H16	C14	9.9463412259E-01	5.6283684822E-01	3.7014170408E-01	-1.9269514415E-01
		7.7078057658E-01	-9.3297855230E-01		

H16	Total	9.9463412259E-01	5.6283684822E-01	3.7014170408E-01	-1.9269514415E-01
		7.7078057658E-01	-9.3297855230E-01		

C17 B25 1.0321262091E+00 7.6865024491E-01 4.4947564596E-01 -3.1917459894E-01
1.2766983958E+00 -1.2181258909E+00

C17 C23 1.1671883578E+00 8.0307841912E-01 2.7333142700E-01 -5.2974699212E-01
2.1189879685E+00 -1.0764098461E+00

C17 H18 9.9240178870E-01 5.5202054960E-01 3.7052306097E-01 -1.8149748862E-01
7.2598995450E-01 -9.2254361057E-01

C17 H19 9.9243583315E-01 5.5206542404E-01 3.7059171037E-01 -1.8147371367E-01
7.2589485468E-01 -9.2265713441E-01

C17 Total 4.1841521887E+00 2.6758146377E+00 1.4639218443E+00 -1.2118927933E+00
4.8475711735E+00 -4.1397364820E+00

H18 C17 9.9240178870E-01 5.5202054960E-01 3.7052306097E-01 -1.8149748862E-01
7.2598995450E-01 -9.2254361057E-01

H18 Total 9.9240178870E-01 5.5202054960E-01 3.7052306097E-01 -1.8149748862E-01
7.2598995450E-01 -9.2254361057E-01

H19 C17 9.9243583315E-01 5.5206542404E-01 3.7059171037E-01 -1.8147371367E-01
7.2589485468E-01 -9.2265713441E-01

H19 Total 9.9243583315E-01 5.5206542404E-01 3.7059171037E-01 -1.8147371367E-01
7.2589485468E-01 -9.2265713441E-01

C20 C4 1.1967125876E+00 8.2599778889E-01 3.1799480253E-01 -5.0800298635E-01
2.0320119454E+00 -1.1439925914E+00

C20 C23 1.1970969821E+00 8.2642024100E-01 3.1816126714E-01 -5.0825897386E-01
2.0330358955E+00 -1.1445815081E+00

C20 H21 9.9460795420E-01 5.6284407921E-01 3.7011495043E-01 -1.9272912877E-01
7.7091651510E-01 -9.3295902964E-01

C20 H22 9.9352879482E-01 5.6131156568E-01 3.6981567356E-01 -1.9149589212E-01
7.6598356848E-01 -9.3112723923E-01

C20 Total 4.3819463187E+00 2.7765736748E+00 1.3760866937E+00 -1.4004869811E+00
5.6019479245E+00 -4.1526603684E+00

H21	C20	9.9460795420E-01	5.6284407921E-01	3.7011495043E-01	-1.9272912877E-01
7.7091651510E-01 -9.3295902964E-01					

H21	Total	9.9460795420E-01	5.6284407921E-01	3.7011495043E-01	-1.9272912877E-01
7.7091651510E-01 -9.3295902964E-01					

H22	C20	9.9352879482E-01	5.6131156568E-01	3.6981567356E-01	-1.9149589212E-01
7.6598356848E-01 -9.3112723923E-01					

H22	Total	9.9352879482E-01	5.6131156568E-01	3.6981567356E-01	-1.9149589212E-01
7.6598356848E-01 -9.3112723923E-01					

C23	C14	1.1967667873E+00	8.2608625921E-01	3.1795327197E-01	-5.0813298724E-01
2.0325319489E+00 -1.1440395312E+00					

C23	C17	1.1671883578E+00	8.0307841912E-01	2.7333142700E-01	-5.2974699212E-01
2.1189879685E+00 -1.0764098461E+00					

C23	C20	1.1970969821E+00	8.2642024100E-01	3.1816126714E-01	-5.0825897386E-01
2.0330358955E+00 -1.1445815081E+00					

C23	H24	9.8121537510E-01	5.5881070653E-01	3.7404638639E-01	-1.8476432014E-01
7.3905728058E-01 -9.3285709292E-01					

C23	Total	4.5422675023E+00	3.0143956259E+00	1.2834923525E+00	-1.7309032734E+00
6.9236130935E+00 -4.2978879783E+00					

H24	C23	9.8121537510E-01	5.5881070653E-01	3.7404638639E-01	-1.8476432014E-01
7.3905728058E-01 -9.3285709292E-01					

H24	Total	9.8121537510E-01	5.5881070653E-01	3.7404638639E-01	-1.8476432014E-01
7.3905728058E-01 -9.3285709292E-01					

B25	C1	1.0323954184E+00	7.6894512658E-01	4.4956855667E-01	-3.1937656991E-01
1.2775062796E+00 -1.2185136833E+00					

B25	C9	1.0324089651E+00	7.6885568536E-01	4.4964975607E-01	-3.1920592929E-01
1.2768237171E+00 -1.2185054414E+00					

B25	C17	1.0321262091E+00	7.6865024491E-01	4.4947564596E-01	-3.1917459894E-01
1.2766983958E+00 -1.2181258909E+00					

B25 Total 3.0969305926E+00 2.3064510568E+00 1.3486939587E+00 -9.5775709814E-01
3.8310283925E+00 -3.6551450156E+00

Total Total 5.7285576550E+01 3.6068841787E+01 1.9284599473E+01 -1.6784242314E+01
6.7136969258E+01 -5.5353441260E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP\_Var\_IDS(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP*ESP\_Int\_IDS(A)$ = Surface Integral of $ESP*ESP$ Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	1.9368739853E+01
H2	4.1626448452E+01
H3	4.2007545888E+01
C4	2.2471977856E+00
H5	4.3680388053E+01
C6	7.3204185363E+00
H7	3.9362164321E+01
H8	4.0095886229E+01
C9	1.9579043090E+01
H10	4.2153437298E+01
H11	4.1906638705E+01
C12	2.3669429774E+00
H13	4.3758226541E+01
C14	7.1078142541E+00
H15	3.9947463805E+01
H16	3.8889599869E+01
C17	1.9181379310E+01
H18	4.1875910622E+01
H19	4.1902966446E+01
C20	7.0454679019E+00
H21	3.9547634093E+01
H22	3.9914685687E+01
C23	2.6131467195E+00
H24	4.3314466355E+01

B25 5.9950323066E+00

Total 7.1280864510E+02

0.001 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 1.8143713376E+01 -5.1603279001E-02 2.4014433775E-02 -9.1414210586E-03 -2.8441409942E-03 5.4337392222E-03 5.1958504395E-05

H2 3.6458707130E+01 2.1695483734E-02 8.6993295356E-03 -8.4778926775E-03 5.9507002419E-04 4.3045572139E-03 2.4465499968E-05

H3 3.6217195158E+01 1.9102823476E-02 8.6787993388E-03 -8.4205445206E-03 5.2745176408E-04 4.3324746204E-03 2.4656192815E-05

C4 3.2132246126E+00 4.3239113824E-04 4.6002803256E-03 -5.5098302997E-03 1.3456611049E-04 1.7250007550E-03 5.4574299592E-06

H5 3.8305099705E+01 1.8840203324E-01 1.1537015852E-02 -4.6189466202E-03 4.9184582389E-03 3.0391610558E-03 1.3160109280E-05

C6 7.2683646194E+00 -3.4346871119E-03 5.2249508234E-03 -2.0319584591E-03 -4.7255294578E-04 1.0942026056E-03 1.9230746838E-06

H7 3.4568850771E+01 1.8049580793E-01 1.1875096037E-02 -1.8387349010E-03 5.2213424485E-03 3.1548797689E-03 1.3696401277E-05

H8 3.5013558381E+01 2.4390486395E-01 1.3865556320E-02 -1.7158053491E-03 6.9660118887E-03 3.6693761650E-03 1.8152353242E-05

C9 1.8028782421E+01 -5.2957428198E-02 2.2878748243E-02 -9.1340287070E-03 -2.9373824012E-03 5.3501000243E-03 4.9985133427E-05

H10 3.6712465655E+01 1.8534388502E-02 8.6918148593E-03 -8.4132290890E-03 5.0485272977E-04 4.3584741136E-03 2.5004834757E-05

H11 3.6368029686E+01 1.9625155597E-02 8.7131060534E-03 -8.4486682499E-03 5.3962658320E-04 4.3292741843E-03 2.4679931781E-05

C12 3.3093958187E+00 2.0263285376E-03 4.7171537325E-03 -4.8732412623E-03 6.1229561184E-04 1.4980990109E-03 4.2805548760E-06

H13 3.8118722177E+01 1.8826937674E-01 1.1514507400E-02 -4.5523926499E-03 4.9390264412E-03 3.0219209173E-03 1.3017488190E-05

C14 7.4583184726E+00 -3.3242595133E-03 4.6389567399E-03 -2.0248478475E-03 -4.4571166081E-04 1.0991872848E-03 1.9474100538E-06

H15 3.5191265628E+01 2.4445271992E-01 1.3870224900E-02 -1.7110348300E-03 6.9464031930E-03 3.6775714085E-03 1.8183466247E-05

H16 3.4708753814E+01 1.8073832870E-01 1.1889292096E-02 -1.8609715268E-03 5.2072837206E-03 3.1648844418E-03 1.3806123916E-05

C17 1.8311934643E+01 -5.4848057094E-02 2.2460192290E-02 -9.1336989111E-03 -2.9952082160E-03 5.3407413621E-03 5.0328688218E-05

H18 3.6429101686E+01 1.9250981406E-02 8.6864043964E-03 -8.5759674375E-03 5.2845062093E-04 4.3322982760E-03 2.4690275478E-05

H19 3.6378986510E+01 1.8918623135E-02 8.6963838506E-03 -8.5001841113E-03 5.2004261114E-04 4.3266513441E-03 2.4639176760E-05

C20 7.3017863244E+00 -3.3482752261E-03 3.4145893898E-03 -2.0260215009E-03 -4.5855562972E-04 1.0752434525E-03 1.6670137959E-06

H21 3.4673291693E+01 1.8075760063E-01 1.1862364738E-02 -1.8566270394E-03 5.2131652868E-03 3.1498108089E-03 1.3657796195E-05

H22 3.5168584283E+01 2.4447018211E-01 1.3879097440E-02 -1.6684255713E-03 6.9513796785E-03 3.6787770626E-03 1.8264587365E-05

C23 2.9603113057E+00 9.3948026482E-04 3.9966133648E-03 -5.2893619601E-03 3.1735860449E-04 1.6073449992E-03 4.7810370993E-06

H24 3.8179305927E+01 1.8869391682E-01 1.1525776672E-02 -4.5457230605E-03 4.9423087255E-03 3.0206822482E-03 1.3045460833E-05

B25 5.9990578815E+00 1.0327103167E-01 3.1555176500E-02 -6.2338808412E-03 1.7214541635E-02 9.2053933507E-03 1.1530390513E-04

Total	6.3448680768E+02	1.8944655314E+00	3.1555176500E-02	-9.1414210586E-03
	2.9858233590E-03	3.3335602542E-05		

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
ESP-_Int_IDS(A)					

C1	1.2163235795E-01	1.0894872124E-03	4.1676317508E+00	3.5014539477E-02	
	1.3976081626E+01	-8.6617818477E-02			
H2	1.5865882383E-01	9.0489083015E-04	2.0237416316E+01	9.0177153782E-02	
	1.6221290814E+01	-6.8481670048E-02			
H3	1.5822830365E-01	9.0305396497E-04	1.9844663149E+01	8.8665563561E-02	
	1.6372532009E+01	-6.9562740085E-02			

C4	5.6601017017E-03 1.1063084245E+00	1.7594133460E-05 -2.6138552817E-03	2.1069161881E+00	3.0462464200E-03
H5	1.9901204192E-01 3.0767984511E+00	1.4307468307E-03 -5.3050043423E-03	3.5228301254E+01	1.9370703758E-01
C6	8.6943424012E-03 4.7876180395E+00	1.5600679505E-05 -6.0645147566E-03	2.4807465799E+00	2.6298276446E-03
H7	1.8587477600E-01 3.1311645368E+00	1.4158992755E-03 -2.6894840354E-03	3.1437686234E+01	1.8318529196E-01
H8	2.4762973082E-01 2.2443823203E+00	2.3346226620E-03 -1.8624334349E-03	3.2769176061E+01	2.4576729738E-01
C9	1.2007415329E-01 1.3789912494E+01	1.0567273124E-03 -8.6515790742E-02	4.2388699269E+00	3.3558362543E-02
H10	1.6134484771E-01 1.6482756304E+01	9.2734627384E-04 -7.1405229604E-02	2.0229709350E+01	8.9939618107E-02
H11	1.5881656927E-01 1.6365886414E+01	9.0815074732E-04 -6.9595706837E-02	2.0002143272E+01	8.9220862434E-02
C12	5.5717555247E-03 9.6340009122E-01	1.5406762480E-05 -1.7727134936E-03	2.3459957275E+00	3.7990420312E-03
H13	1.9840012607E-01 2.9929932169E+00	1.4260774455E-03 -5.0653746640E-03	3.5125728960E+01	1.9333475140E-01
C14	8.8598588757E-03 4.9162060056E+00	1.6006065607E-05 -6.0920591945E-03	2.5421124670E+00	2.7677996812E-03
H15	2.4821167401E-01 2.3597129958E+00	2.3379663450E-03 -1.8794770437E-03	3.2831552632E+01	2.4633219697E-01
H16	1.8637131560E-01 3.1650958609E+00	1.4203491128E-03 -2.8164934514E-03	3.1543657953E+01	1.8355482215E-01
C17	1.2294730074E-01 1.4344125843E+01	1.0858970006E-03 -8.8897678919E-02	3.9678088003E+00	3.4049621825E-02
H18	1.5921780434E-01 1.6425056353E+01	9.0961774913E-04 -6.9983411466E-02	2.0004045334E+01	8.9234392872E-02
H19	1.5868296454E-01 1.6516274384E+01	9.0618676916E-04 -6.9882170702E-02	1.9862712126E+01	8.8800793837E-02
C20	8.4624901298E-03 4.7442925564E+00	1.3707548992E-05 -5.9053826779E-03	2.5574937680E+00	2.5571074518E-03
H21	1.8611771575E-01 3.1388737646E+00	1.4158800003E-03 -2.6800575605E-03	3.1534417929E+01	1.8343765819E-01
H22	2.4843832198E-01 2.4945379277E+00	2.3417447360E-03 -1.9840699391E-03	3.2674046355E+01	2.4645425204E-01

C23	5.0173965425E-03	1.4451510324E-05	1.9562138836E+00	2.9784384037E-03
1.0040974221E+00 -2.0389581388E-03				
H24	1.9914559542E-01	1.4306502317E-03	3.5127675326E+01	1.9391975612E-01
3.0516306013E+00 -5.2258393004E-03				
B25	1.0713584003E-01	2.4694782753E-03	5.4121462603E+00	1.0520343585E-01
5.8691162115E-01 -1.9324041797E-03				

Total	3.3682062081E+00	2.6807539475E-02	4.5022886760E+02	2.6313358697E+00
1.8425794008E+02 -7.3687033837E-01				

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				
C1	7.6327965524E-06	8.4015435073E-03	5.4199953581E-03	4.1284804840E-05
4.6623604028E-04				
H2	8.2358117831E-06	4.4559617874E-03	2.0920424942E-03	5.9348737313E-06
5.2193246183E-04				
H3	2.5682318991E-05	4.4679802774E-03	2.0887966747E-03	5.9223762986E-06
5.1368355196E-04				
C4	2.7052790121E-05	1.4458317977E-03	1.0590819691E-03	1.5951318012E-06
7.7651689519E-06				
H5	1.1431199663E-05	5.4986198790E-03	2.7312527671E-03	9.9905882751E-06
1.4170728210E-03				
C6	3.0763821156E-05	1.0600952414E-03	8.3477262954E-04	1.3188090139E-06
6.0594987226E-06				
H7	6.7735695748E-05	5.8269330191E-03	2.8365835695E-03	1.0982320070E-05
1.4126671588E-03				
H8	2.4069431682E-05	7.4999535211E-03	3.3271605592E-03	1.4932930808E-05
2.3325831461E-03				
C9	6.9741110377E-06	7.9168181902E-03	5.2856903203E-03	3.9312969504E-05
4.3231801918E-04				
H10	1.9985329988E-05	4.4459174647E-03	2.0883801658E-03	5.9299283358E-06
5.1982484561E-04				
H11	3.8276749983E-05	4.4605651115E-03	2.1025082016E-03	5.9986053633E-06
5.1796043010E-04				

C12	3.2246353129E-05	1.6193729540E-03	1.1266051514E-03	1.5699521504E-06
9.8351669534E-06				
H13	2.1782414425E-05	5.5040779828E-03	2.7236461643E-03	9.9346993183E-06
1.4130931041E-03				
C14	6.9947759639E-05	1.0887793979E-03	8.0032938233E-04	1.3572437085E-06
6.4637894226E-06				
H15	9.7105908242E-06	7.5029103780E-03	3.3215869003E-03	1.4854979785E-05
2.3359204477E-03				
H16	1.8120489661E-05	5.8190721705E-03	2.8423571496E-03	1.1057939145E-05
1.4169266074E-03				
C17	4.6300159165E-04	8.5814673888E-03	5.2287684501E-03	3.8452017855E-05
4.4476597413E-04				
H18	9.0166135297E-05	4.4608173689E-03	2.0859817063E-03	5.9208951586E-06
5.1650018480E-04				
H19	4.4755370057E-06	4.4707285327E-03	2.0950627362E-03	5.9369479319E-06
5.1492813041E-04				
C20	1.3345578884E-05	9.9984894738E-04	6.5130285044E-04	7.3904363793E-07
4.4468206923E-06				
H21	2.1405878422E-06	5.8170618088E-03	2.8335416596E-03	1.0960644377E-05
1.4127057363E-03				
H22	9.0340275538E-05	7.5428139314E-03	3.2966439809E-03	1.4708067640E-05
2.3395306496E-03				
C23	7.1741962175E-05	1.5225525331E-03	1.0676526838E-03	1.4353069055E-06
7.3425962318E-06				
H24	2.2207087852E-05	5.5204266812E-03	2.7142184574E-03	9.8486153536E-06
1.4164787582E-03				
B25	6.8865083120E-04	1.9438394824E-02	7.5258922047E-03	7.6835144474E-05
2.4608289628E-03				

Total	2.1405878422E-06	5.8444405924E-03	1.5701311956E-05	2.2447870071E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-4.7953884441E-05	-6.1975753146E-03	2.0884259260E-03	6.1841881641E-06	6.2325117217E-04

H2	-1.4103557550E-05 3.8295836831E-04	-4.2217152034E-03	2.0783105898E-03	5.7854989343E-06
H3	-4.4734257084E-06 3.8937041301E-04	-4.2487466231E-03	2.0675816975E-03	5.7300823065E-06
C4	-1.1102265863E-04 9.8289645083E-06	-2.3626822537E-03	1.6423187633E-03	3.3022030199E-06
H5	-4.3891647158E-05 1.3674009716E-05	-1.7241962470E-03	1.0129047214E-03	1.4713804658E-06
C6	-6.6192388678E-05 9.5411807825E-06	-1.2667081431E-03	5.4729005616E-04	3.8833727779E-07
H7	-3.5797938316E-05 3.2321166985E-06	-8.5894050083E-04	4.6632657859E-04	2.9446230734E-07
H8	-5.5748610739E-05 2.0395158232E-06	-8.2982004362E-04	3.9898621170E-04	2.2011901649E-07
C9	-1.2970493577E-04 6.2440929325E-04	-6.2738462466E-03	2.0661766387E-03	5.9190023340E-06
H10	-2.9737823953E-05 4.0752142822E-04	-4.3321170492E-03	2.1106068214E-03	5.9568687323E-06
H11	-5.3039856380E-05 3.9019031721E-04	-4.2524862433E-03	2.0761278075E-03	5.7580462746E-06
C12	-6.6636085683E-06 5.5715955264E-06	-1.8400595035E-03	1.3100472096E-03	2.3974434263E-06
H13	-5.5712837484E-05 1.2984341476E-05	-1.6924110070E-03	1.0181401135E-03	1.4739911923E-06
C14	-3.1987026774E-06 9.5422761841E-06	-1.2391789904E-03	5.5743336846E-04	4.0541922366E-07
H15	-6.0279201777E-06 2.0458972555E-06	-7.9648543999E-04	4.1808287156E-04	2.3262199953E-07
H16	-3.2929416933E-05 3.4225054549E-06	-8.8986039448E-04	4.6710307437E-04	2.8947606060E-07
C17	-2.0143218293E-05 6.4113102644E-04	-6.1974971423E-03	2.0943774148E-03	6.2874459112E-06
H18	-2.1072224513E-05 3.9311756433E-04	-4.2607714680E-03	2.0751225267E-03	5.7798426677E-06
H19	-2.1727677861E-05 3.9125863875E-04	-4.2311098179E-03	2.0768828867E-03	5.7869891220E-06
C20	-1.2858908791E-06 9.2607283001E-06	-1.2447340900E-03	5.5696365658E-04	4.0260948152E-07

H21	-1.5533496588E-06	-8.5382776164E-04	4.5993460281E-04	2.8225296458E-07
3.1742639734E-06				
H22	-7.1806706395E-06	-7.9536571366E-04	4.3666157057E-04	2.5496714051E-07
2.2140864054E-06				
C23	-2.5044278947E-05	-2.0306377588E-03	1.4780702322E-03	2.9564150265E-06
7.1089140921E-06				
H24	-1.6888944442E-06	-1.7124744057E-03	1.1087226595E-03	1.7113333967E-06
1.4171473413E-05				
B25	-6.9417924297E-04	-3.2924960250E-03	1.7549159366E-03	3.8964630082E-06
8.6493125011E-06				

Total	-1.2858908791E-06	-3.9991239350E-03	7.6676945158E-06	4.3596694038E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	1.8051570010E+01
H2	3.2365882253E+01
H3	3.2318182464E+01
C4	4.4526669527E+00
H5	3.3523088164E+01
C6	8.2741079106E+00
H7	3.1122099224E+01
H8	3.1555137975E+01
C9	1.8168399699E+01
H10	3.2351595133E+01
H11	3.2209249782E+01
C12	4.7977230054E+00
H13	3.3305271836E+01
C14	8.3773789867E+00
H15	3.1559612490E+01
H16	3.1338180172E+01

C17 1.7966870492E+01
 H18 3.2611331911E+01
 H19 3.2339384842E+01
 C20 8.5802047055E+00
 H21 3.1313312958E+01
 H22 3.1611711952E+01
 C23 4.7541014027E+00
 H24 3.3666228926E+01
 B25 5.8715080605E+00

Total 5.8248480131E+02

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
 Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.1661360745E+02	8.8092438241E+01	6.6283689038E+00	7.5243335707E-02	
9.9939903160E+01					
H2	9.0383311823E+01	6.8352285752E+01	1.0075007618E+00	1.4739825461E-02	
9.9069888313E+01					
H3	9.0742060378E+01	6.8395257505E+01	1.0076126922E+00	1.4732201164E-02	
9.9069438612E+01					

C4	1.9999575200E+02 9.9993799930E+01	5.1227838755E+01	5.9581436726E+00	1.1630675464E-01
H5	8.9211782299E+01 9.9053795177E+01	6.7494559340E+01	1.0024106508E+00	1.4851725244E-02
C6	2.0660164702E+02 9.9977420863E+01	5.9364252380E+01	5.9711786586E+00	1.0058542674E-01
H7	8.8835355227E+01 9.9142092199E+01	6.6419657038E+01	1.0061843602E+00	1.5148894244E-02
H8	8.9267285688E+01 9.9128121214E+01	6.7096818187E+01	1.0086478306E+00	1.5032722235E-02
C9	2.1680302715E+02 9.9939672681E+01	8.8047862461E+01	6.6281114054E+00	7.5278504442E-02
H10	9.0891382805E+01 9.9068795428E+01	6.8345077988E+01	1.0075676086E+00	1.4742358020E-02
H11	9.0641107258E+01 9.9070693822E+01	6.8413161386E+01	1.0075310640E+00	1.4727152548E-02
C12	2.0013380477E+02 9.9993551483E+01	5.1273176178E+01	5.9581270575E+00	1.1620358834E-01
H13	8.9299490731E+01 9.9051937858E+01	6.7443104339E+01	1.0024922784E+00	1.4864266529E-02
C14	2.0639925823E+02 9.9977689352E+01	5.9515259840E+01	5.9719137654E+00	1.0034256393E-01
H15	8.9113714653E+01 9.9127547821E+01	6.7055464358E+01	1.0086739935E+00	1.5042383244E-02
H16	8.8353344310E+01 9.9144269991E+01	6.6472949344E+01	1.0061514313E+00	1.5136253787E-02
C17	2.1637701471E+02 9.9939898330E+01	8.7993321294E+01	6.6278754759E+00	7.5322483325E-02
H18	9.0612541964E+01 9.9068279339E+01	6.8365403564E+01	1.0075587856E+00	1.4737845944E-02
H19	9.0630150892E+01 9.9066904517E+01	6.8329528442E+01	1.0074877767E+00	1.4744544557E-02
C20	2.0633235800E+02 9.9976584515E+01	5.9331169732E+01	5.9713392356E+00	1.0064421893E-01
H21	8.9016066540E+01 9.9144490530E+01	6.6501861531E+01	1.0062365778E+00	1.5130953549E-02
H22	8.9081956937E+01 9.9127725908E+01	6.7073094876E+01	1.0086212597E+00	1.5037643060E-02

C23	2.0038499525E+02	5.1463622044E+01	5.9587597960E+00	1.1578586114E-01
9.9992970508E+01				
H24	8.8848275887E+01	6.7462252811E+01	1.0024269178E+00	1.4859078611E-02
9.9052926087E+01				
B25	1.5050038832E+02	2.7370604709E+01	3.0724163993E+00	1.1225241210E-01
9.9958880339E+01				

Total	3.3650696803E+03	1.6369000221E+03	7.3843338359E+01	4.5111697332E-02
9.9788172307E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.7804463372E+02	7.9138649670E+01	6.6225104682E+00	8.3682378911E-02	
9.9851572004E+01					
H2	7.4733425515E+01	5.0945636876E+01	9.9616798078E-01	1.9553548486E-02	
9.7955509652E+01					
H3	7.4497960507E+01	5.0967126216E+01	9.9627473698E-01	1.9547398705E-02	
9.7954680067E+01					
C4	1.6597277954E+02	4.9686095988E+01	5.9571029882E+00	1.1989476874E-01	
9.9976334425E+01					
H5	7.3772827764E+01	5.0060592251E+01	9.9114059877E-01	1.9798818875E-02	
9.7940138389E+01					
C6	1.6920889858E+02	5.5827777048E+01	5.9688572379E+00	1.0691554551E-01	
9.9938552548E+01					
H7	7.3615446342E+01	5.0192252289E+01	9.9562502602E-01	1.9836229311E-02	
9.8101652172E+01					
H8	7.3778539552E+01	5.0428932786E+01	9.9778969272E-01	1.9786056091E-02	
9.8061002666E+01					
C9	1.7791301484E+02	7.9082187141E+01	6.6222698522E+00	8.3739083245E-02	
9.9851592853E+01					
H10	7.4986492648E+01	5.0975442667E+01	9.9625990252E-01	1.9543918609E-02	
9.7956968478E+01					
H11	7.4647428134E+01	5.0986615595E+01	9.9620895950E-01	1.9538636716E-02	
9.7957389440E+01					
C12	1.6607381781E+02	4.9798401184E+01	5.9571380898E+00	1.1962508732E-01	
9.9976953920E+01					

H13	7.3596613908E+01	5.0083644743E+01	9.9126695966E-01	1.9792228875E-02
9.7942812533E+01				
C14	1.6941522456E+02	5.5889210639E+01	5.9695257839E+00	1.0680998561E-01
9.9937711401E+01				
H15	7.3976669963E+01	5.0518908663E+01	9.9792652784E-01	1.9753525051E-02
9.8071339449E+01				
H16	7.3745227665E+01	5.0137930554E+01	9.9551143931E-01	1.9855455307E-02
9.8095825188E+01				
C17	1.7818661397E+02	7.9051929162E+01	6.6220215926E+00	8.3767994820E-02
9.9851629246E+01				
H18	7.4712671597E+01	5.0989745983E+01	9.9625455055E-01	1.9538331312E-02
9.7956789735E+01				
H19	7.4644853848E+01	5.0985301741E+01	9.9619289904E-01	1.9538825211E-02
9.7956272118E+01				
C20	1.6924291547E+02	5.5883086120E+01	5.9690484215E+00	1.0681314931E-01
9.9938230009E+01				
H21	7.3715165958E+01	5.0155645388E+01	9.9559783458E-01	1.9850164959E-02
9.8096255155E+01				
H22	7.3934027336E+01	5.0479233733E+01	9.9782372291E-01	1.9767014059E-02
9.8066539405E+01				
C23	1.6572781061E+02	4.9997023939E+01	5.9577983888E+00	1.1916306051E-01
9.9976837291E+01				
H24	7.3655236881E+01	5.0092379092E+01	9.9120319629E-01	1.9787504891E-02
9.7943875205E+01				
B25	1.2652841502E+02	2.4491139631E+01	3.0705257503E+00	1.2537292248E-01
9.9897369420E+01				

Total	2.7783267117E+03	1.3368448891E+03	7.3648042601E+01	5.5090940768E-02
9.9524259445E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.4991162336E+02	7.2341413009E+01	6.6126951574E+00	9.1409538221E-02	
9.9703580662E+01					
H2	6.2891065672E+01	3.9123924250E+01	9.7914205329E-01	2.5026683086E-02	
9.6281310684E+01					

H3 9.6280298953E+01	6.2832517041E+01	3.9136696540E+01	9.7924498810E-01	2.5021145745E-02
C4 9.9939081018E+01	1.4072782571E+02	4.8184014446E+01	5.9548832391E+00	1.2358628287E-01
H5 9.6281985223E+01	6.1722369745E+01	3.8227440441E+01	9.7436031901E-01	2.5488505319E-02
C6 9.9868504946E+01	1.4190330404E+02	5.2950718876E+01	5.9646736258E+00	1.1264575349E-01
H7 9.6496330574E+01	6.2353143855E+01	3.8854266901E+01	9.7933275854E-01	2.5205282113E-02
H8 9.6450301349E+01	6.2547346700E+01	3.9034941990E+01	9.8140049489E-01	2.5141589685E-02
C9 9.9704504801E+01	1.5001730952E+02	7.2325684984E+01	6.6125148073E+00	9.1426922659E-02
H10 9.6287282118E+01	6.2872649554E+01	3.9158048743E+01	9.7927855248E-01	2.5008359300E-02
H11 9.6288687193E+01	6.2720751385E+01	3.9172231940E+01	9.7923855902E-01	2.4998283491E-02
C12 9.9936955556E+01	1.4106009300E+02	4.8183274821E+01	5.9547547828E+00	1.2358551396E-01
H13 9.6287511965E+01	6.1492091601E+01	3.8254141790E+01	9.7451386958E-01	2.5474728329E-02
C14 9.9866953683E+01	1.4201941294E+02	5.2996356710E+01	5.9652992510E+00	1.1256055362E-01
H15 9.6450890013E+01	6.2556419837E+01	3.9027670568E+01	9.8143761794E-01	2.5147225127E-02
H16 9.6494627014E+01	6.2567038443E+01	3.8849524642E+01	9.7926190885E-01	2.5206535160E-02
C17 9.9704632582E+01	1.4979414715E+02	7.2301015819E+01	6.6122729777E+00	9.1454772839E-02
H18 9.6276792886E+01	6.3126972449E+01	3.9119863783E+01	9.7916839950E-01	2.5029954218E-02
H19 9.6285489146E+01	6.2855247030E+01	3.9163103692E+01	9.7920141808E-01	2.5003161797E-02
C20 9.9866829585E+01	1.4219376963E+02	5.2951785568E+01	5.9647838614E+00	1.1264556610E-01
H21 9.6496595754E+01	6.2529832706E+01	3.8867046525E+01	9.7936258245E-01	2.5197761857E-02

H22	6.2601210326E+01	3.9020759151E+01	9.8135875721E-01	2.5149658247E-02
	9.6448355581E+01			
C23	1.4103641395E+02	4.8309649162E+01	5.9553117964E+00	1.2327375379E-01
	9.9935110192E+01			
H24	6.1868881814E+01	3.8266160822E+01	9.7446574827E-01	2.5465469421E-02
	9.6289995833E+01			
B25	1.0830294198E+02	2.2309259966E+01	3.0673834996E+00	1.3749373597E-01
	9.9795138531E+01			

Total	2.3445043794E+03	1.1261289951E+03	7.3345341026E+01	6.5130496899E-02
	9.9115203766E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	H2	1.6956118147E-02		
C1	H3	1.7073716147E-02		
C1	C4	-2.4222486249E-02		
C1	B25	-6.4216033547E-01		
C1		-6.3235298742E-01	-6.3235473940E-01	
H2	C1	-1.6957870124E-02		
H2		-1.6957870124E-02	-1.6959622100E-02	
H3	C1	-1.7075468124E-02		
H3		-1.7075468124E-02	-1.7077220100E-02	
C4	C1	2.4220734272E-02		
C4	H5	1.1982608247E-02		
C4	C6	2.5040576548E-03		
C4	C20	2.7812472016E-03		
C4		4.1488647376E-02	4.1486895400E-02	

H5	C4	-1.1984360224E-02
H5		-1.1984360224E-02 -1.1986112200E-02
C6	C4	-2.5058096311E-03
C6	H7	1.4887686947E-02
C6	H8	1.7515862147E-02
C6	C12	-2.4231911876E-03
C6		2.7474548276E-02 2.7472796300E-02
H7	C6	-1.4889438924E-02
H7		-1.4889438924E-02 -1.4891190900E-02
H8	C6	-1.7517614124E-02
H8		-1.7517614124E-02 -1.7519366100E-02
C9	B25	-6.4212037941E-01
C9	C12	-2.4003497608E-02
C9	H10	1.7034811947E-02
C9	H11	1.6978436047E-02
C9		-6.3211062902E-01 -6.3211238100E-01
H10	C9	-1.7036563924E-02
H10		-1.7036563924E-02 -1.7038315900E-02
H11	C9	-1.6980188024E-02
H11		-1.6980188024E-02 -1.6981940000E-02
C12	C6	2.4214392113E-03
C12	C9	2.4001902556E-02
C12	H13	1.2083992847E-02
C12	C14	2.9831242619E-03
C12		4.1490458876E-02 4.1488706900E-02
H13	C12	-1.2085744824E-02
H13		-1.2085744824E-02 -1.2087496800E-02
C14	C12	-2.9848762382E-03
C14	H15	1.7548141047E-02
C14	H16	1.4832180847E-02
C14	C23	-2.6401290805E-03
C14		2.6755316576E-02 2.6753564600E-02

H15	C14	-1.7549893024E-02
H15		-1.7549893024E-02 -1.7551645000E-02
H16	C14	-1.4833932824E-02
H16		-1.4833932824E-02 -1.4835684800E-02
C17	B25	-6.4204582230E-01
C17	C23	-2.3818605717E-02
C17	H18	1.7031204147E-02
C17	H19	1.6973640547E-02
C17		-6.3185958332E-01 -6.3186133530E-01
H18	C17	-1.7032956124E-02
H18		-1.7032956124E-02 -1.7034708100E-02
H19	C17	-1.6975392524E-02
H19		-1.6975392524E-02 -1.6977144500E-02
C20	C4	-2.7831404943E-03
C20	C23	-2.3618084244E-03
C20	H21	1.4915804647E-02
C20	H22	1.7493115147E-02
C20		2.7263970876E-02 2.7262218900E-02
H21	C20	-1.4917556624E-02
H21		-1.4917556624E-02 -1.4919308600E-02
H22	C20	-1.7494867124E-02
H22		-1.7494867124E-02 -1.7496619100E-02
C23	C14	2.6383771042E-03
C23	C17	2.3816853741E-02
C23	C20	2.3599151835E-03
C23	H24	1.2007909947E-02
C23		4.0823055976E-02 4.0821304000E-02
H24	C23	-1.2009661924E-02
H24		-1.2009661924E-02 -1.2011413900E-02
B25	C1	6.4215858349E-01
B25	C9	6.4211881196E-01
B25	C17	6.4204407033E-01

B25 1.9263214658E+00 1.9263197138E+00

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	3.4817377688E-01	-4.5342440194E-01	-1.0525062506E-01
H2	-1.4072058376E-01	-1.2178771175E-02	-1.5289935493E-01
H3	8.0905631223E-02	7.6025778325E-03	8.8508209056E-02
C4	-1.2768193686E-02	-4.0919605169E-03	-1.6860154203E-02
H5	-4.9565048982E-02	-3.0392462293E-03	-5.2604295211E-02
C6	-3.9679549367E-02	-2.2052124720E-02	-6.1731674087E-02
H7	-1.4616181998E-01	-1.0646372869E-02	-1.5680819285E-01
H8	-1.2916060467E-02	-4.9021446761E-04	-1.3406274935E-02
C9	6.0794694442E-01	-7.9381878686E-01	-1.8587184244E-01
H10	3.9942526514E-02	4.1879655936E-03	4.4130492108E-02
H11	-1.4463221802E-01	-1.2281783027E-02	-1.5691400105E-01
C12	-2.2945318678E-02	-7.2022088840E-03	-3.0147527562E-02
H13	-8.6950046083E-02	-5.3736065504E-03	-9.2323652633E-02
C14	1.3696774589E-02	8.5125055834E-03	2.2209280172E-02
H15	4.5164446048E-03	1.6659726453E-04	4.6830418693E-03
H16	5.3087958057E-02	3.8536089524E-03	5.6941567009E-02
C17	-9.5371874492E-01	1.2454038606E+00	2.9168511564E-01
H18	1.0081611838E-01	8.0520369279E-03	1.0886815531E-01
H19	6.3836831508E-02	4.7280432657E-03	6.8564874774E-02
C20	2.5488902748E-02	1.4513092570E-02	4.0001995318E-02
H21	9.3140529725E-02	6.7914908667E-03	9.9932020592E-02

H22	7.9923767456E-03	2.9902308684E-04	8.2913998324E-03
C23	3.6492274894E-02	1.2343403713E-02	4.8835678607E-02
H24	1.3628986394E-01	8.3847402678E-03	1.4467460421E-01
B25	-1.3338527976E-03	-4.6223080862E-04	-1.7960836062E-03

Total	9.3551748780E-04	-2.2276157225E-04	7.1275591555E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	9.0153838038E-01	-1.1773604963E+00	-2.7582211590E-01
H2	-3.5020847804E-02	-2.2070482106E-03	-3.7227896015E-02
H3	-1.2033287138E-01	-9.8756051911E-03	-1.3020847657E-01
C4	-3.3628581986E-02	-1.1563346575E-02	-4.5191928561E-02
H5	-1.2896769344E-01	-7.9146647449E-03	-1.3688235818E-01
C6	-6.0336653045E-03	-3.4053866143E-03	-9.4390519188E-03
H7	-2.3059543961E-02	-1.6808419707E-03	-2.4740385932E-02
H8	-2.1712625376E-03	-8.9864989723E-05	-2.2611275273E-03
C9	-7.5049209121E-01	9.7986792046E-01	2.2937582925E-01
H10	1.3954993892E-01	1.1722085719E-02	1.5127202464E-01
H11	-9.8952947916E-03	-1.6339870825E-03	-1.1529281874E-02
C12	2.8044381903E-02	1.0061601315E-02	3.8105983218E-02
H13	1.0719805178E-01	6.6421355669E-03	1.1384018735E-01
C14	3.7732330916E-02	2.1017319299E-02	5.8749650215E-02
H15	1.1876335649E-02	4.3079324384E-04	1.2307128893E-02
H16	1.3818935659E-01	1.0034316177E-02	1.4822367277E-01
C17	-1.4986485994E-01	1.9597383848E-01	4.6108978545E-02
H18	-1.0424809280E-01	-9.4751691713E-03	-1.1372326197E-01
H19	1.3036532720E-01	1.1462135757E-02	1.4182746296E-01
C20	-3.1224314697E-02	-1.7181575390E-02	-4.8405890087E-02
H21	-1.1498218758E-01	-8.3996272582E-03	-1.2338181484E-01
H22	-1.0223849430E-02	-3.8832691319E-04	-1.0612176343E-02
C23	4.1032021385E-03	2.3115649267E-03	6.4147670652E-03

H24 2.1496193935E-02 1.3213610427E-03 2.2817554978E-02
B25 7.0410940136E-04 -4.7024245222E-04 2.3386694914E-04

Total 6.5245195116E-04 -8.0111084681E-04 -1.4865889565E-04

Atom A Mu_Intra_Z(A) Mu_Bond_Z(A) Mu_Z(A)

C1 -4.2096193146E-01 2.3504505026E-01 -1.8591688120E-01
H2 -5.5670009901E-02 -4.0439640625E-03 -5.9713973963E-02
H3 -5.5712683382E-02 -4.0719708259E-03 -5.9784654208E-02
C4 8.9149984875E-03 -2.7984351566E-02 -1.9069353078E-02
H5 6.3191974197E-02 3.3385442983E-03 6.6530518495E-02
C6 2.8792116305E-02 1.8786764451E-02 4.7578880756E-02
H7 -3.8912558091E-02 -3.6239309415E-03 -4.2536489032E-02
H8 1.5312753122E-01 1.3401469856E-02 1.6652900108E-01
C9 -4.2324646461E-01 2.3772769746E-01 -1.8551876715E-01
H10 -5.5304392041E-02 -4.0234955614E-03 -5.9327887602E-02
H11 -5.5761575844E-02 -4.0586878734E-03 -5.9820263717E-02
C12 9.0075674017E-03 -2.7518958844E-02 -1.8511391442E-02
H13 6.3513274504E-02 3.3840993784E-03 6.6897373882E-02
C14 2.9086394734E-02 1.9244211816E-02 4.8330606550E-02
H15 1.5318487555E-01 1.3427220029E-02 1.6661209558E-01
H16 -3.8571107195E-02 -3.5777251620E-03 -4.2148832357E-02
C17 -4.2431799959E-01 2.3880705590E-01 -1.8551094369E-01
H18 -5.5585445987E-02 -4.0572256889E-03 -5.9642671676E-02
H19 -5.5347357167E-02 -4.0195318245E-03 -5.9366888992E-02
C20 2.9014467515E-02 1.8863781573E-02 4.7878249088E-02
H21 -3.8859557669E-02 -3.6231005033E-03 -4.2482658172E-02
H22 1.5313613362E-01 1.3384012694E-02 1.6652014631E-01
C23 8.6562636256E-03 -2.7455603586E-02 -1.8799339961E-02
H24 6.3643131270E-02 3.3660415425E-03 6.7009172813E-02
B25 -1.8562228299E-01 2.1576877967E-01 3.0146496683E-02

Total -1.1406046375E+00 9.1648618249E-01 -2.2411845501E-01

Atom A |Mu_Intra(A)| |Mu_Bond(A)| |Mu(A)|

C1	1.0541372671E+00	1.2833618360E+00	3.4888482399E-01
H2	1.5533155661E-01	1.3021028165E-02	1.6831484684E-01
H3	1.5533713075E-01	1.3111358206E-02	1.6841067460E-01
C4	3.7059216053E-02	3.0554525973E-02	5.1867286738E-02
H5	1.5192954168E-01	9.1117953060E-03	1.6102888483E-01
C6	4.9394915895E-02	2.9169082625E-02	7.8508885998E-02
H7	1.5300067766E-01	1.1371163549E-02	1.6434795082E-01
H8	1.5368662862E-01	1.3410733769E-02	1.6708306050E-01
C9	1.0545024590E+00	1.2832785614E+00	3.4868155361E-01
H10	1.5533243916E-01	1.3081852542E-02	1.6837613851E-01
H11	1.5532465576E-01	1.3037831697E-02	1.6832525662E-01
C12	3.7337799561E-02	3.0172847557E-02	5.1996259368E-02
H13	1.5193968823E-01	9.1894363728E-03	1.6111642909E-01
C14	4.9571653080E-02	2.9741051599E-02	7.9250369435E-02
H15	1.5371093558E-01	1.3435161896E-02	1.6713164481E-01
H16	1.5297829871E-01	1.1328632770E-02	1.6428366715E-01
C17	1.0545542591E+00	1.2831466523E+00	3.4874138673E-01
H18	1.5531032285E-01	1.3079572233E-02	1.6835232056E-01
H19	1.5534989391E-01	1.3034246634E-02	1.6834666260E-01
C20	4.9663682070E-02	2.9354363288E-02	7.8965920245E-02
H21	1.5299061069E-01	1.1393197248E-02	1.6436014486E-01
H22	1.5368500448E-01	1.3392983551E-02	1.6706383429E-01
C23	3.7728680002E-02	3.0191275494E-02	5.2720849049E-02
H24	1.5194558738E-01	9.1312704499E-03	1.6106399709E-01
B25	1.8562841075E-01	2.1576978720E-01	3.0200858802E-02

Total 1.1406052078E+00 9.1648655969E-01 2.2411963769E-01

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

C1	H2	-2.0686863227E-02	
C1	H3	1.2936441198E-02	
C1	C4	-6.6073786763E-04	
C1	B25	-4.4501324204E-01	
C1		-4.5342440194E-01	
H2	C1	-1.2178771175E-02	
H2		-1.2178771175E-02	
H3	C1	7.6025778325E-03	
H3		7.6025778325E-03	
C4	C1	-5.0881752298E-04	
C4	H5	-5.2287222945E-03	
C4	C6	-2.1392842752E-03	
C4	C20	3.7848635757E-03	
C4		-4.0919605169E-03	
H5	C4	-3.0392462293E-03	
H5		-3.0392462293E-03	
C6	C4	-2.1594713973E-03	
C6	H7	-1.8133318243E-02	
C6	H8	-5.7393965022E-04	
C6	C12	-1.1853954290E-03	
C6		-2.2052124720E-02	
H7	C6	-1.0646372869E-02	
H7		-1.0646372869E-02	

H8	C6	-4.9021446761E-04
H8		-4.9021446761E-04
C9	B25	-7.7897929686E-01
C9	C12	-1.1344865638E-03
C9	H10	7.1438206370E-03
C9	H11	-2.0848824075E-02
C9		-7.9381878686E-01
H10	C9	4.1879655936E-03
H10		4.1879655936E-03
H11	C9	-1.2281783027E-02
H11		-1.2281783027E-02
C12	C6	-1.1566433147E-03
C12	C9	-8.7839773280E-04
C12	H13	-9.2444724994E-03
C12	C14	4.0773046628E-03
C12		-7.2022088840E-03
H13	C12	-5.3736065504E-03
H13		-5.3736065504E-03
C14	C12	4.0531277305E-03
C14	H15	1.8840071184E-04
C14	H16	6.5636540981E-03
C14	C23	-2.2926769571E-03
C14		8.5125055834E-03
H15	C14	1.6659726453E-04
H15		1.6659726453E-04
H16	C14	3.8536089524E-03
H16		3.8536089524E-03
C17	B25	1.2218910150E+00
C17	C23	1.8756775364E-03
C17	H18	1.3643277085E-02
C17	H19	7.9938909127E-03
C17		1.2454038606E+00

H18	C17	8.0520369279E-03
H18		8.0520369279E-03
H19	C17	4.7280432657E-03
H19		4.7280432657E-03
C20	C4	3.7753071078E-03
C20	C23	-1.1743286323E-03
C20	H21	1.1569681410E-02
C20	H22	3.4243268386E-04
C20		1.4513092570E-02
H21	C20	6.7914908667E-03
H21		6.7914908667E-03
H22	C20	2.9902308684E-04
H22		2.9902308684E-04
C23	C14	-2.3332888113E-03
C23	C17	1.4669536464E-03
C23	C20	-1.2121060773E-03
C23	H24	1.4421844955E-02
C23		1.2343403713E-02
H24	C23	8.3847402678E-03
H24		8.3847402678E-03
B25	C1	-2.2616568268E-01
B25	C9	-3.9611447823E-01
B25	C17	6.2181793010E-01
B25		-4.6223080862E-04

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	H2	-3.7118127181E-03	
C1	H3	-1.6746135726E-02	
C1	C4	-1.7054940494E-03	
C1	B25	-1.1551970538E+00	
C1		-1.1773604963E+00	

H2	C1	-2.2070482106E-03
H2		-2.2070482106E-03
H3	C1	-9.8756051911E-03
H3		-9.8756051911E-03
C4	C1	-1.3160227624E-03
C4	H5	-1.3614568009E-02
C4	C6	2.7161829419E-03
C4	C20	6.5106125507E-04
C4		-1.1563346575E-02
H5	C4	-7.9146647449E-03
H5		-7.9146647449E-03
C6	C4	2.6812182071E-03
C6	H7	-2.8627338087E-03
C6	H8	-1.1121506034E-04
C6	C12	-3.1126559524E-03
C6		-3.4053866143E-03
H7	C6	-1.6808419707E-03
H7		-1.6808419707E-03
H8	C6	-8.9864989723E-05
H8		-8.9864989723E-05
C9	B25	9.6127378221E-01
C9	C12	1.5167034110E-03
C9	H10	1.9889986402E-02
C9	H11	-2.8125515579E-03
C9		9.7986792046E-01
H10	C9	1.1722085719E-02
H10		1.1722085719E-02
H11	C9	-1.6339870825E-03
H11		-1.6339870825E-03
C12	C6	-3.1390962926E-03
C12	C9	1.1925679627E-03
C12	H13	1.1422927669E-02

C12	C14	5.8520197662E-04
C12		1.0061601315E-02
H13	C12	6.6421355669E-03
H13		6.6421355669E-03
C14	C12	6.2717018180E-04
C14	H15	4.8698279299E-04
C14	H16	1.7091804938E-02
C14	C23	2.8113613863E-03
C14		2.1017319299E-02
H15	C14	4.3079324384E-04
H15		4.3079324384E-04
H16	C14	1.0034316177E-02
H16		1.0034316177E-02
C17	B25	1.9227844859E-01
C17	C23	3.3164033373E-04
C17	H18	-1.6112117228E-02
C17	H19	1.9475866787E-02
C17		1.9597383848E-01
H18	C17	-9.4751691713E-03
H18		-9.4751691713E-03
H19	C17	1.1462135757E-02
H19		1.1462135757E-02
C20	C4	6.0670276462E-04
C20	C23	-3.0269267776E-03
C20	H21	-1.4304911916E-02
C20	H22	-4.5643946116E-04
C20		-1.7181575390E-02
H21	C20	-8.3996272582E-03
H21		-8.3996272582E-03
H22	C20	-3.8832691319E-04
H22		-3.8832691319E-04
C23	C14	2.7987561313E-03

C23	C17	2.6660721825E-04
C23	C20	-3.0267414431E-03
C23	H24	2.2729430203E-03
C23		2.3115649267E-03
H24	C23	1.3213610427E-03
H24		1.3213610427E-03
B25	C1	-5.8771620015E-01
B25	C9	4.8933382356E-01
B25	C17	9.7912134141E-02
B25		-4.7024245222E-04

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	H2	-6.5375752237E-03	
C1	H3	-6.5828909541E-03	
C1	C4	-3.5777427622E-02	
C1	B25	2.8394294406E-01	
C1		2.3504505026E-01	
H2	C1	-4.0439640625E-03	
H2		-4.0439640625E-03	
H3	C1	-4.0719708259E-03	
H3		-4.0719708259E-03	
C4	C1	-3.6132072023E-02	
C4	H5	5.7287238865E-03	
C4	C6	1.1451381747E-03	
C4	C20	1.2738583964E-03	
C4		-2.7984351566E-02	
H5	C4	3.3385442983E-03	
H5		3.3385442983E-03	
C6	C4	1.1788267870E-03	
C6	H7	-6.3805455869E-03	
C6	H8	2.2853841452E-02	

C6	C12	1.1346417985E-03
C6		1.8786764451E-02
H7	C6	-3.6239309415E-03
H7		-3.6239309415E-03
H8	C6	1.3401469856E-02
H8		1.3401469856E-02
C9	B25	2.8623377867E-01
C9	C12	-3.5440786841E-02
C9	H10	-6.5024545824E-03
C9	H11	-6.5628397868E-03
C9		2.3772769746E-01
H10	C9	-4.0234955614E-03
H10		-4.0234955614E-03
H11	C9	-4.0586878734E-03
H11		-4.0586878734E-03
C12	C6	1.1016292450E-03
C12	C9	-3.5794215177E-02
C12	H13	5.8075467184E-03
C12	C14	1.3660803696E-03
C12		-2.7518958844E-02
H13	C12	3.3840993784E-03
H13		3.3840993784E-03
C14	C12	1.4067241547E-03
C14	H15	2.2897058780E-02
C14	H16	-6.3025601865E-03
C14	C23	1.2429890672E-03
C14		1.9244211816E-02
H15	C14	1.3427220029E-02
H15		1.3427220029E-02
H16	C14	-3.5777251620E-03
H16		-3.5777251620E-03
C17	B25	2.8702679041E-01

C17	C23	-3.5164749290E-02
C17	H18	-6.5581679041E-03
C17	H19	-6.4968173213E-03
C17		2.3880705590E-01
H18	C17	-4.0572256889E-03
H18		-4.0572256889E-03
H19	C17	-4.0195318245E-03
H19		-4.0195318245E-03
C20	C4	1.3113872656E-03
C20	C23	1.1065971857E-03
C20	H21	-6.3786701909E-03
C20	H22	2.2824467312E-02
C20		1.8863781573E-02
H21	C20	-3.6231005033E-03
H21		-3.6231005033E-03
H22	C20	1.3384012694E-02
H22		1.3384012694E-02
C23	C14	1.2067406231E-03
C23	C17	-3.5514920903E-02
C23	C20	1.0739385425E-03
C23	H24	5.7786381514E-03
C23		-2.7455603586E-02
H24	C23	3.3660415425E-03
H24		3.3660415425E-03
B25	C1	7.1073989816E-02
B25	C9	7.2346843606E-02
B25	C17	7.2347946251E-02
B25		2.1576877967E-01

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	H2	2.2010537332E-02	

C1	H3	2.2161205426E-02
C1	C4	3.5824148443E-02
C1	B25	1.2700947264E+00
C1		1.2833618360E+00
H2	C1	1.3021028165E-02
H2		1.3021028165E-02
H3	C1	1.3111358206E-02
H3		1.3111358206E-02
C4	C1	3.6159610616E-02
C4	H5	1.5668895184E-02
C4	C6	3.6421873130E-03
C4	C20	4.0462066505E-03
C4		3.0554525973E-02
H5	C4	9.1117953060E-03
H5		9.1117953060E-03
C6	C4	3.6389394586E-03
C6	H7	1.9435118661E-02
C6	H8	2.2861317649E-02
C6	C12	3.5186931398E-03
C6		2.9169082625E-02
H7	C6	1.1371163549E-02
H7		1.1371163549E-02
H8	C6	1.3410733769E-02
H8		1.3410733769E-02
C9	B25	1.2699550407E+00
C9	C12	3.5491362624E-02
C9	H10	2.2111708391E-02
C9	H11	2.2037576492E-02
C9		1.2832785614E+00
H10	C9	1.3081852542E-02
H10		1.3081852542E-02
H11	C9	1.3037831697E-02

H11		1.3037831697E-02
C12	C6	3.5221209923E-03
C12	C9	3.5824846700E-02
C12	H13	1.5800985640E-02
C12	C14	4.3397062392E-03
C12		3.0172847557E-02
H13	C12	9.1894363728E-03
H13		9.1894363728E-03
C14	C12	4.3359035603E-03
C14	H15	2.2903011764E-02
C14	H16	1.9363202629E-02
C14	C23	3.8347284513E-03
C14		2.9741051599E-02
H15	C14	1.3435161896E-02
H15		1.3435161896E-02
H16	C14	1.1328632770E-02
H16		1.1328632770E-02
C17	B25	1.2697925156E+00
C17	C23	3.5216299410E-02
C17	H18	2.2107666033E-02
C17	H19	2.2032256224E-02
C17		1.2831466523E+00
H18	C17	1.3079572233E-02
H18		1.3079572233E-02
H19	C17	1.3034246634E-02
H19		1.3034246634E-02
C20	C4	4.0423716508E-03
C20	C23	3.4301444263E-03
C20	H21	1.9472428360E-02
C20	H22	2.2831598832E-02
C20		2.9354363288E-02
H21	C20	1.1393197248E-02

H21		1.1393197248E-02
H22	C20	1.3392983551E-02
H22		1.3392983551E-02
C23	C14	3.8384235685E-03
C23	C17	3.5546204287E-02
C23	C20	3.4327407271E-03
C23	H24	1.5701864245E-02
C23		3.0191275494E-02
H24	C23	9.1312704499E-03
H24		9.1312704499E-03
B25	C1	6.3372924816E-01
B25	C9	6.3370997824E-01
B25	C17	6.3362334990E-01
B25		2.1576978720E-01

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	1.3633114353E+00	-1.2831316764E+00	6.1693741587E-01	-1.4680355437E+00	1.6025739389E+00	1.0472410837E-01
H2	3.4178941639E-01	7.5000669637E-02	1.5633010511E-01	-1.8273340284E-01	3.7890328383E-02	-1.5905601354E-01

H3 3.0756377661E-02 -2.6855333235E-01 -9.0622902437E-02 1.2827828912E-01 1.3306274401E-01 -1.5903466678E-01

C4 -1.3870270046E-02 -5.2145762012E-03 -4.7832596640E-03 -4.8158336491E-03 -2.1988078803E-02 1.8686103695E-02

H5 -1.2202125585E-01 1.6458118600E-01 -6.4225243404E-02 2.4342733834E-01 -1.6730474006E-01 -1.2140608248E-01

C6 -6.4054587638E-03 1.0056397181E-03 1.5960045056E-02 -1.5091604426E-03 4.1893679857E-03 7.9146192064E-03

H7 2.9056956179E-01 7.4434416307E-02 1.9263627049E-01 -1.6925558648E-01 3.0584556118E-02 -1.2131397531E-01

H8 -1.9830076362E-01 -2.3742584788E-03 4.8552032947E-04 -1.8351310555E-01 -4.4681494880E-04 3.8181386917E-01

C9 3.4369056329E-01 1.8669886453E+00 1.0872878326E+00 -4.4089803612E-01 -1.3329543460E+00 9.7207472829E-02

H10 -1.1715873001E-01 1.8945900533E-01 -4.4483262796E-02 2.7707303248E-01 -1.5285986243E-01 -1.5991430247E-01

H11 3.3609677055E-01 9.1860778765E-02 1.6106067606E-01 -1.7721584642E-01 1.2061407474E-02 -1.5888092413E-01

C12 -1.3760124725E-02 -7.2975971327E-04 -1.4623933038E-02 -7.9210893013E-03 1.8515843398E-02 2.1681214026E-02

H13 8.9030495971E-03 -2.4019286084E-01 -1.1320368441E-01 1.1168631726E-01 1.3995501599E-01 -1.2058936686E-01

C14 -2.7021573146E-03 1.6335797574E-03 -4.6406219383E-03 -1.4826001915E-03 -1.4390204963E-02 4.1847575060E-03

H15 -1.8514618563E-01 -5.3163940130E-03 -6.6141445487E-04 -1.9656111488E-01 -2.0295502908E-03 3.8170730050E-01

H16 -1.1870226526E-01 1.6217227382E-01 -6.9308712742E-02 2.4133723120E-01 -1.8091736682E-01 -1.2263496594E-01

C17 -1.8617818151E+00 -5.8421335949E-01 -1.7027388548E+00 1.7680564437E+00 -2.6622612385E-01 9.3725371349E-02

H18 1.4322785671E-02 -2.6504324159E-01 -1.1114986875E-01 1.4483711773E-01 1.1629790099E-01 -1.5915990340E-01

H19 -1.2849267499E-01 1.7672622570E-01 -6.9524268344E-02 2.8815663971E-01 -1.4394668156E-01 -1.5966396472E-01

C20 -3.1126322839E-03 7.6799622973E-04 -1.0842051889E-02 -3.0235574339E-03 1.1659416658E-02 6.1361897179E-03

H21 1.0251157787E-02 -2.3652611771E-01 -1.2234142904E-01 1.1160975017E-01 1.5145847190E-01 -1.2186090796E-01

H22 -1.8943523973E-01 7.5806710152E-03 -7.9979395217E-04 -1.9236562644E-01 3.5345325276E-04 3.8180086616E-01

C23 -8.6153801568E-03 8.0336906034E-03 2.8072298530E-02 -1.6952896961E-02 -2.8745657042E-03 2.5568277118E-02

H24 2.9385444766E-01 7.5526443585E-02 1.7787275161E-01 -1.7349075682E-01 2.7959954695E-02 -1.2036369084E-01

B25 2.1746326527E-01 -5.5367562245E-03 -2.5174843859E-03 2.3038648043E-01 2.4167892484E-03 -4.4784974569E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
C1	1	-2.9335683699E+00	3.1320833658E-01	8.1227814484E-01	-4.9204141422E-01
C1	2	1.0752855884E+00	1.7830411168E-01	4.5859985353E-01	8.7057097247E-01
C1	3	1.8582827814E+00	9.3279589496E-01	-3.6040309344E-01	-1.1952357734E-03
H2	1	-2.1545832764E-01	-1.4315061579E-01	-5.9105101452E-01	7.9383033416E-01
H2	2	-1.8285356027E-01	-2.7498246292E-01	7.9426259241E-01	5.4178554741E-01
H2	3	3.9831188791E-01	9.5073263659E-01	1.4073248569E-01	2.7622784289E-01
H3	1	-2.1544047795E-01	-2.9103826744E-01	-5.3455515864E-01	7.9344029974E-01
H3	2	-1.8309722385E-01	7.3682420278E-01	4.0375203558E-01	5.4228626017E-01
H3	3	3.9853770180E-01	-6.1023505397E-01	7.4245206992E-01	2.7636588570E-01
C4	1	-2.3178533822E-02	5.9872068574E-01	6.7891228578E-01	4.2498429227E-01
C4	2	-8.7328201599E-03	-8.0033016892E-01	5.2809567768E-01	2.8387774819E-01
C4	3	3.1911353982E-02	-3.1704276923E-02	-5.1009123049E-01	8.5953579065E-01
H5	1	-1.8652992138E-01	-1.1425210367E-01	-3.2197215096E-01	-9.3982997974E-01
H5	2	-1.8521378615E-01	9.3458834324E-01	-3.5563611405E-01	8.2208915252E-03
H5	3	3.7174370753E-01	3.3688437999E-01	8.7741488954E-01	-3.4154359331E-01

C6	1	-1.6875729875E-02	8.2951614856E-01	9.5719147757E-02	-5.5021886921E-01
C6	2	-2.1765965015E-03	-1.8617215176E-01	9.7624481076E-01	-1.1084222739E-01
C6	3	1.9052326376E-02	5.2653859230E-01	1.9438084838E-01	8.2763107518E-01
H7	1	-1.9744075479E-01	-3.5755552134E-01	-6.6546529455E-02	9.3151790567E-01
H7	2	-1.8100286721E-01	-1.5959587844E-01	9.8713899701E-01	9.2604627028E-03
H7	3	3.7844362200E-01	9.2015390275E-01	1.4535528887E-01	3.6357755053E-01
H8	1	-1.9867290656E-01	9.8795984645E-01	1.5470889307E-01	-7.0724840114E-04
H8	2	-1.8314172526E-01	-1.5470822823E-01	9.8795978063E-01	9.1431821160E-04
H8	3	3.8181463182E-01	8.4018613367E-04	-7.9389253288E-04	9.9999933191E-01
C9	1	-2.9328833695E+00	-5.4839859473E-01	6.7493062834E-01	4.9368778415E-01
C9	2	1.0737116710E+00	3.0758995059E-01	-3.8617807180E-01	8.6962918486E-01
C9	3	1.8591716986E+00	7.7759076872E-01	6.2875682405E-01	4.1776332677E-03
H10	1	-2.1543282095E-01	4.4637383592E-01	-4.1738521971E-01	-7.9154278278E-01
H10	2	-1.8291264243E-01	8.2248365697E-01	-1.5710092445E-01	5.4666254084E-01
H10	3	3.9834546338E-01	3.5252096763E-01	8.9504685794E-01	-2.7316677960E-01
H11	1	-2.1542889354E-01	-3.1824227406E-01	5.1349748816E-01	7.9689534109E-01
H11	2	-1.8301229297E-01	1.7238741307E-02	8.4359411961E-01	-5.3670456226E-01
H11	3	3.9844118650E-01	9.4785266830E-01	1.5706460776E-01	2.7731936137E-01
C12	1	-2.2684423302E-02	7.0645959207E-01	-5.3954711035E-01	4.5804340459E-01
C12	2	-1.1730954429E-02	6.5301042093E-01	7.4647783820E-01	-1.2786018631E-01
C12	3	3.4415377731E-02	-2.7293265641E-01	3.8943517149E-01	8.7968631470E-01
H13	1	-1.8640451118E-01	2.2957232512E-01	-2.5590429876E-01	9.3904714334E-01
H13	2	-1.8533419858E-01	-7.7364110124E-01	-6.3340862162E-01	1.6521638329E-02
H13	3	3.7173870976E-01	-5.9057259843E-01	7.3027837702E-01	3.4339117352E-01
C14	1	-1.3594827723E-02	-1.6344275721E-01	-7.4555710039E-01	-6.4608906133E-01
C14	2	-3.5066350764E-03	9.5977733425E-01	-2.7170502979E-01	7.0737864316E-02
C14	3	1.7101462799E-02	-2.2828476466E-01	-6.0854004539E-01	7.5997702556E-01
H15	1	-1.9866142179E-01	3.6621327816E-01	9.3052369973E-01	3.6713959923E-03
H15	2	-1.8305373061E-01	9.3053025152E-01	-3.6621496393E-01	-2.2626477471E-04
H15	3	3.8171515240E-01	-1.1339754156E-03	-3.4992062010E-03	9.9999323480E-01
H16	1	-1.9753414642E-01	1.2115911272E-01	3.3971564290E-01	9.3269167005E-01
H16	2	-1.8097645993E-01	9.3465510614E-01	-3.5546436552E-01	8.0571343588E-03

H16	3	3.7851060634E-01	3.3427578730E-01	8.7076883661E-01	-3.6058470740E-01
C17	1	-2.9343709997E+00	8.5859908918E-01	1.3467335411E-01	4.9464198340E-01
C17	2	1.0746028801E+00	-4.8847560001E-01	-7.7868034467E-02	8.6909617270E-01
C17	3	1.8597681196E+00	-1.5556089564E-01	9.8782572193E-01	1.0727760139E-03
H18	1	-2.1549963965E-01	5.8300992755E-01	1.7259256633E-01	7.9392142585E-01
H18	2	-1.8303317116E-01	-5.4933733283E-01	-6.3622120045E-01	5.4171125045E-01
H18	3	3.9853281081E-01	-5.9860497754E-01	7.5195371543E-01	2.7611173592E-01
H19	1	-2.1535448759E-01	6.0760947088E-01	1.3763216526E-02	7.9411668209E-01
H19	2	-1.8304919542E-01	-7.1865902221E-01	4.3520822857E-01	5.4233108668E-01
H19	3	3.9840368301E-01	3.3814189431E-01	9.0022462289E-01	-2.7432770121E-01
C20	1	-1.5530965058E-02	5.5320820007E-01	-5.8595371604E-01	5.9213083861E-01
C20	2	-2.3050362865E-03	7.3013163555E-01	6.8328030047E-01	-5.9854622094E-03
C20	3	1.7836001344E-02	-4.0108413350E-01	4.3564466443E-01	8.0581961021E-01
H21	1	-1.9760961443E-01	2.2447861501E-01	-2.8476723598E-01	9.3194258016E-01
H21	2	-1.8096381194E-01	7.7869927883E-01	6.2738369815E-01	4.1386519725E-03
H21	3	3.7857342638E-01	-5.8586413489E-01	7.2477397622E-01	3.6258226493E-01
H22	1	-1.9862245495E-01	-6.3651299286E-01	7.7126480289E-01	-1.3467503235E-03
H22	2	-1.8317973576E-01	7.7126472222E-01	6.3651413744E-01	6.9360765080E-04
H22	3	3.8180219071E-01	-1.3921807886E-03	5.9721073250E-04	9.9999885259E-01
C23	1	-2.9876948598E-02	-7.3550172594E-01	5.4632023680E-01	4.0071362592E-01
C23	2	-1.1501350909E-02	4.6527117019E-01	8.3720442415E-01	-2.8742214663E-01
C23	3	4.1378299507E-02	4.9250375564E-01	2.4958987276E-02	8.6995235481E-01
H24	1	-1.8626216533E-01	-3.5036415164E-01	2.2028054909E-02	9.3635448738E-01
H24	2	-1.8538816520E-01	-1.2927549437E-01	9.8901753270E-01	-7.1639141301E-02
H24	3	3.7165033053E-01	9.2764907578E-01	1.4614747623E-01	3.4366860111E-01
B25	1	-4.4786773491E-01	3.7543599207E-03	-3.5325547653E-03	9.9998671283E-01
B25	2	2.1541907477E-01	9.3776292974E-01	3.4726852037E-01	-2.2939849727E-03
B25	3	2.3244866015E-01	-3.4725580253E-01	9.3775908197E-01	4.6164699208E-03

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r * r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1 1.2162133047E+01	1.3788750007E+02		1.5301707837E+01	6.6323547394E+00	7.4146379094E+00
H2 1.7066307460E+00	2.9531509442E+00		1.2917423978E+00	1.0169596221E+00	1.1439764654E+00
H3 1.7070211169E+00	2.9534313723E+00		1.2918748083E+00	1.0170772201E+00	1.1441503537E+00
C4 8.5190190815E+00	1.3765993869E+02		1.4968165248E+01	5.9585131046E+00	5.9005343948E+00
H5 1.6592917933E+00	2.9856003601E+00		1.2969878756E+00	1.0119861122E+00	1.1260385347E+00
C6 8.7295615788E+00	1.3771539423E+02		1.4986074212E+01	5.9725272037E+00	5.9501365902E+00
H7 1.6727799275E+00	2.9707754148E+00		1.2951095116E+00	1.0148911909E+00	1.1336670964E+00
H8 1.6855104872E+00	2.9692029113E+00		1.2962187770E+00	1.0175193661E+00	1.1390807674E+00
C9 1.2159775311E+01	1.3788739659E+02		1.5301683067E+01	6.6321123810E+00	7.4138314064E+00
H10 1.7067928553E+00	2.9533486367E+00		1.2918369035E+00	1.0170383159E+00	1.1440709228E+00
H11 1.7067474115E+00	2.9533172232E+00		1.2917912935E+00	1.0169819400E+00	1.1440071573E+00
C12 8.5198955038E+00	1.3766001706E+02		1.4968200141E+01	5.9585112931E+00	5.9006262182E+00
H13 1.6594896233E+00	2.9856801762E+00		1.2970747355E+00	1.0120874968E+00	1.1261714781E+00
C14 8.7356823867E+00	1.3771514998E+02		1.4986218996E+01	5.9732464354E+00	5.9522861181E+00
H15 1.6854617006E+00	2.9693235347E+00		1.2962694904E+00	1.0175516450E+00	1.1390938747E+00

H16	2.9706458582E+00	1.2950417941E+00	1.0148356848E+00	1.1336115280E+00
	1.6727180006E+00			
C17	1.3788759422E+02	1.5301641788E+01	6.6318613353E+00	7.4130283899E+00
	1.2157341988E+01			
H18	2.9531623054E+00	1.2917866205E+00	1.0170347081E+00	1.1441260680E+00
	1.7069997860E+00			
H19	2.9532720392E+00	1.2917751993E+00	1.0169771445E+00	1.1440213984E+00
	1.7068222913E+00			
C20	1.3771512650E+02	1.4986042211E+01	5.9727377811E+00	5.9509163312E+00
	8.7320132746E+00			
H21	2.9706432088E+00	1.2950930804E+00	1.0149193086E+00	1.1337558452E+00
	1.6730173434E+00			
H22	2.9692004645E+00	1.2962038418E+00	1.0174966191E+00	1.1390390680E+00
	1.6854070610E+00			
C23	1.3766013625E+02	1.4968403383E+01	5.9591786960E+00	5.9030342498E+00
	8.5289908303E+00			
H24	2.9856484620E+00	1.2970174272E+00	1.0120114139E+00	1.1260600771E+00
	1.6593000919E+00			
B25	9.2239723479E+01	1.0526880372E+01	3.0736802862E+00	1.9512441725E+00
	2.1751892291E+00			

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3630957543E+02	-2.7658370372E+01	-1.4067152869E+01	-1.7365215598E+01	-3.3132831273E+01
H2	-2.2780570128E+00	-1.8333313388E+00	-2.1132094293E+00	-3.2038911848E+00	-6.1167188028E+00

H3	-2.2783336089E+00	-1.8336618802E+00	-2.1137876654E+00	-3.2051680660E+00	-
6.1199937297E+00					
C4	-1.3584037123E+02	-2.6719085078E+01	-1.1978367703E+01	-1.2319171241E+01	-
1.9893797094E+01					
H5	-2.3104865089E+00	-1.8539024067E+00	-2.1282098649E+00	-3.2092884494E+00	-
6.0800820756E+00					
C6	-1.3595503705E+02	-2.6922335053E+01	-1.2407680052E+01	-1.3327655036E+01	-
2.2507535600E+01					
H7	-2.2931909247E+00	-1.8369974817E+00	-2.0987908170E+00	-3.1387128141E+00	-
5.8832216689E+00					
H8	-2.2931057621E+00	-1.8399631482E+00	-2.1072808386E+00	-3.1615599344E+00	-
5.9483028978E+00					
C9	-1.3630913546E+02	-2.7657911479E+01	-1.4066064075E+01	-1.7362221732E+01	-
3.3123943600E+01					
H10	-2.2782465667E+00	-1.8335243347E+00	-2.1135023846E+00	-3.2044774310E+00	-
6.1181224636E+00					
H11	-2.2782098770E+00	-1.8334984689E+00	-2.1135114776E+00	-3.2045959636E+00	-
6.1185908556E+00					
C12	-1.3584018623E+02	-2.6718901768E+01	-1.1978311161E+01	-1.2320174684E+01	-
1.9900247871E+01					
H13	-2.3105543939E+00	-1.8540111107E+00	-2.1283714899E+00	-3.2095401599E+00	-
6.0805113983E+00					
C14	-1.3595545655E+02	-2.6923480838E+01	-1.2410818364E+01	-1.3336814828E+01	-
2.2535611989E+01					
H15	-2.2931381324E+00	-1.8399344937E+00	-2.1071432086E+00	-3.1611383239E+00	-
5.9470483188E+00					
H16	-2.2930866535E+00	-1.8369016972E+00	-2.0986795868E+00	-3.1385446508E+00	-
5.8828655542E+00					
C17	-1.3630937784E+02	-2.7657994251E+01	-1.4065907247E+01	-1.7361054527E+01	-
3.3118582700E+01					
H18	-2.2781643400E+00	-1.8335493936E+00	-2.1136803736E+00	-3.2050185309E+00	-
6.1196864586E+00					
H19	-2.2781938914E+00	-1.8335056239E+00	-2.1135699424E+00	-3.2048138801E+00	-
6.1193394104E+00					
C20	-1.3595517628E+02	-2.6922789819E+01	-1.2409006086E+01	-1.3331978368E+01	-
2.2523126167E+01					
H21	-2.2931269057E+00	-1.8370208088E+00	-2.0989266114E+00	-3.1390910501E+00	-
5.8842144999E+00					

H22 -2.2930767888E+00 -1.8399047373E+00 -2.1071632384E+00 -3.1612848969E+00 -
5.9475461219E+00

C23 -1.3584043943E+02 -2.6719553334E+01 -1.1980610114E+01 -1.2328981596E+01 -
1.9935505498E+01

H24 -2.3105242773E+00 -1.8539269020E+00 -2.1282147189E+00 -3.2092388408E+00 -
6.0798616507E+00

B25 -9.0900360940E+01 -1.9355717009E+01 -6.9274303927E+00 -4.4349817445E+00 -
5.3684506410E+00

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

C1	3.3161773697E+00	3.3161773697E+00	6.6323547394E+00	0.0000000000E+00
H2	5.0847981104E-01	5.0847981104E-01	1.0169596221E+00	0.0000000000E+00
H3	5.0853861005E-01	5.0853861005E-01	1.0170772201E+00	0.0000000000E+00
C4	2.9792565523E+00	2.9792565523E+00	5.9585131046E+00	0.0000000000E+00
H5	5.0599305612E-01	5.0599305612E-01	1.0119861122E+00	0.0000000000E+00
C6	2.9862636018E+00	2.9862636018E+00	5.9725272037E+00	0.0000000000E+00
H7	5.0744559543E-01	5.0744559543E-01	1.0148911909E+00	0.0000000000E+00
H8	5.0875968307E-01	5.0875968307E-01	1.0175193661E+00	0.0000000000E+00
C9	3.3160561905E+00	3.3160561905E+00	6.6321123810E+00	0.0000000000E+00
H10	5.0851915797E-01	5.0851915797E-01	1.0170383159E+00	0.0000000000E+00
H11	5.0849097002E-01	5.0849097002E-01	1.0169819400E+00	0.0000000000E+00
C12	2.9792556466E+00	2.9792556466E+00	5.9585112931E+00	0.0000000000E+00
H13	5.0604374842E-01	5.0604374842E-01	1.0120874968E+00	0.0000000000E+00
C14	2.9866232177E+00	2.9866232177E+00	5.9732464354E+00	0.0000000000E+00
H15	5.0877582251E-01	5.0877582251E-01	1.0175516450E+00	0.0000000000E+00

H16	5.0741784242E-01	5.0741784242E-01	1.0148356848E+00	0.0000000000E+00
C17	3.3159306676E+00	3.3159306676E+00	6.6318613353E+00	0.0000000000E+00
H18	5.0851735406E-01	5.0851735406E-01	1.0170347081E+00	0.0000000000E+00
H19	5.0848857227E-01	5.0848857227E-01	1.0169771445E+00	0.0000000000E+00
C20	2.9863688905E+00	2.9863688905E+00	5.9727377811E+00	0.0000000000E+00
H21	5.0745965430E-01	5.0745965430E-01	1.0149193086E+00	0.0000000000E+00
H22	5.0874830956E-01	5.0874830956E-01	1.0174966191E+00	0.0000000000E+00
C23	2.9795893480E+00	2.9795893480E+00	5.9591786960E+00	0.0000000000E+00
H24	5.0600570696E-01	5.0600570696E-01	1.0120114139E+00	0.0000000000E+00
B25	1.5368401431E+00	1.5368401431E+00	3.0736802862E+00	0.0000000000E+00

Total	3.7000045522E+01	3.7000045522E+01	7.4000091044E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A)

into interatomic ($VeeX(A,B)$ and $VeeX(A,A')$) and intraatomic ($VeeX(A,A)$) contributions is ambiguous. Currently, interatomic contributions $VeeX(A,B)$ and $VeeX(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$. For wavefunctions of non-supported DFT models, $VeeX$ is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E\_IQA(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

C2H4

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\c2h4\c2h4.wfn

Sum File: D:\calc\ellipticity\c2h4\c2h4.sum

SumViz File: D:\calc\ellipticity\c2h4\c2h4.sumviz

Wfn Title: c2h4.wfn

Total memory allocated for AIMSum = 0.450 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

```

Number of electrons (from MO Occs)      =      15.9999998000
Number of Alpha electrons (from MO Occs) =      7.9999999000
Number of Beta electrons (from MO Occs)  =      7.9999999000
Number of electron pairs (N*(N-1)/2)     =     119.9999969000
Number of electron pairs (from Muller 2EDM) =     119.9999796500
Number of electron pairs (from Muller 2EDM, no SOSI) =     120.2036200199

```

Nuclear Charges and Cartesian Coordinates:

```

-----
Atom   Charge      X      Y      Z
-----
C1     6.0      0.0000000000E+00 0.0000000000E+00 1.2653135300E+00
H2     1.0      0.0000000000E+00 1.7506659500E+00 2.3339722900E+00
H3     1.0      0.0000000000E+00 -1.7506659500E+00 2.3339722900E+00
C4     6.0      0.0000000000E+00 0.0000000000E+00 -1.2653135300E+00
H5     1.0      0.0000000000E+00 -1.7506659500E+00 -2.3339722900E+00
H6     1.0      0.0000000000E+00 1.7506659500E+00 -2.3339722900E+00

```

Some Atomic Properties:

 $q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

```

-----
Atom A    q(A)      L(A)      K(A)      K_Scaled(A)  |Mu_Intra(A)|
-----
C1        -4.8687574700E-02 9.6617031720E-05 3.7913136691E+01 -3.7954152260E+01 8.3889259422E-02

```


H2	2.4408356120E-02	1.6006299744E-05	6.0891432426E-01	-6.0957306604E-01	1.4691747138E-01
H3	2.4408919320E-02	1.5994075482E-05	6.0891403561E-01	-6.0957277708E-01	1.4691778748E-01
C4	-4.8687213300E-02	9.6987699753E-05	3.7913136279E+01	-3.7954151847E+01	8.3887858936E-02
H5	2.4408730160E-02	1.6138670974E-05	6.0891423587E-01	-6.0957297756E-01	1.4691761978E-01
H6	2.4409011490E-02	1.6081894272E-05	6.0891406672E-01	-6.0957280822E-01	1.4691775184E-01

Total	2.6022909000E-04	2.5782567195E-04	7.8261929632E+01	-7.8346595736E+01	

Molecular charge q(Mol) from the wfn file: 2.0000000035E-07

Molecular energy E(Mol) from the wfn file: -7.8346527479E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0010818300E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	
C1	22	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	6	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

H3	6	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C4	26	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H5	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H6	7	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 74

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 5.93262573278155E-20 -9.29908508811704E-20 1.26531564755810E+00

Type = (3,-3) NACP C1

Rho = 1.1955746835E+02 Rho at Nucleus = 1.1955746795E+02

GradRho = 1.2122333392E-22 2.8533059275E-17 4.3245935721E-09

HessRho_EigVals = -1.8126222127E+05 -1.8126023844E+05 -1.8125956460E+05

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

DelSqRho = -5.4378202432E+05

Bond Ellipticity = NA

V = -1.3596068159E+05

G = 7.5877552828E+00

K = 1.3595309384E+05

L = 1.3594550608E+05

Vnuc = 2.8334562134E+06

Ven = -3.3876085156E+08

Vrep = 3.3862489088E+08

DelSqV = 4.6076569954E+09

DelSqVen = 1.5407826207E+12

DelSqVrep = -1.5361749637E+12

DelSqG = 2.0613192816E+08

DelSqK = -4.8137889235E+09

Stress_EigVals = -4.5320623571E+04 -4.5320383390E+04 -4.5319674629E+04

Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

-DivStress = -8.8723185214E-11 1.3931361766E-10 -3.1760656948E+03

CP# 2 Coords = -1.24268464619257E-17 1.72607441613526E+00 2.31907171965092E+00

Type = (3,-3) NACP H2

Rho = 4.2748452624E-01 Rho at Nucleus = 4.2413816581E-01

GradRho = -4.1908235590E-31 -8.4567769454E-16 -1.7288687842E-15

HessRho_EigVals = -8.5271079919E+00 -8.5179987670E+00 -7.8460085499E+00

HessRho_EigVec1 = 0.0000000000E+00 -5.1875528118E-01 8.5492277911E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5492277911E-01 5.1875528118E-01

DelSqRho = -2.4891115309E+01

Bond Ellipticity = NA

V = -6.2426683112E+00

G = 9.9447419968E-03

K = 6.2327235692E+00

L = 6.2227788272E+00

Vnuc = 3.9927999566E+01

Ven = -1.7068601978E+01

Vrep = 1.0825933667E+01

DelSqV = 1.6071922966E+03

DelSqVen = 9.9385244124E+02

DelSqVrep = 6.1333985532E+02

DelSqG = 1.2196743521E+02

DelSqK = -1.7291597318E+03

Stress_EigVals = -2.1379093204E+00 -2.1373529054E+00 -1.9674060854E+00

Stress_EigVec1 = 0.0000000000E+00 -5.1924571339E-01 8.5462499912E-01
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 8.5462499912E-01 5.1924571339E-01
-DivStress = 6.4726605928E-15 1.2824366827E+01 7.7710341641E+00

CP# 3 Coords = -4.66944739186723E-18 -1.72607441613526E+00 2.31907171965092E+00

Type = (3,-3) NACP H3

Rho = 4.2748452624E-01 Rho at Nucleus = 4.2413816581E-01

GradRho = -2.4651903288E-31 1.3209919270E-15 -1.8184238837E-15

HessRho_EigVals = -8.5271079919E+00 -8.5179987670E+00 -7.8460085499E+00

HessRho_EigVec1 = 0.0000000000E+00 5.1875528118E-01 8.5492277911E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5492277911E-01 -5.1875528118E-01

DelSqRho = -2.4891115309E+01

Bond Ellipticity = NA

V = -6.2426683112E+00

G = 9.9447419968E-03

K = 6.2327235692E+00

L = 6.2227788272E+00

Vnuc = 3.9927999566E+01

Ven = -1.7068601978E+01

Vrep = 1.0825933667E+01

DelSqV = 1.6071922966E+03

DelSqVen = 9.9385244124E+02

DelSqVrep = 6.1333985532E+02

DelSqG = 1.2196743521E+02

DelSqK = -1.7291597318E+03

Stress_EigVals = -2.1379093204E+00 -2.1373529054E+00 -1.9674060854E+00

Stress_EigVec1 = 0.0000000000E+00 5.1924571339E-01 8.5462499912E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.5462499912E-01 -5.1924571339E-01

-DivStress = 2.2365588262E-15 -1.2824366827E+01 7.7710341641E+00

CP# 4 Coords = -3.85272049908914E-20 1.02935849074648E-19 -1.26531564755811E+00

Type = (3,-3) NACP C4

Rho = 1.1955746641E+02 Rho at Nucleus = 1.1955746600E+02

GradRho = -7.7372471549E-23 -7.4079886527E-18 -4.3178447484E-09

HessRho_EigVals = -1.8126221967E+05 -1.8126023684E+05 -1.8125956301E+05

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 4.3400320436E-14

HessRho_EigVec3 = 0.0000000000E+00 -4.3400320436E-14 1.0000000000E+00

DelSqRho = -5.4378201952E+05

Bond Ellipticity = NA

V = -1.3596068039E+05

G = 7.5877552828E+00

K = 1.3595309264E+05

L = 1.3594550488E+05

Vnuc = 2.8334561985E+06

Ven = -3.3876084427E+08

Vrep = 3.3862488359E+08

DelSqV = 4.6076569586E+09

DelSqVen = 1.5407825551E+12

DelSqVrep = -1.5361748982E+12

DelSqG = 2.0613192788E+08

DelSqK = -4.8137888865E+09

Stress_EigVals = -4.5320623171E+04 -4.5320382990E+04 -4.5319674229E+04

Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

-DivStress = 5.8107166009E-11 -1.4746361468E-10 3.1760656852E+03

CP# 5 Coords = -1.52401658089922E-18 -1.72607441613526E+00 -2.31907171965093E+00

Type = (3,-3) NACP H5

Rho = 4.2748452624E-01 Rho at Nucleus = 4.2413816581E-01

GradRho = 8.6281661509E-32 -3.8163916471E-17 7.7238562768E-16
HessRho_EigVals = -8.5271079919E+00 -8.5179987670E+00 -7.8460085499E+00
HessRho_EigVec1 = 0.0000000000E+00 -5.1875528118E-01 8.5492277911E-01
HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec3 = 0.0000000000E+00 8.5492277911E-01 5.1875528118E-01
DelSqRho = -2.4891115309E+01
Bond Ellipticity = NA
V = -6.2426683112E+00
G = 9.9447419968E-03
K = 6.2327235692E+00
L = 6.2227788272E+00
Vnuc = 3.9927999566E+01
Ven = -1.7068601978E+01
Vrep = 1.0825933667E+01
DelSqV = 1.6071922966E+03
DelSqVen = 9.9385244124E+02
DelSqVrep = 6.1333985532E+02
DelSqG = 1.2196743521E+02
DelSqK = -1.7291597318E+03
Stress_EigVals = -2.1379093204E+00 -2.1373529054E+00 -1.9674060854E+00
Stress_EigVec1 = 0.0000000000E+00 -5.1924571339E-01 8.5462499912E-01
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 8.5462499912E-01 5.1924571339E-01
-DivStress = 9.9269514990E-16 -1.2824366827E+01 -7.7710341641E+00

CP# 6 Coords = -1.11184746824674E-17 1.72607441613526E+00 -2.31907171965093E+00

Type = (3,-3) NACP H6

Rho = 4.2748452624E-01 Rho at Nucleus = 4.2413816581E-01

GradRho = -5.3617889652E-31 -1.4328815912E-15 -1.1503385050E-15

HessRho_EigVals = -8.5271079919E+00 -8.5179987670E+00 -7.8460085499E+00

HessRho_EigVec1 = 0.0000000000E+00 5.1875528118E-01 8.5492277911E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5492277911E-01 -5.1875528118E-01

DelSqRho = -2.4891115309E+01

Bond Ellipticity = NA

V = -6.2426683112E+00

G = 9.9447419968E-03

K = 6.2327235692E+00

L = 6.2227788272E+00

Vnuc = 3.9927999566E+01

Ven = -1.7068601978E+01

Vrep = 1.0825933667E+01

DelSqV = 1.6071922966E+03

DelSqVen = 9.9385244124E+02

DelSqVrep = 6.1333985532E+02

DelSqG = 1.2196743521E+02

DelSqK = -1.7291597318E+03

Stress_EigVals = -2.1379093204E+00 -2.1373529054E+00 -1.9674060854E+00

Stress_EigVec1 = 0.0000000000E+00 5.1924571339E-01 8.5462499912E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.5462499912E-01 -5.1924571339E-01

-DivStress = 5.6245377815E-15 1.2824366827E+01 -7.7710341641E+00

CP# 7 Coords = -2.21697456709825E-16 8.96728462913939E-16 -2.39596069086202E-11

Type = (3,-1) BCP C1 C4

Rho = 3.3453643207E-01

GradRho = 7.8905812045E-26 -3.1091614566E-17 2.7047701196E-13

HessRho_EigVals = -7.1285660262E-01 -5.2316178464E-01 2.6061517372E-01

HessRho_EigVec1 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

DelSqRho = -9.7540321355E-01

Bond Ellipticity = 3.6259303249E-01

V = -5.2835294109E-01

G = 1.4225106885E-01
K = 3.8610187224E-01
L = 2.4385080339E-01
Vnuc = 1.0854815918E+01
Ven = -3.6313313880E+00
Vrep = 3.1029784469E+00
DelSqV = -1.2844434171E+00
DelSqVen = 1.0587822329E+01
DelSqVrep = -1.1872265746E+01
DelSqG = 1.2446948017E+00
DelSqK = 3.9748615432E-02
Stress_EigVals = -3.0082101637E-01 -2.6555024956E-01 3.8018324843E-02
Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
-DivStress = 2.1408857969E-17 -5.4046240867E-16 -1.2194723111E-10
BPL = 2.5306312951E+00 = 1.2653156476E+00 + 1.2653156475E+00
GBL_I = 2.5306312951E+00
GBL_II = 2.5306270600E+00
GBL_III = 2.5306312951E+00 = 1.2653156476E+00 + 1.2653156475E+00
GBL_IV = 2.5306270600E+00 = 1.2653135300E+00 + 1.2653135300E+00

CP# 8 Coords = -7.82851024942208E-17 1.12326729737665E+00 1.95312820286630E+00

Type = (3,-1) BCP H2 C1

Rho = 2.7842306271E-01

GradRho = 2.7117093617E-31 -1.0408340856E-16 -5.0740661672E-17

HessRho_EigVals = -7.2797223345E-01 -7.1573433580E-01 4.8161580595E-01

HessRho_EigVec1 = 0.0000000000E+00 -5.1874081378E-01 8.5493155756E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5493155756E-01 5.1874081378E-01

DelSqRho = -9.6209076330E-01

Bond Ellipticity = 1.7098380006E-02

V = -3.2876905442E-01
G = 4.4123181799E-02
K = 2.8464587262E-01
L = 2.4052269082E-01
Vnuc = 8.4475074827E+00
Ven = -2.3519809056E+00
Vrep = 2.0232118512E+00
DelSqV = -2.5674727803E+00
DelSqVen = 8.1272689220E+00
DelSqVrep = -1.0694741702E+01
DelSqG = 1.5856759802E+00
DelSqK = 9.8179680010E-01
Stress_EigVals = -2.1754194335E-01 -2.1543192465E-01 1.0420481358E-01
Stress_EigVec1 = 0.0000000000E+00 -5.2047885992E-01 8.5387455541E-01
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 8.5387455541E-01 5.2047885992E-01
-DivStress = -1.9201493481E-17 -9.2436372687E-02 -5.6944126113E-02
BPL = 2.0223450933E+00 = 7.0518868987E-01 + 1.3171564034E+00
GBL_I = 2.0223092616E+00
GBL_II = 2.0510638249E+00
GBL_III = 2.0223126464E+00 = 7.0518868391E-01 + 1.3171239625E+00
GBL_IV = 2.0510673603E+00 = 7.3394229202E-01 + 1.3171250683E+00

CP# 9 Coords = -6.49616913461314E-18 -1.12326729737664E+00 1.95312820286630E+00

Type = (3,-1) BCP C1 H3

Rho = 2.7842306271E-01

GradRho = 2.2186712959E-31 9.0205620751E-17 -6.3317406873E-17

HessRho_EigVals = -7.2797223345E-01 -7.1573433580E-01 4.8161580595E-01

HessRho_EigVec1 = 0.0000000000E+00 5.1874081378E-01 8.5493155756E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5493155756E-01 -5.1874081378E-01

DelSqRho = -9.6209076330E-01

Bond Ellipticity = 1.7098380006E-02

V = -3.2876905442E-01

G = 4.4123181799E-02

K = 2.8464587262E-01

L = 2.4052269082E-01

Vnuc = 8.4475074827E+00

Ven = -2.3519809056E+00

Vrep = 2.0232118512E+00

DelSqV = -2.5674727803E+00

DelSqVen = 8.1272689220E+00

DelSqVrep = -1.0694741702E+01

DelSqG = 1.5856759802E+00

DelSqK = 9.8179680010E-01

Stress_EigVals = -2.1754194335E-01 -2.1543192465E-01 1.0420481358E-01

Stress_EigVec1 = 0.0000000000E+00 5.2047885992E-01 8.5387455541E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.5387455541E-01 -5.2047885992E-01

-DivStress = 2.0967552597E-17 9.2436372687E-02 -5.6944126113E-02

BPL = 2.0223450933E+00 = 1.3171564034E+00 + 7.0518868987E-01

GBL_I = 2.0223092616E+00

GBL_II = 2.0510638249E+00

GBL_III = 2.0223126464E+00 = 1.3171239625E+00 + 7.0518868391E-01

GBL_IV = 2.0510673603E+00 = 1.3171250683E+00 + 7.3394229202E-01

CP# 10 Coords = 2.30596600542530E-18 -1.12326729736957E+00 -1.95312820286181E+00

Type = (3,-1) BCP C4 H5

Rho = 2.7842306271E-01

GradRho = -2.0954117795E-31 3.6429192996E-17 -9.5409791179E-18

HessRho_EigVals = -7.2797223344E-01 -7.1573433579E-01 4.8161580592E-01

HessRho_EigVec1 = 0.0000000000E+00 -5.1874081378E-01 8.5493155756E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5493155756E-01 5.1874081378E-01

DelSqRho = -9.6209076331E-01

Bond Ellipticity = 1.7098380006E-02

V = -3.2876905442E-01

G = 4.4123181798E-02

K = 2.8464587263E-01

L = 2.4052269083E-01

Vnuc = 8.4475074827E+00

Ven = -2.3519809056E+00

Vrep = 2.0232118512E+00

DelSqV = -2.5674727802E+00

DelSqVen = 8.1272689222E+00

DelSqVrep = -1.0694741702E+01

DelSqG = 1.5856759801E+00

DelSqK = 9.8179680004E-01

Stress_EigVals = -2.1754194335E-01 -2.1543192465E-01 1.0420481357E-01

Stress_EigVec1 = 0.0000000000E+00 -5.2047885992E-01 8.5387455541E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.5387455541E-01 5.2047885992E-01

-DivStress = 1.1737884380E-17 9.2436372717E-02 5.6944126133E-02

BPL = 2.0223450933E+00 = 1.3171564034E+00 + 7.0518868988E-01

GBL_I = 2.0223092616E+00

GBL_II = 2.0510638249E+00

GBL_III = 2.0223126464E+00 = 1.3171239625E+00 + 7.0518868392E-01

GBL_IV = 2.0510673603E+00 = 1.3171250683E+00 + 7.3394229203E-01

CP# 11 Coords = -1.48367866813746E-16 1.12326729736957E+00 -1.95312820286181E+00

Type = (3,-1) BCP H6 C4

Rho = 2.7842306271E-01

GradRho = 6.7792734042E-32 8.8470897275E-17 4.7704895589E-18

HessRho_EigVals = -7.2797223344E-01 -7.1573433579E-01 4.8161580592E-01

HessRho_EigVec1 = 0.0000000000E+00 5.1874081378E-01 8.5493155756E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 8.5493155756E-01 -5.1874081378E-01

DelSqRho = -9.6209076331E-01

Bond Ellipticity = 1.7098380006E-02

V = -3.2876905442E-01

G = 4.4123181798E-02

K = 2.8464587263E-01

L = 2.4052269083E-01

Vnuc = 8.4475074827E+00

Ven = -2.3519809056E+00

Vrep = 2.0232118512E+00

DelSqV = -2.5674727802E+00

DelSqVen = 8.1272689222E+00

DelSqVrep = -1.0694741702E+01

DelSqG = 1.5856759801E+00

DelSqK = 9.8179680004E-01

Stress_EigVals = -2.1754194335E-01 -2.1543192465E-01 1.0420481357E-01

Stress_EigVec1 = 0.0000000000E+00 5.2047885992E-01 8.5387455541E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.5387455541E-01 -5.2047885992E-01

-DivStress = 7.7305693299E-18 -9.2436372717E-02 5.6944126132E-02

BPL = 2.0223450933E+00 = 7.0518868988E-01 + 1.3171564034E+00

GBL_I = 2.0223092616E+00

GBL_II = 2.0510638249E+00

GBL_III = 2.0223126464E+00 = 7.0518868392E-01 + 1.3171239625E+00

GBL_IV = 2.0510673603E+00 = 7.3394229203E-01 + 1.3171250683E+00

Number of NACPs = 6

Number of NNACPs = 0

Number of BCPs = 5

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H2	C1	C4	122.08638588	121.40376642	121.40113735	121.48047079	121.48054934
H3	C1	C4	122.08638588	121.40376642	121.40113735	121.48047079	121.48054934
H3	C1	H2	115.82722824	117.19246716	117.19772531	117.03905843	117.03890131
H5	C4	C1	122.08638588	121.40376642	121.40113735	121.48047079	121.48054934
H6	C4	C1	122.08638588	121.40376642	121.40113735	121.48047079	121.48054934
H6	C4	H5	115.82722824	117.19246716	117.19772531	117.03905843	117.03890131

Total time for electron density critical point search, analysis and connectivity = 3 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$E_e(A) = E(A) - W(A) = -T(A)$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A) = V_{ee}(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7913136691E+01	3.7913136691E+01	-1.1231022411E+02	-8.9863924968E+01		
H2	-6.0891432426E-01	6.0891432426E-01	-5.8536185724E+00	-1.2500888994E+00		
H3	-6.0891403561E-01	6.0891403561E-01	-5.8536146769E+00	-1.2500883623E+00		
C4	-3.7913136279E+01	3.7913136279E+01	-1.1231022265E+02	-8.9863923814E+01		
H5	-6.0891423587E-01	6.0891423587E-01	-5.8536162586E+00	-1.2500886227E+00		
H6	-6.0891406672E-01	6.0891406672E-01	-5.8536143014E+00	-1.2500883417E+00		
Total	-7.8261929632E+01	7.8261929632E+01	-2.4803491057E+02	-1.8472820301E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
C1	-3.7913136691E+01					
H2	-6.0891432426E-01					
H3	-6.0891403561E-01					
C4	-3.7913136279E+01					
H5	-6.0891423587E-01					
H6	-6.0891406672E-01					
Total	-7.8261929632E+01					

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
VeeC(A)	$VeeX(A)$					
C1			3.7913136691E+01	-5.5815189149E+01	-5.6155112056E+01	
1.1537250692E+01						

H2 2.5477984088E+00	6.0891432426E-01 -3.0968917250E+00 -2.9268092862E+00
H3 2.5477984088E+00	6.0891403561E-01 -3.0968917250E+00 -2.9268073384E+00
C4 1.1537250692E+01	3.7913136279E+01 -5.5815188721E+01 -5.6155111327E+01
H5 2.5477984088E+00	6.0891423587E-01 -3.0968917231E+00 -2.9268081293E+00
H6 2.5477984088E+00	6.0891406672E-01 -3.0968917231E+00 -2.9268071507E+00

Total 3.3265695019E+01	7.8261929632E+01 -1.2401794477E+02 -1.2401745529E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

$$= \text{Intraatomic ("Self") Contribution to } E\_IQA(A)$$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$

C1	3.7913136691E+01 -8.9863924968E+01
H2	6.0891432426E-01 -1.2500888994E+00
H3	6.0891403561E-01 -1.2500883623E+00
C4	3.7913136279E+01 -8.9863923814E+01
H5	6.0891423587E-01 -1.2500886227E+00
H6	6.0891406672E-01 -1.2500883417E+00

Total 7.8261929632E+01 -1.8472820301E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$

C1	-1.0883226665E+01	-1.1223149572E+01		1.1537250692E+01		
H2	-2.4718472754E+00	-2.3017648365E+00		2.5477984088E+00		
H3	-2.4718475439E+00	-2.3017631573E+00		2.5477984088E+00		
C4	-1.0883226813E+01	-1.1223149420E+01		1.1537250692E+01		
H5	-2.4718474117E+00	-2.3017638180E+00		2.5477984088E+00		
H6	-2.4718475522E+00	-2.3017629798E+00		2.5477984088E+00		

Total	-3.1653843261E+01	-3.1653353784E+01		3.3265695019E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$
C1	6.0486875745E+00	4.3607334456E+00	7.2093878083E+01	1.6879541289E+00	
	2.7906121917E+01				
H2	9.7559164402E-01	4.9248517533E-01	5.0480667639E+01	4.8310646869E-01	
	4.9519332361E+01				
H3	9.7559108078E-01	4.9248469474E-01	5.0480647521E+01	4.8310638604E-01	
	4.9519352479E+01				
C4	6.0486872132E+00	4.3607330718E+00	7.2093876210E+01	1.6879541414E+00	
	2.7906123790E+01				
H5	9.7559126981E-01	4.9248489897E-01	5.0480658674E+01	4.8310637084E-01	
	4.9519341326E+01				
H6	9.7559098872E-01	4.9248466217E-01	5.0480648946E+01	4.8310632656E-01	
	4.9519351054E+01				
Total	1.5999739771E+01	1.0691405949E+01	6.6822373999E+01	5.3083338224E+00	
	3.3177626001E+01				

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$DI(A,A')/2$	$DI\_Bond(A,A')/2$	$DI\_NonBond(A,A')/2$

C1	6.0486875745E+00	4.3607334456E+00	1.6879541289E+00	1.6365577371E+00	5.1396391789E-02
H2	9.7559164402E-01	4.9248517533E-01	4.8310646869E-01	4.3272031858E-01	5.0386150110E-02
H3	9.7559108078E-01	4.9248469474E-01	4.8310638604E-01	4.3268667134E-01	5.0419714705E-02
C4	6.0486872132E+00	4.3607330718E+00	1.6879541414E+00	1.6365574333E+00	5.1396708109E-02
H5	9.7559126981E-01	4.9248489897E-01	4.8310637084E-01	4.3271992232E-01	5.0386448523E-02
H6	9.7559098872E-01	4.9248466217E-01	4.8310632656E-01	4.3268676381E-01	5.0419562746E-02

Total	1.5999739771E+01	1.0691405949E+01	5.3083338224E+00	5.0039288465E+00	3.0440497598E-01

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

C1	1.6112943964E+01	2.9252210560E+01	4.5365154524E+01
H2	2.2964694027E-01	7.0872868197E+00	7.3169337600E+00
H3	2.2964663108E-01	7.0872829046E+00	7.3169295357E+00
C4	1.6112941966E+01	2.9252209849E+01	4.5365151815E+01
H5	2.2964671338E-01	7.0872842400E+00	7.3169309534E+00
H6	2.2964655756E-01	7.0872822877E+00	7.3169288452E+00

Total	3.3144472772E+01	8.6853556661E+01	1.1999802943E+02

Diatomic Electron Pair Contributions and Delocalization Data:

2*D2(A,B) = 2*D2(B,A) = Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

DI(A,B) = DI(B,A) = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	
C1	H2	5.4683287364E+00	8.6544063716E-01	7.1539538660E+00	4.4354656093E+01	(Bonded)
C1	H3	5.4683589768E+00	8.6537334268E-01	7.1533975926E+00	4.4351232792E+01	(Bonded)
H2	H3	9.3619410229E-01	3.1168808207E-02	1.5974310767E+00	1.5974319990E+00	
C1	C4	3.5815468441E+01	1.5423014944E+00	1.2749058993E+01	1.2749059755E+01	(Bonded)
H2	C4	5.8753955049E+00	5.1306395240E-02	2.6295015724E+00	4.2411182320E-01	
H3	C4	5.8753837970E+00	5.1322997337E-02	2.6303539643E+00	4.2424906039E-01	
C1	H5	5.8753936219E+00	5.1306339189E-02	4.2411133454E-01	2.6294997084E+00	
H2	H5	9.4577772955E-01	1.2001922513E-02	6.1510994824E-01	6.1511018418E-01	
H3	H5	9.4863329208E-01	6.2896984769E-03	3.2235321749E-01	3.2235315503E-01	
C4	H5	5.4683265167E+00	8.6543984464E-01	7.1539477421E+00	4.4354632489E+01	(Bonded)
C1	H6	5.8753836129E+00	5.1322956767E-02	4.2424869970E-01	2.6303521332E+00	
H2	H6	9.4863356629E-01	6.2897005766E-03	3.2235313900E-01	3.2235335552E-01	
H3	H6	9.4577690806E-01	1.2001918051E-02	6.1511007468E-01	6.1511013272E-01	
C4	H6	5.4683579750E+00	8.6537352762E-01	7.1533995487E+00	4.4351246456E+01	(Bonded)
H5	H6	9.3619366596E-01	3.1168771084E-02	1.5974297868E+00	1.5974302471E+00	

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	C4	5.9983699424E+01	4.6968611578E+01	3.7646006079E+01
C1	H2	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
C1	H3	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
C1	Total	1.4249357622E+02	1.1066304153E+02	8.8484001127E+01
H2	C1	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
H2	Total	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
H3	C1	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
H3	Total	4.1254938396E+01	3.1847214974E+01	2.5418997524E+01
C4	C1	5.9983699424E+01	4.6968611578E+01	3.7646006079E+01
C4	H5	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
C4	H6	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
C4	Total	1.4249106587E+02	1.1065983607E+02	8.8487969171E+01
H5	C4	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
H5	Total	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
H6	C4	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
H6	Total	4.1253683225E+01	3.1845612244E+01	2.5420981546E+01
Total	Total	4.5000188533E+02	3.4870853203E+02	2.7865192844E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta \rho\_IAS(A B)$	$V\_IAS(A B)$

C1	C4	1.5624867752E+00	1.0054779654E+00	7.1795198117E-01	-2.8752598426E-01	1.1501039371E+00	-1.7234299466E+00

C1	H2	9.5037991557E-01	5.1498588250E-01	4.0750668993E-01	-1.0747919257E-01	4.2991677027E-01	-9.2249257243E-01

C1	H3	9.5037991557E-01	5.1498588250E-01	4.0750668993E-01	-1.0747919257E-01	4.2991677027E-01	-9.2249257243E-01

C1	Total	3.4632466063E+00	2.0354497304E+00	1.5329653610E+00	-5.0248436940E-01	2.0099374776E+00	-3.5684150915E+00

H2	C1	9.5037991557E-01	5.1498588250E-01	4.0750668993E-01	-1.0747919257E-01	4.2991677027E-01	-9.2249257243E-01

H2	Total	9.5037991557E-01	5.1498588250E-01	4.0750668993E-01	-1.0747919257E-01	4.2991677027E-01	-9.2249257243E-01

H3	C1	9.5037991557E-01	5.1498588250E-01	4.0750668993E-01	-1.0747919257E-01	4.2991677027E-01	-9.2249257243E-01

H3 Total 9.5037991557E-01 5.1498588250E-01 4.0750668993E-01 -1.0747919257E-01
4.2991677027E-01 -9.2249257243E-01

C4 C1 1.5624867752E+00 1.0054779654E+00 7.1795198117E-01 -2.8752598426E-01
1.1501039371E+00 -1.7234299466E+00

C4 H5 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

C4 H6 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

C4 Total 3.4632466627E+00 2.0354497480E+00 1.5329653722E+00 -5.0248437580E-01
2.0099375033E+00 -3.5684151203E+00

H5 C4 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

H5 Total 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

H6 C4 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

H6 Total 9.5037994373E-01 5.1498589130E-01 4.0750669553E-01 -1.0747919577E-01
4.2991678310E-01 -9.2249258683E-01

Total Total 1.0728012988E+01 6.1308430260E+00 4.6959575042E+00 -1.4348855219E+00
5.7395420877E+00 -1.0826800530E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1 5.7647397840E+01

H2 5.2943911907E+01

H3 5.3188214947E+01

C4 5.7647397840E+01

H5 5.2943911907E+01

H6 5.3188214947E+01

Total 3.2755904939E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	5.0181641238E+01	-4.9420384615E-01	1.0544917901E-02	-2.3620709767E-02	-9.8482997757E-03
	7.0003660736E-03	7.1655198842E-05			

H2	4.3754960673E+01	4.0894501308E-01	2.0568277008E-02	-7.0762495479E-03	9.3462548426E-03
	5.4881623702E-03	4.4394644946E-05			

H3	4.3711069068E+01	4.0631067133E-01	2.0577091766E-02	-7.0135312433E-03	9.2953725451E-03
	5.5468383215E-03	4.5272569850E-05			

C4	5.0181641238E+01	-4.9420380236E-01	1.0544917958E-02	-2.3620709752E-02	-9.8482989030E-03
	7.0003663595E-03	7.1655204651E-05			

H5	4.3754960673E+01	4.0894505914E-01	2.0568277981E-02	-7.0762486577E-03	9.3462558952E-03
	5.4881623059E-03	4.4394644611E-05			

H6	4.3711069068E+01	4.0631071746E-01	2.0577092741E-02	-7.0135302223E-03	9.2953736004E-03
	5.5468382609E-03	4.5272569481E-05			

Total	2.7529534196E+02	6.4210381250E-01	2.0577092741E-02	-2.3620709767E-02	2.3324180058E-03
		1.3973595065E-04			

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
	ESP-_Int_IDS(A)				

C1	5.6157009200E-01	8.4628431084E-03	7.5953959378E+00	3.3683122924E-02	4.2586245301E+01
	-5.2788696908E-01				

H2	4.3538773365E-01	5.7645902526E-03	3.9035058471E+01	4.2216637336E-01	4.7199022026E+00
	-1.3221360281E-02				

H3	4.3451680690E-01	5.7557214867E-03	3.8787701832E+01	4.2041373912E-01	4.9233672358E+00
	-1.4103067785E-02				

C4	5.6157006947E-01	8.4628425372E-03	7.5953959378E+00	3.3683133557E-02
4.2586245301E+01 -5.2788693591E-01				
H5	4.3538777033E-01	5.7645910989E-03	3.9035058471E+01	4.2216641473E-01
4.7199022026E+00 -1.3221355595E-02				
H6	4.3451684309E-01	5.7557223281E-03	3.8787701832E+01	4.2041378027E-01
4.9233672358E+00 -1.4103062814E-02				

Total	2.8629493154E+00	3.9966310812E-02	1.7083631248E+02	1.7525265640E+00
1.0445902948E+02 -1.1104227515E+00				

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				
C1	2.4354749660E-05	4.4346763750E-03	2.2311669434E-03	6.7645271857E-06
2.0075301177E-04				
H2	3.6826131043E-05	1.0815056770E-02	4.5575122388E-03	2.9328122796E-05
5.7105782823E-03				
H3	2.7956462776E-05	1.0838841160E-02	4.5621913418E-03	2.9416798846E-05
5.6978077622E-03				
C4	2.4356320684E-05	4.4346777748E-03	2.2311669237E-03	6.7645267306E-06
2.0075310262E-04				
H5	3.6827565981E-05	1.0815057829E-02	4.5575121763E-03	2.9328122200E-05
5.7105791539E-03				
H6	2.7957338885E-05	1.0838842221E-02	4.5621912789E-03	2.9416798247E-05
5.6978086312E-03				

Total	2.4354749660E-05	1.0258513184E-02	3.0672419730E-05	2.3218279944E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
C1	-1.2171561453E-04	-1.2395715221E-02	5.4038279223E-03	4.0354662566E-05	8.2620900966E-03

H2	-6.5670739280E-05	-2.8011936929E-03	1.6167104408E-03	3.5967650577E-06
5.4011970348E-05				
H3	-6.2846346870E-05	-2.8645167241E-03	1.6064359967E-03	3.5575755590E-06
5.7913724478E-05				
C4	-1.2171399277E-04	-1.2395714442E-02	5.4038281709E-03	4.0354666327E-05
8.2620894346E-03				
H5	-6.5669917440E-05	-2.8011927002E-03	1.6167104972E-03	3.5967652440E-06
5.4011944978E-05				
H6	-6.2844803929E-05	-2.8645157143E-03	1.6064360411E-03	3.5575757483E-06
5.7913696929E-05				

Total	-6.2844803929E-05	-1.0630222749E-02	4.7329462081E-05	1.6748030868E-02

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	4.4383858252E+01
H2	3.6618982188E+01
H3	3.6504290122E+01
C4	4.4383858252E+01
H5	3.6618982188E+01
H6	3.6504290122E+01

Total	2.3501426112E+02

Atomic Surface Area and Volume Data:

$$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$$
$$\text{Vol}(A) = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$$

Isosurface of the Electron Density Distribution (IsoDensity Surface)

$$N(\text{Vol}(A)) = \text{Average Number of Electrons in Vol}(A)$$

$N(\text{Vol(A)})/\text{Vol(A)}$ = Average Electron Density in Vol(A)

$\%N(\text{Vol(A)}) = 100 * N(\text{Vol(A)}) / N(\text{A})$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.0014097405E+02	1.2698948432E+02	6.0344211964E+00	4.7519062139E-02	9.9764140929E+01
H2	9.4198850303E+01	6.9824111160E+01	9.6387386390E-01	1.3804312692E-02	9.8798905254E+01
H3	9.4443153343E+01	6.9730437029E+01	9.6383586408E-01	1.3822312109E-02	9.8795067233E+01
C4	2.0013846371E+02	1.2698787364E+02	6.0344206040E+00	4.7519660193E-02	9.9764137096E+01
H5	9.4197595132E+01	6.9833037920E+01	9.6387718862E-01	1.3802595696E-02	9.8799283923E+01
H6	9.4441898172E+01	6.9724739827E+01	9.6383352594E-01	1.3823407994E-02	9.8794836903E+01
Total	7.7756093471E+02	5.3308968390E+02	1.5924262243E+01	2.9871638345E-02	9.9528257777E+01

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.6084468277E+02	1.0074178162E+02	6.0173823108E+00	5.9730751373E-02	9.9482445348E+01
H2	7.5602175647E+01	5.0127469288E+01	9.5116522806E-01	1.8974930144E-02	9.7496245896E+01
H3	7.5558284042E+01	5.0064321738E+01	9.5110114754E-01	1.8997583799E-02	9.7489733801E+01
C4	1.6084147731E+02	1.0074452028E+02	6.0173850700E+00	5.9729155030E-02	9.9482496909E+01

H5	7.5600572917E+01	5.0125260056E+01	9.5116259588E-01	1.8975713938E-02
9.7496013473E+01				
H6	7.5556681312E+01	5.0065482300E+01	9.5110230254E-01	1.8997166488E-02
9.7489861401E+01				

Total	6.2400387399E+02	4.0186883528E+02	1.5839298655E+01	3.9414100483E-02
9.8997226714E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.3286785938E+02	8.2297087207E+01	5.9909908850E+00	7.2797119416E-02	
9.9046128784E+01					
H2	6.2037979712E+01	3.7188108493E+01	9.3260183208E-01	2.5077958247E-02	
9.5593462483E+01					
H3	6.1923287646E+01	3.7143112247E+01	9.3251067836E-01	2.5105884293E-02	
9.5584174233E+01					
C4	1.3287182742E+02	8.2296354683E+01	5.9909893781E+00	7.2797749076E-02	
9.9046109789E+01					
H5	6.2039963734E+01	3.7187306537E+01	9.3259985041E-01	2.5078445772E-02	
9.5593296008E+01					
H6	6.1925271668E+01	3.7143192345E+01	9.3251100840E-01	2.5105839039E-02	
9.5584217093E+01					

Total	5.1366618956E+02	3.1325516151E+02	1.5712203632E+01	5.0157844348E-02	
9.8202869904E+01					

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	C4	1.1414790000E-05
C1	H2	-2.4361041740E-02
C1	H3	-2.4361604940E-02
C1		-4.8711231890E-02 -4.8687574700E-02
H2	C1	2.4384698930E-02
H2		2.4384698930E-02 2.4408356120E-02
H3	C1	2.4385262130E-02
H3		2.4385262130E-02 2.4408919320E-02
C4	C1	1.2242400000E-05
C4	H5	-2.4361415780E-02
C4	H6	-2.4361697110E-02
C4		-4.8710870490E-02 -4.8687213300E-02
H5	C4	2.4385072970E-02
H5		2.4385072970E-02 2.4408730160E-02
H6	C4	2.4385354300E-02
H6		2.4385354300E-02 2.4409011490E-02

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	3.0082980405E-04	-2.0628331257E-18	3.0082980405E-04
H2	-9.4749840425E-07	1.9089586550E-18	-9.4749840425E-07
H3	2.0189198566E-07	1.5841078719E-19	2.0189198566E-07
C4	-3.0107816172E-04	-3.5556023266E-18	-3.0107816172E-04
H5	1.0537597896E-06	-5.6231149309E-20	1.0537597896E-06
H6	3.7789147575E-07	3.6180029990E-18	3.7789147575E-07

Total 4.3768717676E-07 1.0705839646E-20 4.3768717676E-07

Atom A Mu_Intra_Y(A) Mu_Bond_Y(A) Mu_Y(A)

C1 -6.4042148865E-04 -6.3262414160E-07 -6.4105411279E-04

H2 -1.2154215306E-01 1.5298927253E-02 -1.0624322581E-01

H3 1.2154241578E-01 -1.5299280604E-02 1.0624313518E-01

C4 6.3871982904E-04 3.1600878874E-07 6.3903583783E-04

H5 1.2154187931E-01 -1.5299161926E-02 1.0624271738E-01

H6 -1.2154210009E-01 1.5299338432E-02 -1.0624276166E-01

Total -1.6597196100E-06 -4.9346021131E-07 -2.1531798213E-06

Atom A Mu_Intra_Z(A) Mu_Bond_Z(A) Mu_Z(A)

C1 -8.3886275446E-02 3.3526594576E-02 -5.0359680870E-02

H2 -8.2536346085E-02 9.2867684040E-03 -7.3249577681E-02

H3 -8.2536521882E-02 9.2869828954E-03 -7.3249538987E-02

C4 8.3884886993E-02 -3.3527962428E-02 5.0356924565E-02

H5 8.2537013368E-02 -9.2869108551E-03 7.3250102513E-02

H6 8.2536923322E-02 -9.2870179979E-03 7.3249905324E-02

Total -3.1973000002E-07 -1.5454055301E-06 -1.8651355301E-06

Atom A |Mu_Intra(A)| |Mu_Bond(A)| |Mu(A)|

C1 8.3889259422E-02 3.3526594582E-02 5.0364659299E-02

H2 1.4691747138E-01 1.7896961823E-02 1.2904698238E-01

H3 1.4691778748E-01 1.7897375179E-02 1.2904688580E-01

C4 8.3887858936E-02 3.3527962429E-02 5.0361879101E-02

H5 1.4691761978E-01 1.7897236347E-02 1.2904686171E-01

H6 1.4691775184E-01 1.7897442827E-02 1.2904678622E-01

Total 1.7459858308E-06 1.6222765586E-06 2.8820971450E-06

Bond Contributions to Atomic Dipole Moments:

 $\text{Mu\_Bond}(A|B) = \text{Contribution of Bond Between Atom A and Atom B to Mu\_Bond}(A)$

$\text{Mu\_Bond}(A) = \text{Sum of Mu\_Bond}(A|B) \text{ Over All B}$

$= \text{Total Bonding Dipole Moment Contribution of Atom A}$

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	C4	2.5306299119E-21	
C1	H2	-1.9071066495E-18	
C1	H3	-1.5825710608E-19	
C1		-2.0628331257E-18	
H2	C1	1.9089586550E-18	
H2		1.9089586550E-18	
H3	C1	1.5841078719E-19	
H3		1.5841078719E-19	
C4	C1	2.7141089440E-21	
C4	H5	5.6176596633E-20	
C4	H6	-3.6144930322E-18	
C4		-3.5556023266E-18	
H5	C4	-5.6231149309E-20	
H5		-5.6231149309E-20	
H6	C4	3.6180029990E-18	
H6		3.6180029990E-18	

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1 C4 -1.0235967091E-20

C1	H2	2.7363961517E-02
C1	H3	-2.7364594141E-02
C1		-6.3262414160E-07
H2	C1	1.5298927253E-02
H2		1.5298927253E-02
H3	C1	-1.5299280604E-02
H3		-1.5299280604E-02
C4	C1	-1.0978108534E-20
C4	H5	-2.7364381663E-02
C4	H6	2.7364697672E-02
C4		3.1600878874E-07
H5	C4	-1.5299161926E-02
H5		-1.5299161926E-02
H6	C4	1.5299338432E-02
H6		1.5299338432E-02

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	C4	1.4443288230E-05	
C1	H2	1.6755881955E-02	
C1	H3	1.6756269332E-02	
C1		3.3526594576E-02	
H2	C1	9.2867684040E-03	
H2		9.2867684040E-03	
H3	C1	9.2869828954E-03	
H3		9.2869828954E-03	
C4	C1	-1.5490474359E-05	
C4	H5	-1.6756139225E-02	
C4	H6	-1.6756332728E-02	
C4		-3.3527962428E-02	
H5	C4	-9.2869108551E-03	
H5		-9.2869108551E-03	

H6 C4 -9.2870179979E-03
H6 -9.2870179979E-03

Atom A Atom B |Mu_Bond(A|B)| |Mu_Bond(A)|

C1 C4 1.4443288230E-05
C1 H2 3.2086538766E-02
C1 H3 3.2087280571E-02
C1 3.3526594582E-02
H2 C1 1.7896961823E-02
H2 1.7896961823E-02
H3 C1 1.7897375179E-02
H3 1.7897375179E-02
C4 C1 1.5490474359E-05
C4 H5 3.2087031423E-02
C4 H6 3.2087401970E-02
C4 3.3527962429E-02
H5 C4 1.7897236347E-02
H5 1.7897236347E-02
H6 C4 1.7897442827E-02
H6 1.7897442827E-02

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$

$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$

$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$

$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	-3.4478950176E+00	2.6365024327E-03	-5.5220416996E-04	1.2750403080E+00	1.5328309299E-03	2.1728547095E+00
H2	-3.0760140193E-01	-2.1228725796E-06	2.3101447049E-06	3.0281865737E-01	2.8283660139E-01	4.7827445616E-03
H3	-3.0760182160E-01	4.5237452667E-06	6.0111947586E-06	3.0281852630E-01	-2.8283619903E-01	4.7832952996E-03
C4	-3.4478857189E+00	2.6374218183E-03	-5.5476767373E-04	1.2750333465E+00	1.5384113870E-03	2.1728523724E+00
H5	-3.0760124318E-01	-2.6909416431E-06	3.3376630516E-06	3.0281812270E-01	2.8283589138E-01	4.7831204771E-03
H6	-3.0760050543E-01	4.1071051346E-06	5.7605415421E-06	3.0281722562E-01	-2.8283598531E-01	4.7832798119E-03

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
C1	1	-3.4478965438E+00	9.9999983933E-01	-5.5826552766E-04	9.8396065398E-05
C1	2	1.2750391639E+00	5.5843267353E-04	9.9999838725E-01	-1.7069431425E-03
C1	3	2.1728573799E+00	-9.7442979195E-05	1.7069978159E-03	9.9999853833E-01
H2	1	-3.0760140199E-01	9.999999976E-01	1.1894091935E-05	-1.8164267637E-05
H2	2	-1.6589117315E-01	2.1697275532E-05	-5.1665755226E-01	8.5619213569E-01
H2	3	4.7349257515E-01	-7.9892192024E-07	8.5619213589E-01	5.1665755239E-01
H3	1	-3.0760182200E-01	9.9999999860E-01	-2.8126628546E-05	-4.4708991195E-05
H3	2	-1.6589044810E-01	5.2811321902E-05	5.1665770434E-01	8.5619204257E-01
H3	3	4.7349227010E-01	9.8255079176E-07	8.5619204374E-01	-5.1665770510E-01

C4	1	-3.4478872467E+00	9.9999983917E-01	-5.5846237907E-04	9.8852956558E-05
C4	2	1.2750321843E+00	5.5863091202E-04	9.9999837653E-01	-1.7131481329E-03
C4	3	2.1728550624E+00	-9.7896067291E-05	1.7132030797E-03	9.9999852767E-01
H5	1	-3.0760124331E-01	9.9999999955E-01	1.6122774401E-05	-2.5282194740E-05
H5	2	-1.6589041208E-01	2.9976369558E-05	-5.1665764835E-01	8.5619207746E-01
H5	3	4.7349165539E-01	-7.4195242956E-07	8.5619207783E-01	5.1665764860E-01
H6	1	-3.0760050578E-01	9.9999999876E-01	-2.6310627866E-05	-4.2262545304E-05
H6	2	-1.6589061762E-01	4.9778444158E-05	5.1665833234E-01	8.5619166379E-01
H6	3	4.7349112340E-01	6.9164407132E-07	8.5619166484E-01	-5.1665833301E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3771707001E+02	1.4977320828E+01	6.0486875747E+00	6.3802783741E+00	1.0469499239E+01
H2	2.8778517202E+00	1.2500888994E+00	9.7559164388E-01	1.0935082232E+00	1.6406975542E+00
H3	2.8778511696E+00	1.2500883623E+00	9.7559108068E-01	1.0935075613E+00	1.6406966161E+00
C4	1.3771706778E+02	1.4977320636E+01	6.0486872133E+00	6.3802765538E+00	1.0469490388E+01
H5	2.8778514839E+00	1.2500886227E+00	9.7559126984E-01	1.0935076091E+00	1.6406962997E+00
H6	2.8778511668E+00	1.2500883417E+00	9.7559098851E-01	1.0935072219E+00	1.6406954300E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x*(d\rho/dx) + y*(d\rho/dy) + z*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (\text{A})$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (\text{A})$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (\text{A})$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (\text{A})$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (\text{A})$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3623645674E+02	-2.7536105179E+01	-1.4009412631E+01	-1.8007797368E+01	-3.7596826042E+01
H2	-2.2157946111E+00	-1.8083897557E+00	-2.1259679968E+00	-3.3072398056E+00	-6.5027869603E+00
H3	-2.2157941475E+00	-1.8083891849E+00	-2.1259671881E+00	-3.3072383823E+00	-6.5027837669E+00
C4	-1.3623645436E+02	-2.7536104093E+01	-1.4009408797E+01	-1.8007779423E+01	-3.7596740726E+01
H5	-2.2157942952E+00	-1.8083892750E+00	-2.1259671276E+00	-3.3072379182E+00	-6.5027820873E+00
H6	-2.2157941259E+00	-1.8083890380E+00	-2.1259666208E+00	-3.3072363752E+00	-6.5027767174E+00

Atomic Electronic Spin Populations:

$$N\_alpha(A) = \text{Average number of Alpha electrons in Atom A}$$

$$N\_beta(A) = \text{Average number of Beta electrons in Atom A}$$

$$N\_total(A) = N\_alpha(A) + N\_beta(A)$$

$$N\_spin(A) = N\_alpha(A) - N\_beta(A)$$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)
C1	3.0243437874E+00	3.0243437874E+00	6.0486875747E+00	0.0000000000E+00
H2	4.8779582194E-01	4.8779582194E-01	9.7559164388E-01	0.0000000000E+00

H3	4.8779554034E-01	4.8779554034E-01	9.7559108068E-01	0.0000000000E+00
C4	3.0243436067E+00	3.0243436067E+00	6.0486872133E+00	0.0000000000E+00
H5	4.8779563492E-01	4.8779563492E-01	9.7559126984E-01	0.0000000000E+00
H6	4.8779549425E-01	4.8779549425E-01	9.7559098851E-01	0.0000000000E+00

Total	7.9998698855E+00	7.9998698855E+00	1.5999739771E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A)

will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

C2H6

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\c2h6\c2h6.wfn

Sum File: D:\calc\ellipticity\c2h6\c2h6.sum

SumViz File: D:\calc\ellipticity\c2h6\c2h6.sumviz

Wfn Title: c2h6_mp2

Total memory allocated for AIMSum = 0.549 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	17.9999997000
Number of Alpha electrons (from MO Occs)	=	8.9999998500
Number of Beta electrons (from MO Occs)	=	8.9999998500
Number of electron pairs ($N*(N-1)/2$)	=	152.9999947500

Number of electron pairs (from Muller 2EDM) = 152.9999582000

Number of electron pairs (from Muller 2EDM, no SOSI) = 153.2061451831

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	0.0000000000E+00	0.0000000000E+00	1.4448378600E+00
H2	1.0	-9.6359892000E-01	1.6690025500E+00	2.1900151300E+00
H3	1.0	-9.6359915000E-01	-1.6690024200E+00	2.1900151300E+00
H4	1.0	1.9271980700E+00	-1.3000000000E-07	2.1900151300E+00
C5	6.0	0.0000000000E+00	0.0000000000E+00	-1.4448378600E+00
H6	1.0	9.6359915000E-01	-1.6690024200E+00	-2.1900151300E+00
H7	1.0	-1.9271980700E+00	-1.3000000000E-07	-2.1900151300E+00
H8	1.0	9.6359892000E-01	1.6690025500E+00	-2.1900151300E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
C1	2.8353851500E-02	5.3229216040E-05	3.7866370847E+01	-3.7915159393E+01	5.2024081266E-02
H2	-9.3981914000E-03	3.5388319444E-05	6.2424722087E-01	-6.2505152596E-01	1.5821852880E-01
H3	-9.3977037000E-03	3.5608376536E-05	6.2424714470E-01	-6.2505144969E-01	1.5821880167E-01

H4	-9.4009473000E-03	3.3504864941E-05	6.2424746952E-01	-6.2505177493E-01	1.5821711353E-01
C5	2.8367605900E-02	6.4915044154E-05	3.7866372579E+01	-3.7915161128E+01	5.2017464431E-02
H6	-9.4049704000E-03	3.1900979617E-05	6.2424852018E-01	-6.2505282695E-01	1.5821495263E-01
H7	-9.4015142000E-03	3.3764414689E-05	6.2424790235E-01	-6.2505220832E-01	1.5821658088E-01
H8	-9.4056064000E-03	3.0820582967E-05	6.2424802554E-01	-6.2505233166E-01	1.5821508319E-01

Total	3.1252400000E-04	3.1913179839E-04	7.9478229709E+01	-7.9580632639E+01	

Molecular charge q(Mol) from the wfn file: 2.9999999999E-07

Molecular energy E(Mol) from the wfn file: -7.9251730534E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0012884400E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	
C1	35	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

H3	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	9	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C5	33	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H6	9	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H7	9	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	9	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 124

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -3.32382374488136E-15 -9.31357669844972E-16 1.44483715983616E+00

Type = (3,-3) NACP C1

Rho = 1.1936888736E+02 Rho at Nucleus = 1.1936888732E+02

GradRho = 5.4199372337E-18 -4.0428345164E-17 -1.5633583317E-10

HessRho_EigVals = -1.8097254483E+05 -1.8097192858E+05 -1.8097192858E+05

HessRho_EigVec1 = 1.1527593761E-09 2.1545357887E-10 1.0000000000E+00

HessRho_EigVec2 = 6.8575516530E-01 7.2783229749E-01 -9.4732476982E-10

HessRho_EigVec3 = 7.2783229749E-01 -6.8575516530E-01 -6.9126710058E-10

DelSqRho = -5.4291640199E+05

Bond Ellipticity = NA

V = -1.3574431046E+05

G = 7.6049792187E+00

K = 1.3573670548E+05

L = 1.3572910050E+05

Vnuc = 8.5694270886E+06

Ven = -1.0229229769E+09

Vrep = 1.0227872326E+09

DelSqV = 4.6003551824E+09
DelSqVen = 4.6524819046E+12
DelSqVrep = -4.6478815495E+12
DelSqG = 2.0580068262E+08
DelSqK = -4.8061558650E+09
Stress_EigVals = -4.5248156410E+04 -4.5248156410E+04 -4.5247997636E+04
Stress_EigVec1 = 7.8076431854E-01 -6.2482563879E-01 -1.7204741200E-09
Stress_EigVec2 = 6.2482563879E-01 7.8076431854E-01 1.3612966754E-10
Stress_EigVec3 = 1.2582274974E-09 -1.1812815282E-09 1.0000000000E+00
-DivStress = 4.6017003292E-06 1.5605121950E-06 1.0487586852E+03

CP# 2 Coords = -9.50890785173727E-01 1.64699141126356E+00 2.17993852169848E+00

Type = (3,-3) NACP H2

Rho = 4.2897564380E-01 Rho at Nucleus = 4.2593029764E-01

GradRho = 1.2906762742E-09 -2.2355165705E-09 -1.0235173785E-09

HessRho_EigVals = -8.5585623987E+00 -8.5566376695E+00 -7.9214140011E+00

HessRho_EigVec1 = -1.8437385159E-01 3.1934499138E-01 -9.2952948277E-01

HessRho_EigVec2 = 8.6602544400E-01 4.9999993035E-01 2.8791195559E-08

HessRho_EigVec3 = -4.6476468583E-01 8.0499617771E-01 3.6874780090E-01

DelSqRho = -2.5036614069E+01

Bond Ellipticity = NA

V = -6.2796671475E+00

G = 1.0256815088E-02

K = 6.2694103324E+00

L = 6.2591535173E+00

Vnuc = 4.2178213708E+01

Ven = -1.8093426380E+01

Vrep = 1.1813759232E+01

DelSqV = 1.6207346905E+03

DelSqVen = 1.0559996662E+03

DelSqVrep = 5.6473502439E+02

DelSqG = 1.2299345976E+02

DelSqK = -1.7437281503E+03

Stress_EigVals = -2.1465753238E+00 -2.1463757510E+00 -1.9867160726E+00

Stress_EigVec1 = 1.8407922805E-01 -3.1883468767E-01 9.2976302343E-01

Stress_EigVec2 = 8.6602544401E-01 4.9999993032E-01 2.8408364784E-08

Stress_EigVec3 = -4.6488145599E-01 8.0519842997E-01 3.6815855315E-01

-DivStress = -6.6658766394E+00 1.1545638881E+01 5.2844222785E+00

CP# 3 Coords = -9.50891012176370E-01 -1.64699128317406E+00 2.17993852179106E+00

Type = (3,-3) NACP H3

Rho = 4.2897564359E-01 Rho at Nucleus = 4.2593029746E-01

GradRho = 1.2906718229E-09 2.2355097634E-09 -1.0235135542E-09

HessRho_EigVals = -8.5585624280E+00 -8.5566376988E+00 -7.9214140340E+00

HessRho_EigVec1 = -1.8437396338E-01 -3.1934492592E-01 -9.2952948308E-01

HessRho_EigVec2 = 8.6602536029E-01 -5.0000007533E-01 -4.4165306697E-08

HessRho_EigVec3 = 4.6476479746E-01 8.0499611363E-01 -3.6874780011E-01

DelSqRho = -2.5036614161E+01

Bond Ellipticity = NA

V = -6.2796671703E+00

G = 1.0256815040E-02

K = 6.2694103552E+00

L = 6.2591535402E+00

Vnuc = 4.2178213943E+01

Ven = -1.8093426472E+01

Vrep = 1.1813759301E+01

DelSqV = 1.6207346979E+03

DelSqVen = 1.0559996759E+03

DelSqVrep = 5.6473502205E+02

DelSqG = 1.2299346070E+02

DelSqK = -1.7437281587E+03

Stress_EigVals = -2.1465753311E+00 -2.1463757583E+00 -1.9867160808E+00

Stress_EigVec1 = 1.8407939106E-01 3.1883459258E-01 9.2976302377E-01

Stress_EigVec2 = 8.6602534954E-01 -5.0000009396E-01 -9.9746473334E-08

Stress_EigVec3 = 4.6488156744E-01 8.0519836600E-01 -3.6815855231E-01

-DivStress = -6.6658782389E+00 -1.1545637926E+01 5.2844222518E+00

CP# 4 Coords = 1.90178179722078E+00 -1.28285786085323E-07 2.17993852169683E+00

Type = (3,-3) NACP H4

Rho = 4.2897564504E-01 Rho at Nucleus = 4.2593029892E-01

GradRho = -3.8337388819E-16 5.2041704279E-18 2.5847379792E-16

HessRho_EigVals = -8.5585624781E+00 -8.5566377489E+00 -7.9214140759E+00

HessRho_EigVec1 = -3.6874780030E-01 1.0622660734E-07 9.2952948301E-01

HessRho_EigVec2 = 9.6998048481E-08 1.0000000000E+00 -7.5800490056E-08

HessRho_EigVec3 = 9.2952948301E-01 -6.2211281888E-08 3.6874780030E-01

DelSqRho = -2.5036614303E+01

Bond Ellipticity = NA

V = -6.2796672058E+00

G = 1.0256815060E-02

K = 6.2694103908E+00

L = 6.2591535757E+00

Vnuc = 4.2178213635E+01

Ven = -1.8093426401E+01

Vrep = 1.1813759195E+01

DelSqV = 1.6207347091E+03

DelSqVen = 1.0559996668E+03

DelSqVrep = 5.6473504235E+02

DelSqG = 1.2299346157E+02

DelSqK = -1.7437281707E+03

Stress_EigVals = -2.1465753437E+00 -2.1463757709E+00 -1.9867160913E+00

Stress_EigVec1 = -3.6815855282E-01 1.9593148812E-07 9.2976302356E-01

Stress_EigVec2 = 1.2964663189E-07 1.0000000000E+00 -1.5939649996E-07

Stress_EigVec3 = 9.2976302356E-01 -6.1857459715E-08 3.6815855282E-01

-DivStress = 1.3331755056E+01 -8.9834728242E-07 5.2844223347E+00

CP# 5 Coords = 9.51200757332645E-15 3.03362809854582E-15 -1.44483715983616E+00

Type = (3,-3) NACP C5

Rho = 1.1936888758E+02 Rho at Nucleus = 1.1936888753E+02

GradRho = -2.8816490172E-17 1.1428389692E-17 1.3572742930E-10

HessRho_EigVals = -1.8097254506E+05 -1.8097192881E+05 -1.8097192881E+05

HessRho_EigVec1 = 2.1269993060E-09 4.7088555154E-10 1.0000000000E+00

HessRho_EigVec2 = 9.9204523357E-01 -1.2588190719E-01 -2.0508035520E-09

HessRho_EigVec3 = 1.2588190719E-01 9.9204523357E-01 -7.3489049619E-10

DelSqRho = -5.4291640268E+05

Bond Ellipticity = NA

V = -1.3574431063E+05

G = 7.6049791924E+00

K = 1.3573670565E+05

L = 1.3572910067E+05

Vnuc = 8.5694271076E+06

Ven = -1.0229229810E+09

Vrep = 1.0227872367E+09

DelSqV = 4.6003551866E+09

DelSqVen = 4.6524819046E+12

DelSqVrep = -4.6478815495E+12

DelSqG = 2.0580068277E+08

DelSqK = -4.8061558693E+09

Stress_EigVals = -4.5248156467E+04 -4.5248156467E+04 -4.5247997694E+04

Stress_EigVec1 = 3.4536234194E-01 9.3846942026E-01 -2.3805848174E-09

Stress_EigVec2 = 9.3846942026E-01 -3.4536234194E-01 -1.1769852669E-09

Stress_EigVec3 = 1.9267290288E-09 1.8276196653E-09 1.0000000000E+00

-DivStress = -1.3221529020E-05 -3.9405816160E-06 -1.0487586841E+03

CP# 6 Coords = 9.50891012020945E-01 -1.64699128294667E+00 -2.17993852170157E+00

Type = (3,-3) NACP H6

Rho = 4.2897564150E-01 Rho at Nucleus = 4.2593029534E-01

GradRho = -1.2906730025E-09 2.2355110506E-09 1.0235113896E-09

HessRho_EigVals = -8.5585623554E+00 -8.5566376262E+00 -7.9214139566E+00

HessRho_EigVec1 = -1.8437397711E-01 3.1934491765E-01 -9.2952948320E-01

HessRho_EigVec2 = 8.6602535688E-01 5.0000008123E-01 -5.8701819910E-08

HessRho_EigVec3 = -4.6476479836E-01 8.0499611325E-01 3.6874779981E-01

DelSqRho = -2.5036613938E+01

Bond Ellipticity = NA

V = -6.2796671145E+00

G = 1.0256814981E-02

K = 6.2694102995E+00

L = 6.2591534846E+00

Vnuc = 4.2178213558E+01

Ven = -1.8093426218E+01

Vrep = 1.1813759104E+01

DelSqV = 1.6207346812E+03

DelSqVen = 1.0559996569E+03

DelSqVrep = 5.6473502436E+02

DelSqG = 1.2299345914E+02

DelSqK = -1.7437281404E+03

Stress_EigVals = -2.1465753130E+00 -2.1463757401E+00 -1.9867160614E+00

Stress_EigVec1 = 1.8407939886E-01 -3.1883458763E-01 9.2976302392E-01

Stress_EigVec2 = 8.6602534726E-01 5.0000009791E-01 -1.0786146342E-07

Stress_EigVec3 = -4.6488156860E-01 8.0519836551E-01 3.6815855192E-01

-DivStress = 6.6658782552E+00 -1.1545637934E+01 -5.2844222472E+00

CP# 7 Coords = -1.90178179692366E+00 -1.28252167777400E-07 -2.17993852161698E+00

Type = (3,-3) NACP H7

Rho = 4.2897564226E-01 Rho at Nucleus = 4.2593029610E-01

GradRho = 3.9378222905E-16 0.0000000000E+00 1.2524703497E-15

HessRho_EigVals = -8.5585623972E+00 -8.5566376680E+00 -7.9214139903E+00

HessRho_EigVec1 = -3.6874779977E-01 -1.0064672913E-07 9.2952948322E-01

HessRho_EigVec2 = -9.5994065852E-08 1.0000000000E+00 7.0195867624E-08

HessRho_EigVec3 = 9.2952948322E-01 6.3344742684E-08 3.6874779977E-01

DelSqRho = -2.5036614056E+01

Bond Ellipticity = NA

V = -6.2796671439E+00

G = 1.0256815016E-02

K = 6.2694103289E+00

L = 6.2591535139E+00

Vnuc = 4.2178213227E+01

Ven = -1.8093426108E+01

Vrep = 1.1813758965E+01

DelSqV = 1.6207346900E+03

DelSqVen = 1.0559996461E+03

DelSqVrep = 5.6473504384E+02

DelSqG = 1.2299345995E+02

DelSqK = -1.7437281499E+03

Stress_EigVals = -2.1465753234E+00 -2.1463757506E+00 -1.9867160699E+00

Stress_EigVec1 = -3.6815855210E-01 -1.8520842483E-07 9.2976302385E-01

Stress_EigVec2 = -1.2702766980E-07 1.0000000000E+00 1.4890041687E-07

Stress_EigVec3 = 9.2976302385E-01 6.3286668500E-08 3.6815855210E-01

-DivStress = -1.3331755063E+01 -9.1604861401E-07 -5.2844223167E+00

CP# 8 Coords = 9.50890785093788E-01 1.64699141112902E+00 -2.17993852168812E+00

Type = (3,-3) NACP H8

Rho = 4.2897564354E-01 Rho at Nucleus = 4.2593029736E-01

GradRho = -1.2906767669E-09 -2.2355164941E-09 1.0235174843E-09

HessRho_EigVals = -8.5585623817E+00 -8.5566376524E+00 -7.9214139796E+00

HessRho_EigVec1 = -1.8437383810E-01 -3.1934499828E-01 -9.2952948307E-01

HessRho_EigVec2 = 8.6602544687E-01 -4.9999992538E-01 4.2791437224E-08

HessRho_EigVec3 = 4.6476468584E-01 8.0499617806E-01 -3.6874780013E-01

DelSqRho = -2.5036614014E+01

Bond Ellipticity = NA

V = -6.2796671335E+00

G = 1.0256815031E-02

K = 6.2694103185E+00

L = 6.2591535034E+00
Vnuc = 4.2178213509E+01
Ven = -1.8093426283E+01
Vrep = 1.1813759150E+01
DelSqV = 1.6207346844E+03
DelSqVen = 1.0559996588E+03
DelSqVrep = 5.6473502562E+02
DelSqG = 1.2299345930E+02
DelSqK = -1.7437281437E+03
Stress_EigVals = -2.1465753196E+00 -2.1463757467E+00 -1.9867160672E+00
Stress_EigVec1 = 1.8407912729E-01 3.1883474479E-01 9.2976302379E-01
Stress_EigVec2 = 8.6602546537E-01 -4.9999989333E-01 1.3606278554E-07
Stress_EigVec3 = 4.6488145610E-01 8.0519843031E-01 -3.6815855224E-01
-DivStress = 6.6658766592E+00 1.1545638910E+01 -5.2844222648E+00

CP# 9 Coords = -1.07365575431581E-11 1.08443900029450E-10 -7.48491107960398E-12

Type = (3,-1) BCP C1 C5
Rho = 2.3947532486E-01
GradRho = 1.8945290447E-19 6.5804630608E-20 -3.8249350911E-17
HessRho_EigVals = -4.3920313394E-01 -4.3920313390E-01 3.2190432428E-01
HessRho_EigVec1 = 9.8198964256E-01 1.8893475568E-01 1.0205089674E-10
HessRho_EigVec2 = -1.8893475568E-01 9.8198964256E-01 2.4444990200E-11
HessRho_EigVec3 = -9.5594415365E-11 -4.3285688432E-11 1.0000000000E+00
DelSqRho = -5.5650194357E-01
Bond Ellipticity = 9.0866203450E-11
V = -2.6154198769E-01
G = 6.1208250901E-02
K = 2.0033373679E-01
L = 1.3912548589E-01
Vnuc = 1.0362172455E+01
Ven = -2.4814846150E+00
Vrep = 2.2199426273E+00

DelSqV = -1.4647376047E+00

DelSqVen = 5.7665691109E+00

DelSqVrep = -7.2313067156E+00

DelSqG = 1.0464419159E+00

DelSqK = 4.1829568885E-01

Stress_EigVals = -1.5997784287E-01 -1.5997784286E-01 5.8413698040E-02

Stress_EigVec1 = -2.2460982523E-01 9.7444878080E-01 1.0229359917E-10

Stress_EigVec2 = 9.7444878080E-01 2.2460982523E-01 -1.8897705282E-10

Stress_EigVec3 = 2.0712460615E-10 -5.7233770189E-11 1.0000000000E+00

-DivStress = -3.3189503876E-12 -1.2250496644E-11 -7.6356858372E-12

BPL = 2.8896743197E+00 = 1.4448371598E+00 + 1.4448371598E+00

GBL_I = 2.8896743197E+00

GBL_II = 2.8896757200E+00

GBL_III = 2.8896743197E+00 = 1.4448371598E+00 + 1.4448371598E+00

GBL_IV = 2.8896757200E+00 = 1.4448378600E+00 + 1.4448378600E+00

CP# 10 Coords = -6.13457102930711E-01 1.06253903668012E+00 1.91234411276968E+00

Type = (3,-1) BCP H2 C1

Rho = 2.7250446533E-01

GradRho = -4.1633363423E-17 6.9388939039E-18 1.8388068845E-16

HessRho_EigVals = -6.8853790637E-01 -6.8301644408E-01 4.5930468409E-01

HessRho_EigVec1 = -1.8440057549E-01 3.1939121810E-01 -9.2950829881E-01

HessRho_EigVec2 = 8.6602543817E-01 4.9999994044E-01 8.9914817399E-10

HessRho_EigVec3 = -4.6475409433E-01 8.0497783160E-01 3.6880119637E-01

DelSqRho = -9.1224966636E-01

Bond Ellipticity = 8.0839375572E-03

V = -3.2580948161E-01

G = 4.8873532510E-02

K = 2.7693594910E-01

L = 2.2806241659E-01

Vnuc = 8.9424933667E+00

Ven = -2.4368693736E+00

Vrep = 2.1110598919E+00
DelSqV = -2.2515091282E+00
DelSqVen = 8.1577865902E+00
DelSqVrep = -1.0409295718E+01
DelSqG = 1.5525492968E+00
DelSqK = 6.9895983138E-01
Stress_EigVals = -2.1179389604E-01 -2.1120273571E-01 9.7187150136E-02
Stress_EigVec1 = 8.6602544101E-01 4.9999993552E-01 1.5188413485E-08
Stress_EigVec2 = 1.8396913583E-01 -3.1864397332E-01 9.2985018972E-01
Stress_EigVec3 = -4.6492503975E-01 8.0527391783E-01 3.6793834358E-01
-DivStress = 7.0423893217E-02 -1.2197777926E-01 -5.2142843978E-02
BPL = 2.0390570554E+00 = 7.2598404821E-01 + 1.3130730072E+00
GBL_I = 2.0389085333E+00
GBL_II = 2.0662481831E+00
GBL_III = 2.0389507533E+00 = 7.2598404670E-01 + 1.3129667066E+00
GBL_IV = 2.0662914063E+00 = 7.5332494905E-01 + 1.3129664573E+00

CP# 11 Coords = -6.13457249023778E-01 -1.06253895476579E+00 1.91234411331404E+00

Type = (3,-1) BCP C1 H3
Rho = 2.7250446425E-01
GradRho = -2.0816681712E-17 -9.0205620751E-17 -1.7347234760E-18
HessRho_EigVals = -6.8853790369E-01 -6.8301644137E-01 4.5930468604E-01
HessRho_EigVec1 = -1.8440063835E-01 -3.1939118104E-01 -9.2950829908E-01
HessRho_EigVec2 = 8.6602536532E-01 -5.0000006662E-01 -1.9785796707E-08
HessRho_EigVec3 = 4.6475420514E-01 8.0497776793E-01 -3.6880119570E-01
DelSqRho = -9.1224965902E-01
Bond Ellipticity = 8.0839376398E-03
V = -3.2580947913E-01
G = 4.8873532186E-02
K = 2.7693594694E-01
L = 2.2806241476E-01
Vnuc = 8.9424933579E+00

Ven = -2.4368693616E+00
Vrep = 2.1110598824E+00
DelSqV = -2.2515091389E+00
DelSqVen = 8.1577865166E+00
DelSqVrep = -1.0409295655E+01
DelSqG = 1.5525492915E+00
DelSqK = 6.9895984734E-01
Stress_EigVals = -2.1179389508E-01 -2.1120273476E-01 9.7187150718E-02
Stress_EigVec1 = 8.6602537003E-01 -5.0000005846E-01 2.6641392231E-09
Stress_EigVec2 = 1.8396919079E-01 3.1864394077E-01 9.2985019000E-01
Stress_EigVec3 = 4.6492515021E-01 8.0527385439E-01 -3.6793834286E-01
-DivStress = 7.0423908639E-02 1.2197776858E-01 -5.2142843559E-02
BPL = 2.0390570579E+00 = 1.3130730094E+00 + 7.2598404848E-01
GBL_I = 2.0389085357E+00
GBL_II = 2.0662481854E+00
GBL_III = 2.0389507557E+00 = 1.3129667088E+00 + 7.2598404696E-01
GBL_IV = 2.0662914086E+00 = 1.3129664595E+00 + 7.5332494914E-01

CP# 12 Coords = 1.22691435059250E+00 -8.30063164502057E-08 1.91234411255810E+00

Type = (3,-1) BCP H4 C1
Rho = 2.7250446477E-01
GradRho = 4.8572257327E-17 -2.0816681712E-17 3.1225022568E-17
HessRho_EigVals = -6.8853790421E-01 -6.8301644199E-01 4.5930468354E-01
HessRho_EigVec1 = -3.6880119583E-01 4.7541497812E-08 9.2950829902E-01
HessRho_EigVec2 = 7.5519674475E-08 1.0000000000E+00 -2.1182975535E-08
HessRho_EigVec3 = 9.2950829902E-01 -6.2383857456E-08 3.6880119583E-01
DelSqRho = -9.1224966266E-01
Bond Ellipticity = 8.0839374788E-03
V = -3.2580948051E-01
G = 4.8873532421E-02
K = 2.7693594809E-01
L = 2.2806241566E-01

Vnuc = 8.9424933608E+00

Ven = -2.4368693670E+00

Vrep = 2.1110598865E+00

DelSqV = -2.2515091040E+00

DelSqVen = 8.1577865518E+00

DelSqVrep = -1.0409295656E+01

DelSqG = 1.5525492920E+00

DelSqK = 6.9895981197E-01

Stress_EigVals = -2.1179389544E-01 -2.1120273508E-01 9.7187150020E-02

Stress_EigVec1 = 4.6925401339E-08 1.0000000000E+00 4.8785358455E-08

Stress_EigVec2 = -3.6793834312E-01 -2.8097420405E-08 9.2985018990E-01

Stress_EigVec3 = 9.2985018990E-01 -6.1583597305E-08 3.6793834312E-01

-DivStress = -1.4084780367E-01 9.5784795876E-09 -5.2142844534E-02

BPL = 2.0390570583E+00 = 7.2598405033E-01 + 1.3130730079E+00

GBL_I = 2.0389085361E+00

GBL_II = 2.0662481857E+00

GBL_III = 2.0389507561E+00 = 7.2598404881E-01 + 1.3129667073E+00

GBL_IV = 2.0662914089E+00 = 7.5332495086E-01 + 1.3129664580E+00

CP# 13 Coords = 6.13457250760822E-01 -1.06253895836730E+00 -1.91234411475652E+00

Type = (3,-1) BCP C5 H6

Rho = 2.7250446456E-01

GradRho = 4.1633363423E-17 -6.2450045135E-17 -7.6327832943E-17

HessRho_EigVals = -6.8853790800E-01 -6.8301644577E-01 4.5930469089E-01

HessRho_EigVec1 = -1.8440065886E-01 3.1939116999E-01 -9.2950829880E-01

HessRho_EigVec2 = 8.6602536102E-01 5.0000007408E-01 -4.1432860584E-08

HessRho_EigVec3 = -4.6475420502E-01 8.0497776768E-01 3.6880119638E-01

DelSqRho = -9.1224966289E-01

Bond Ellipticity = 8.0839374548E-03

V = -3.2580947887E-01

G = 4.8873531573E-02

K = 2.7693594730E-01

L = 2.2806241572E-01
Vnuc = 8.9424933483E+00
Ven = -2.4368693617E+00
Vrep = 2.1110598829E+00
DelSqV = -2.2515092087E+00
DelSqVen = 8.1577865423E+00
DelSqVrep = -1.0409295751E+01
DelSqG = 1.5525492979E+00
DelSqK = 6.9895991076E-01
Stress_EigVals = -2.1179389567E-01 -2.1120273537E-01 9.7187152169E-02
Stress_EigVec1 = 8.6602537944E-01 5.0000004216E-01 5.2972884537E-08
Stress_EigVec2 = 1.8396914442E-01 -3.1864396786E-01 9.2985018990E-01
Stress_EigVec3 = -4.6492515103E-01 8.0527385378E-01 3.6793834314E-01
-DivStress = -7.0423904093E-02 1.2197776079E-01 5.2142840083E-02
BPL = 2.0390570576E+00 = 1.3130730136E+00 + 7.2598404395E-01
GBL_I = 2.0389085354E+00
GBL_II = 2.0662481854E+00
GBL_III = 2.0389507554E+00 = 1.3129667130E+00 + 7.2598404244E-01
GBL_IV = 2.0662914086E+00 = 1.3129664637E+00 + 7.5332494490E-01

CP# 14 Coords = -1.22691435498101E+00 -8.23440303617138E-08 -1.91234411433536E+00

Type = (3,-1) BCP C5 H7
Rho = 2.7250446448E-01
GradRho = 0.0000000000E+00 -3.4694469520E-18 1.1796119637E-16
HessRho_EigVals = -6.8853790788E-01 -6.8301644558E-01 4.5930468941E-01
HessRho_EigVec1 = -3.6880119638E-01 -4.5048276854E-08 9.2950829880E-01
HessRho_EigVec2 = -7.5192683205E-08 1.0000000000E+00 1.8630414974E-08
HessRho_EigVec3 = 9.2950829880E-01 6.3021303717E-08 3.6880119638E-01
DelSqRho = -9.1224966405E-01
Bond Ellipticity = 8.0839375671E-03
V = -3.2580947949E-01
G = 4.8873531737E-02

K = 2.7693594775E-01
L = 2.2806241601E-01
Vnuc = 8.9424933500E+00
Ven = -2.4368693615E+00
Vrep = 2.1110598820E+00
DelSqV = -2.2515091870E+00
DelSqVen = 8.1577865543E+00
DelSqVrep = -1.0409295741E+01
DelSqG = 1.5525493001E+00
DelSqK = 6.9895988690E-01
Stress_EigVals = -2.1179389585E-01 -2.1120273546E-01 9.7187151817E-02
Stress_EigVec1 = -3.6093603641E-08 1.0000000000E+00 -7.9113404233E-08
Stress_EigVec2 = -3.6793834332E-01 6.0283393215E-08 9.2985018982E-01
Stress_EigVec3 = 9.2985018982E-01 6.2670499085E-08 3.6793834332E-01
-DivStress = 1.4084779342E-01 9.3820970129E-09 5.2142840577E-02
BPL = 2.0390570580E+00 = 1.3130730127E+00 + 7.2598404529E-01
GBL_I = 2.0389085358E+00
GBL_II = 2.0662481857E+00
GBL_III = 2.0389507558E+00 = 1.3129667121E+00 + 7.2598404377E-01
GBL_IV = 2.0662914089E+00 = 1.3129664627E+00 + 7.5332494613E-01

CP# 15 Coords = 6.13457104449618E-01 1.06253903927055E+00 -1.91234411409466E+00

Type = (3,-1) BCP H8 C5
Rho = 2.7250446579E-01
GradRho = -5.5511151231E-17 -1.1796119637E-16 2.3418766926E-17
HessRho_EigVals = -6.8853791105E-01 -6.8301644872E-01 4.5930469076E-01
HessRho_EigVec1 = -1.8440056656E-01 -3.1939122395E-01 -9.2950829857E-01
HessRho_EigVec2 = 8.6602544014E-01 -4.9999993703E-01 1.0807332797E-08
HessRho_EigVec3 = 4.6475409421E-01 8.0497783139E-01 -3.6880119697E-01
DelSqRho = -9.1224966902E-01
Bond Ellipticity = 8.0839375693E-03
V = -3.2580948125E-01

G = 4.8873531996E-02
K = 2.7693594925E-01
L = 2.2806241725E-01
Vnuc = 8.9424933591E+00
Ven = -2.4368693757E+00
Vrep = 2.1110598944E+00
DelSqV = -2.2515092033E+00
DelSqVen = 8.1577866071E+00
DelSqVrep = -1.0409295810E+01
DelSqG = 1.5525493087E+00
DelSqK = 6.9895989457E-01
Stress_EigVals = -2.1179389680E-01 -2.1120273649E-01 9.7187152042E-02
Stress_EigVec1 = 8.6602542175E-01 -4.9999996889E-01 -8.2463627812E-08
Stress_EigVec2 = 1.8396922688E-01 3.1864392106E-01 9.2985018962E-01
Stress_EigVec3 = 4.6492503961E-01 8.0527391780E-01 -3.6793834383E-01
-DivStress = -7.0423890068E-02 -1.2197777438E-01 5.2142841861E-02
BPL = 2.0390570553E+00 = 7.2598404479E-01 + 1.3130730105E+00
GBL_I = 2.0389085332E+00
GBL_II = 2.0662481831E+00
GBL_III = 2.0389507531E+00 = 7.2598404327E-01 + 1.3129667099E+00
GBL_IV = 2.0662914063E+00 = 7.5332494577E-01 + 1.3129664606E+00

Number of NACPs = 8

Number of NNACPs = 0

Number of BCPs = 7

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H2	C1	C5	110.01689718	111.13316049	111.13967008	110.85898498	110.85895643
H3	C1	C5	110.01689728	111.13316047	111.13967005	110.85898498	110.85895643
H3	C1	H2	108.92007496	107.75936279	107.75246614	108.04851147	108.04854145
H4	C1	C5	110.01689721	111.13316047	111.13967005	110.85898496	110.85895641
H4	C1	H2	108.92007511	107.75936280	107.75246615	108.04851153	108.04854150
H4	C1	H3	108.92007507	107.75936291	107.75246627	108.04851159	108.04854156
H6	C5	C1	110.01689735	111.13316047	111.13967005	110.85898498	110.85895642
H7	C5	C1	110.01689733	111.13316047	111.13967005	110.85898497	110.85895642
H7	C5	H6	108.92007504	107.75936291	107.75246627	108.04851160	108.04854157
H8	C5	C1	110.01689721	111.13316050	111.13967008	110.85898499	110.85895644
H8	C5	H6	108.92007490	107.75936279	107.75246614	108.04851148	108.04854146
H8	C5	H7	108.92007497	107.75936280	107.75246615	108.04851150	108.04854147

Total time for electron density critical point search, analysis and connectivity = 7 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, \text{Mol})$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7866370847E+01	3.7866370847E+01	-1.1466998718E+02	-8.9764759581E+01		
H2	-6.2424722087E-01	6.2424722087E-01	-6.4976429472E+00	-1.2789279809E+00		
H3	-6.2424714470E-01	6.2424714470E-01	-6.4976397586E+00	-1.2789276266E+00		
H4	-6.2424746952E-01	6.2424746952E-01	-6.4976602224E+00	-1.2789298519E+00		
C5	-3.7866372579E+01	3.7866372579E+01	-1.1466991732E+02	-8.9764730567E+01		
H6	-6.2424852018E-01	6.2424852018E-01	-6.4976871855E+00	-1.2789329161E+00		
H7	-6.2424790235E-01	6.2424790235E-01	-6.4976654827E+00	-1.2789304644E+00		
H8	-6.2424802554E-01	6.2424802554E-01	-6.4976891891E+00	-1.2789329296E+00		
Total	-7.9478229709E+01	7.9478229709E+01	-2.6832588929E+02	-1.8720307192E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)
C1	-3.7866370847E+01					
H2	-6.2424722087E-01					
H3	-6.2424714470E-01					
H4	-6.2424746952E-01					
C5	-3.7866372579E+01					
H6	-6.2424852018E-01					
H7	-6.2424790235E-01					
H8	-6.2424802554E-01					
Total	-7.9478229709E+01					

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	E_IQA(A) VeeX(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2
C1 1.2772364325E+01			3.7866370847E+01	-5.7073305150E+01	-5.7334993592E+01	
H2 2.7753498199E+00			6.2424722087E-01	-3.3361932557E+00	-3.2488214736E+00	
H3 2.7753498179E+00			6.2424714470E-01	-3.3361932525E+00	-3.2488198793E+00	
H4 2.7753498177E+00			6.2424746952E-01	-3.3361932540E+00	-3.2488301112E+00	
C5 1.2772364325E+01			3.7866372579E+01	-5.7073305164E+01	-5.7334958658E+01	
H6 2.7753498179E+00			6.2424852018E-01	-3.3361932500E+00	-3.2488435927E+00	
H7 2.7753498177E+00			6.2424790235E-01	-3.3361932493E+00	-3.2488327413E+00	
H8 2.7753498199E+00			6.2424802554E-01	-3.3361932540E+00	-3.2488445945E+00	
Total 4.2196827561E+01			7.9478229709E+01	-1.3416376983E+02	-1.3416294464E+02	

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)
C1	3.7866370847E+01	-8.9764759581E+01				
H2	6.2424722087E-01	-1.2789279809E+00				
H3	6.2424714470E-01	-1.2789276266E+00				
H4	6.2424746952E-01	-1.2789298519E+00				
C5	3.7866372579E+01	-8.9764730567E+01				
H6	6.2424852018E-01	-1.2789329161E+00				
H7	6.2424790235E-01	-1.2789304644E+00				
H8	6.2424802554E-01	-1.2789329296E+00				
Total	7.9478229709E+01	-1.8720307192E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$$VeeC(A,A') = \text{Coulomb Part of } Vee(A,A')$$

$$VeeX(A,A') = \text{Exchange-Correlation Part of } Vee(A,A')$$

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Inter(A)	Vne(A,A')/2	Ven(A,A')/2	Vee(A,A')	Vnn(A)	VeeC(A,A')
VeeX(A,A')						
C1	-1.2190925359E+01	-1.2452613801E+01		1.2772364325E+01		
H2	-2.6967292653E+00	-2.6093574832E+00		2.7753498199E+00		
H3	-2.6967294392E+00	-2.6093560660E+00		2.7753498179E+00		
H4	-2.6967283280E+00	-2.6093651852E+00		2.7753498177E+00		
C5	-1.2190939880E+01	-1.2452593374E+01		1.2772364325E+01		
H6	-2.6967267920E+00	-2.6093771347E+00		2.7753498179E+00		
H7	-2.6967280171E+00	-2.6093675091E+00		2.7753498177E+00		
H8	-2.6967267892E+00	-2.6093781298E+00		2.7753498199E+00		
Total	-4.0562233870E+01	-4.0561408683E+01		4.2196827561E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')

C1	5.9716461485E+00	4.2070210025E+00	7.0449937888E+01	1.7646251460E+00
	2.9550062112E+01			
H2	1.0093981917E+00	5.2160908462E-01	5.1675254513E+01	4.8778910709E-01
	4.8324745487E+01			
H3	1.0093977038E+00	5.2160866144E-01	5.1675237567E+01	4.8778904237E-01
	4.8324762433E+01			
H4	1.0094009474E+00	5.2161137665E-01	5.1675340507E+01	4.8778957074E-01
	4.8324659493E+01			
C5	5.9716323942E+00	4.2070083552E+00	7.0449888363E+01	1.7646240390E+00
	2.9550111637E+01			
H6	1.0094049704E+00	5.2161471500E-01	5.1675465277E+01	4.8779025543E-01
	4.8324534723E+01			
H7	1.0094015139E+00	5.2161186049E-01	5.1675359436E+01	4.8778965346E-01
	4.8324640564E+01			
H8	1.0094056064E+00	5.2161505209E-01	5.1675466115E+01	4.8779055430E-01
	4.8324533885E+01			

Total	1.7999687476E+01	1.1543700108E+01	6.4132780767E+01	6.4559873684E+00
	3.5867219233E+01			

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that

are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that

are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1 5.4445709056E-02	5.9716461485E+00		4.2070210025E+00	1.7646251460E+00	1.7101794369E+00
H2 6.2605525914E-02	1.0093981917E+00		5.2160908462E-01	4.8778910709E-01	4.2518358118E-01
H3 6.2583207551E-02	1.0093977038E+00		5.2160866144E-01	4.8778904237E-01	4.2520583482E-01
H4 6.2637052450E-02	1.0094009474E+00		5.2161137665E-01	4.8778957074E-01	4.2515251829E-01
C5 5.4443712379E-02	5.9716323942E+00		4.2070083552E+00	1.7646240390E+00	1.7101803266E+00
H6 6.2606501644E-02	1.0094049704E+00		5.2161471500E-01	4.8779025543E-01	4.2518375378E-01
H7 6.2640762908E-02	1.0094015139E+00		5.2161186049E-01	4.8778965346E-01	4.2514889055E-01
H8 6.2580374623E-02	1.0094056064E+00		5.2161505209E-01	4.8779055430E-01	4.2521017968E-01
Total 4.8454284653E-01	1.7999687476E+01		1.1543700108E+01	6.4559873684E+00	5.9714445219E+00

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

C1	1.5726768360E+01	3.5032220177E+01	5.0758988537E+01
H2	2.4863781241E-01	8.3312415144E+00	8.5798793268E+00
H3	2.4863753151E-01	8.3312376481E+00	8.5798751796E+00
H4	2.4863944797E-01	8.3312633021E+00	8.5799027500E+00
C5	1.5726692548E+01	3.5032179078E+01	5.0758871626E+01
H6	2.4864183966E-01	8.3312951063E+00	8.5799369460E+00
H7	2.4863977794E-01	8.3312677879E+00	8.5799075658E+00
H8	2.4864231306E-01	8.3313000385E+00	8.5799423515E+00

Total 3.2945299631E+01 1.2005200465E+02 1.5299730428E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized
 (Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$
C1	H2	5.6025852426E+00	8.5036716236E-01	7.1200397781E+00	4.2122482948E+01 (Bonded)
C1	H3	5.6025600754E+00	8.5041166964E-01	7.1204124332E+00	4.2124707954E+01 (Bonded)
H2	H3	1.0010732197E+00	3.5621994420E-02	1.7645164571E+00	1.7645173100E+00
C1	H4	5.6026327615E+00	8.5030503658E-01	7.1195196051E+00	4.2119290594E+01 (Bonded)
H2	H4	1.0010763236E+00	3.5622334834E-02	1.7645333193E+00	1.7645285021E+00

H3	H4	1.0010758594E+00	3.5622278280E-02	1.7645313708E+00	1.7645257007E+00
C1	C5	3.5225838084E+01	8.6927500527E-01	7.2783532686E+00	7.2783700326E+00 (Bonded)
H2	C5	6.0096332456E+00	3.6243389318E-02	1.7952969213E+00	3.0346299743E-01
H3	C5	6.0096282976E+00	3.6247458190E-02	1.7954993385E+00	3.0349706577E-01
H4	C5	6.0096526875E+00	3.6237417244E-02	1.7949961974E+00	3.0341299373E-01
C1	H6	6.0096874654E+00	3.6243676907E-02	3.0346470643E-01	1.7952991103E+00
H2	H6	1.0134520847E+00	1.0878934362E-02	5.3888219986E-01	5.3887858097E-01
H3	H6	1.0171849050E+00	3.4123087048E-03	1.6902696984E-01	1.6902575303E-01
H4	H6	1.0171881611E+00	3.4123446516E-03	1.6902820730E-01	1.6902753363E-01
C5	H6	5.6026116665E+00	8.5036750757E-01	7.1200590679E+00	4.2122217172E+01 (Bonded)
C1	H7	6.0096699144E+00	3.6237497352E-02	3.0341296563E-01	1.7949991580E+00
H2	H7	1.0171818787E+00	3.4123683252E-03	1.6902984141E-01	1.6902928508E-01
H3	H7	1.0171813363E+00	3.4124681337E-03	1.6903486707E-01	1.6903422902E-01
H4	H7	1.0134513819E+00	1.0878925112E-02	5.3888027054E-01	5.3887996808E-01
C5	H7	5.6026258889E+00	8.5029778111E-01	7.1194752538E+00	4.2118907559E+01 (Bonded)
H6	H7	1.0010835321E+00	3.5622746438E-02	1.7645418579E+00	1.7645479002E+00
C1	H8	6.0096891237E+00	3.6247955930E-02	3.0350053426E-01	1.7955099368E+00
H2	H8	1.0171860192E+00	3.4123491795E-03	1.6902889303E-01	1.6902765142E-01
H3	H8	1.0134522330E+00	1.0878936610E-02	5.3888257172E-01	5.3887835283E-01
H4	H8	1.0171887875E+00	3.4123758120E-03	1.6902975080E-01	1.6902897063E-01
C5	H8	5.6025890383E+00	8.5042035935E-01	7.1205015916E+00	4.2124808599E+01 (Bonded)
H6	H8	1.0010874228E+00	3.5623227015E-02	1.7645656629E+00	1.7645645511E+00
H7	H8	1.0010841092E+00	3.5622876060E-02	1.7645543210E+00	1.7645471669E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
C1	C5	5.6803164989E+01	4.4162208289E+01	3.5191073122E+01
C1	H2	4.2300237096E+01	3.2775125955E+01	2.6211893475E+01
C1	H3	4.2300237093E+01	3.2775125951E+01	2.6211893471E+01
C1	H4	4.2300093348E+01	3.2775187267E+01	2.6213220633E+01
C1	Total	1.8370373253E+02	1.4248764746E+02	1.1382808070E+02
H2	C1	4.2300237096E+01	3.2775125955E+01	2.6211893475E+01
H2	Total	4.2300237096E+01	3.2775125955E+01	2.6211893475E+01
H3	C1	4.2300237093E+01	3.2775125951E+01	2.6211893471E+01
H3	Total	4.2300237093E+01	3.2775125951E+01	2.6211893471E+01
H4	C1	4.2300093348E+01	3.2775187267E+01	2.6213220633E+01
H4	Total	4.2300093348E+01	3.2775187267E+01	2.6213220633E+01
C5	C1	5.6803164988E+01	4.4162208287E+01	3.5191073122E+01
C5	H6	4.2300093316E+01	3.2775187245E+01	2.6213220617E+01
C5	H7	4.2300237059E+01	3.2775125930E+01	2.6211893458E+01
C5	H8	4.2300093314E+01	3.2775187245E+01	2.6213220618E+01
C5	Total	1.8370358868E+02	1.4248770871E+02	1.1382940781E+02
H6	C5	4.2300093316E+01	3.2775187245E+01	2.6213220617E+01

H6	Total	4.2300093316E+01	3.2775187245E+01	2.6213220617E+01

H7	C5	4.2300237059E+01	3.2775125930E+01	2.6211893458E+01

H7	Total	4.2300237059E+01	3.2775125930E+01	2.6211893458E+01

H8	C5	4.2300093314E+01	3.2775187245E+01	2.6213220618E+01

H8	Total	4.2300093314E+01	3.2775187245E+01	2.6213220618E+01

Total	Total	6.2120831243E+02	4.8162629576E+02	3.8493283079E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N_{IAS}(A B)$	$G_{IAS}(A B)$	$K_{IAS}(A B)$	$L_{IAS}(A B)$	$\Delta \rho_{IAS}(A B)$ $V_{IAS}(A B)$

C1	C5	1.1508135297E+00	7.7502869684E-01	3.4073644809E-01	-4.3429224875E-01	1.7371689950E+00 -1.1157651449E+00

C1	H2	9.6269415296E-01	5.4394775263E-01	3.9986868436E-01	-1.4407906827E-01	5.7631627309E-01 -9.4381643699E-01

C1	H3	9.6269414932E-01	5.4394774979E-01	3.9986868112E-01	-1.4407906867E-01	5.7631627467E-01 -9.4381643091E-01

C1	H4	9.6269186584E-01	5.4394678466E-01	3.9986759964E-01	-1.4407918502E-01
		5.7631674007E-01	-9.4381438430E-01		

C1	Total	4.0388936978E+00	2.4068709839E+00	1.5403414132E+00	-8.6652957071E-01
		3.4661182828E+00	-3.9472123971E+00		

H2	C1	9.6269415296E-01	5.4394775263E-01	3.9986868436E-01	-1.4407906827E-01
		5.7631627309E-01	-9.4381643699E-01		

H2	Total	9.6269415296E-01	5.4394775263E-01	3.9986868436E-01	-1.4407906827E-01
		5.7631627309E-01	-9.4381643699E-01		

H3	C1	9.6269414932E-01	5.4394774979E-01	3.9986868112E-01	-1.4407906867E-01
		5.7631627467E-01	-9.4381643091E-01		

H3	Total	9.6269414932E-01	5.4394774979E-01	3.9986868112E-01	-1.4407906867E-01
		5.7631627467E-01	-9.4381643091E-01		

H4	C1	9.6269186584E-01	5.4394678466E-01	3.9986759964E-01	-1.4407918502E-01
		5.7631674007E-01	-9.4381438430E-01		

H4	Total	9.6269186584E-01	5.4394678466E-01	3.9986759964E-01	-1.4407918502E-01
		5.7631674007E-01	-9.4381438430E-01		

C5	C1	1.1508135297E+00	7.7502869684E-01	3.4073644809E-01	-4.3429224875E-01
		1.7371689950E+00	-1.1157651449E+00		

C5	H6	9.6269185886E-01	5.4394678002E-01	3.9986759688E-01	-1.4407918314E-01
		5.7631673258E-01	-9.4381437690E-01		

C5	H7	9.6269414375E-01	5.4394774798E-01	3.9986868002E-01	-1.4407906796E-01
		5.7631627185E-01	-9.4381642800E-01		

C5	H8	9.6269186313E-01	5.4394678336E-01	3.9986759973E-01	-1.4407918363E-01
		5.7631673454E-01	-9.4381438309E-01		

C5	Total	4.0388913954E+00	2.4068700082E+00	1.5403403247E+00	-8.6652968348E-01
		3.4661187340E+00	-3.9472103329E+00		

H6 C5 9.6269185886E-01 5.4394678002E-01 3.9986759688E-01 -1.4407918314E-01
5.7631673258E-01 -9.4381437690E-01

H6 Total 9.6269185886E-01 5.4394678002E-01 3.9986759688E-01 -1.4407918314E-01
5.7631673258E-01 -9.4381437690E-01

H7 C5 9.6269414375E-01 5.4394774798E-01 3.9986868002E-01 -1.4407906796E-01
5.7631627185E-01 -9.4381642800E-01

H7 Total 9.6269414375E-01 5.4394774798E-01 3.9986868002E-01 -1.4407906796E-01
5.7631627185E-01 -9.4381642800E-01

H8 C5 9.6269186313E-01 5.4394678336E-01 3.9986759973E-01 -1.4407918363E-01
5.7631673454E-01 -9.4381438309E-01

H8 Total 9.6269186313E-01 5.4394678336E-01 3.9986759973E-01 -1.4407918363E-01
5.7631673454E-01 -9.4381438309E-01

Total Total 1.3853943127E+01 8.0774245906E+00 5.4798905797E+00 -2.5975340109E+00
1.0390136044E+01 -1.3557315170E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

$ESP*ESP\_Int\_IDS(A)$ = Surface Integral of $ESP*ESP$ Over Atom A's Part of IDS

$Area\_ESP+_IDS(A)$ = Surface Area of Positive ESP Regions of Atom A's Part of IDS

$ESP+_Int\_IDS(A)$ = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

$Area\_ESP-_IDS(A)$ = Surface Area of Negative ESP Regions of Atom A's Part of IDS

$ESP-_Int\_IDS(A)$ = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

$ESP+_Min\_IDS(A)$ = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_Avg\_IDS(A)$ = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_MAD\_IDS(A)$ = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_Var\_IDS(A)$ = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP*ESP+_Int\_IDS(A)$ = Surface Integral of $ESP*ESP$ Over Positive Regions of Atom A's Part of IDS

$ESP-_Min\_IDS(A)$ = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_Avg\_IDS(A)$ = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_MAD\_IDS(A)$ = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_Var\_IDS(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-*ESP-_Int\_IDS(A)$ = Surface Integral of $ESP*ESP$ Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	2.1832344495E+01						

H2	5.2554436041E+01						

H3	5.2311424405E+01						

H4	5.3040947641E+01						

C5	2.1783360937E+01						

H6	5.2628061771E+01						

H7	5.3040947257E+01						

H8	5.2311424161E+01						

Total	3.5950294671E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	2.0997016725E+01	-3.9209492589E-02	1.8045207072E-03	-4.1508722117E-03	-1.8673839766E-03
	1.9334225165E-03	4.5226864417E-06			

H2	4.3323028184E+01	1.4774946366E-01	1.1018298260E-02	-3.7467127691E-03	3.4104140420E-03
	3.4441660706E-03	1.6511610748E-05			

H3	4.3171221780E+01	1.4752001286E-01	1.1012236624E-02	-3.7841275601E-03	3.4170914506E-03
	3.4500738765E-03	1.6573161646E-05			

H4	4.3401453777E+01	1.4763315146E-01	1.1011340686E-02	-3.7284642753E-03	3.4015715745E-03
	3.4479724489E-03	1.6560125791E-05			

C5	2.0997016684E+01	-3.9209451525E-02	1.8045203182E-03	-4.1508692480E-03	-1.8673820246E-03
	1.9334215872E-03	4.5226819922E-06			

H6	4.3323027957E+01	1.4774956592E-01	1.1018300816E-02	-3.7467097260E-03	3.4104164203E-03
	3.4441660883E-03	1.6511610313E-05			

H7	4.3401453436E+01	1.4763329071E-01	1.1011344269E-02	-3.7284603401E-03	3.4015748096E-03
	3.4479726178E-03	1.6560126737E-05			

H8	4.3171221559E+01	1.4752006071E-01	1.1012237625E-02	-3.7841250474E-03	3.4170925765E-03
	3.4500736935E-03	1.6573158998E-05			

Total	3.0178544010E+02	8.0738660121E-01	1.1018300816E-02	-4.1508722117E-03	2.6753663163E-03
	1.8210729826E-05				

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
	ESP-_Int_IDS(A)				

C1	5.1818412279E-02	1.6818210105E-04	5.7826714783E+00	6.3044598452E-03	
	1.5214345246E+01	-4.5513952434E-02			

H2	1.8682361636E-01	1.2192198234E-03	3.2892503915E+01	1.6728654001E-01	
	1.0430524269E+01	-1.9537076348E-02			

H3	1.8680427210E-01	1.2195730117E-03	3.2877704286E+01	1.6716214248E-01	
	1.0293517494E+01	-1.9642129624E-02			

H4	1.8733057067E-01 1.0439563652E+01 -1.9848709607E-02	1.2209182655E-03	3.2961890125E+01	1.6748186107E-01
C5	5.1818376418E-02 1.5214345191E+01 -4.5513913972E-02	1.6818185422E-04	5.7826714925E+00	6.3044624467E-03
H6	1.8682366143E-01 1.0430524210E+01 -1.9537047751E-02	1.2192205009E-03	3.2892503747E+01	1.6728661367E-01
H7	1.8733064005E-01 1.0439563596E+01 -1.9848674674E-02	1.2209192522E-03	3.2961889840E+01	1.6748196538E-01
H8	1.8680427835E-01 1.0293517420E+01 -1.9642108821E-02	1.2195732233E-03	3.2877704139E+01	1.6716216953E-01

Total	1.2255538277E+00 9.2755901078E+01 -2.0908361323E-01	7.6557880323E-03	2.0902953902E+02	1.0164702144E+00

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A) ESP+*ESP+_Int_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
C1	5.4037718214E-05 8.3841723336E-06	1.0902330988E-03	4.3902357890E-04	2.6127051240E-07
H2	1.5121488829E-06 1.1704966212E-03	5.0858560492E-03	2.6985817899E-03	9.7195811129E-06
H3	1.2893852300E-05 1.1702446476E-03	5.0843617615E-03	2.7013952501E-03	9.7431329045E-06
H4	6.7029463624E-06 1.1708147126E-03	5.0810757645E-03	2.6966462923E-03	9.7029231674E-06
C5	5.4038407537E-05 8.3841758864E-06	1.0902335460E-03	4.3902327802E-04	2.6127014811E-07
H6	1.5144906144E-06 1.1704974088E-03	5.0858583147E-03	2.6985819621E-03	9.7195821935E-06
H7	6.7035704543E-06 1.1708158339E-03	5.0810789732E-03	2.6966465481E-03	9.7029248854E-06
H8	1.2893079847E-05 1.1702449455E-03	5.0843626070E-03	2.7013953758E-03	9.7431335246E-06

Total	1.5121488829E-06 4.8628065640E-03		1.0032000725E-05	7.0398825178E-03

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
C1	-1.3291792427E-05	-2.9915156845E-03	1.0438683816E-03	1.5539430558E-06	1.5979792872E-04
H2	-2.3204043958E-05	-1.8730675318E-03	9.3661204574E-04	1.1628311717E-06	4.8723202131E-05
H3	-3.1622985338E-05	-1.9082038414E-03	9.2929590340E-04	1.1509357135E-06	4.9328364103E-05
H4	-2.9243552591E-05	-1.9012968614E-03	9.4557939414E-04	1.1844617310E-06	5.0103552913E-05
C5	-1.3290881022E-05	-2.9915131673E-03	1.0438679079E-03	1.5539416971E-06	1.5979767833E-04
H6	-2.3202182681E-05	-1.8730648007E-03	9.3661193370E-04	1.1628308828E-06	4.8723092128E-05
H7	-2.9241980435E-05	-1.9012935254E-03	9.4557931799E-04	1.1844615477E-06	5.0103418299E-05
H8	-3.1621804352E-05	-1.9082018342E-03	9.2929563607E-04	1.1509350316E-06	4.9328277878E-05
Total	-1.3290881022E-05	-2.2541273472E-03	1.5589781609E-06	6.1590551450E-04	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
C1	2.2417095811E+01				
H2	3.6422812407E+01				
H3	3.6389045147E+01				
H4	3.6329016134E+01				
C5	2.2417095760E+01				
H6	3.6422812207E+01				

H7 3.6329015823E+01

H8 3.6389044966E+01

Total 2.6311593825E+02

Atomic Surface Area and Volume Data:

 $\text{Area}(A) = \text{Area\_IAS}(A | \text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an

Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.0553607702E+02	8.0826746500E+01	5.9673837543E+00	7.3829320277E-02	
	9.9928622794E+01				
H2	9.4854673137E+01	7.1204751762E+01	9.9771818313E-01	1.4011960697E-02	
	9.8842874064E+01				
H3	9.4611661498E+01	7.1232440048E+01	9.9773004756E-01	1.4006680761E-02	
	9.8844097218E+01				
H4	9.5341040989E+01	7.1207526431E+01	9.9772117252E-01	1.4011456689E-02	
	9.8842900355E+01				
C5	2.0548694962E+02	8.0841595755E+01	5.9673791031E+00	7.3815701525E-02	
	9.9928775070E+01				
H6	9.4928155087E+01	7.1215682935E+01	9.9772921381E-01	1.4009964838E-02	
	9.8843303042E+01				
H7	9.5341184316E+01	7.1217412472E+01	9.9772582626E-01	1.4009577035E-02	
	9.8843305882E+01				

H8	9.4611517475E+01	7.1236277115E+01	9.9773931883E-01	1.4006056454E-02
9.8844241849E+01				

Total	9.8071125914E+02	5.8898243302E+02	1.7921126620E+01	3.0427268480E-02
9.9563543217E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.6348466419E+02	7.0893512953E+01	5.9609071138E+00	8.4082546703E-02	9.9820166258E+01
H2	7.6098154139E+01	5.1536909482E+01	9.8503165352E-01	1.9113130054E-02	9.7586033135E+01
H3	7.5946347731E+01	5.1453569434E+01	9.8494867781E-01	1.9142475219E-02	9.7577859965E+01
H4	7.6176641044E+01	5.1496719766E+01	9.8499291099E-01	1.9127294233E-02	9.7581928531E+01
C5	1.6348472539E+02	7.0907644421E+01	5.9609124218E+00	8.4065864413E-02	9.9820485060E+01
H6	7.6098215202E+01	5.1529535520E+01	9.8503113860E-01	1.9115855182E-02	9.7585326750E+01
H7	7.6176579366E+01	5.1495044338E+01	9.8499227468E-01	1.9127904196E-02	9.7581810689E+01
H8	7.5946408804E+01	5.1449140141E+01	9.8495170438E-01	1.9144182034E-02	9.7577395859E+01
Total	7.8341173586E+02	4.5076207606E+02	1.7831767896E+01	3.9559157353E-02	9.9067097243E+01

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.3624517651E+02	6.3019099619E+01	5.9494945928E+00	9.4407800632E-02	9.9629054449E+01

H2	6.2634705882E+01	3.8401292242E+01	9.6622067293E-01	2.5161149964E-02
	9.5722449392E+01			
H3	6.2600938618E+01	3.8395156882E+01	9.6620870722E-01	2.5164858948E-02
	9.5721310211E+01			
H4	6.2542236767E+01	3.8419794180E+01	9.6626058621E-01	2.5150071905E-02
	9.5726142203E+01			
C5	1.3624650358E+02	6.3015437855E+01	5.9494798789E+00	9.4413053078E-02
	9.9629037527E+01			
H6	6.2636032824E+01	3.8392339552E+01	9.6620932077E-01	2.5166721592E-02
	9.5720681897E+01			
H7	6.2540909281E+01	3.8396301526E+01	9.6621394336E-01	2.5164245122E-02
	9.5721467599E+01			
H8	6.2602265584E+01	3.8396224471E+01	9.6621779278E-01	2.5164395878E-02
	9.5721460893E+01			

Total	6.4804876905E+02	3.5643564633E+02	1.7696305495E+01	4.9647967809E-02
	9.8314515284E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	C5	1.1164566667E-05		
C1	H2	9.4398612667E-03		
C1	H3	9.4393735667E-03		
C1	H4	9.4426171667E-03		
C1		2.8333016567E-02	2.8353851500E-02	
H2	C1	-9.4190263333E-03		
H2		-9.4190263333E-03	-9.3981914000E-03	
H3	C1	-9.4185386333E-03		
H3		-9.4185386333E-03	-9.3977037000E-03	

H4	C1	-9.4217822333E-03
H4		-9.4217822333E-03 -9.4009473000E-03
C5	C1	9.6703666663E-06
C5	H6	9.4466402667E-03
C5	H7	9.4431840667E-03
C5	H8	9.4472762667E-03
C5		2.8346770967E-02 2.8367605900E-02
H6	C5	-9.4258053333E-03
H6		-9.4258053333E-03 -9.4049704000E-03
H7	C5	-9.4223491333E-03
H7		-9.4223491333E-03 -9.4015142000E-03
H8	C5	-9.4264413333E-03
H8		-9.4264413333E-03 -9.4056064000E-03

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)
C1	2.8767200579E-04	-3.6804235021E-06	2.8399158229E-04
H2	7.2175272959E-02	3.2979949954E-03	7.5473267954E-02
H3	7.2177000504E-02	3.2978250215E-03	7.5474825525E-02
H4	-1.4434428288E-01	-6.5979207058E-03	-1.5094220359E-01
C5	-3.1925972285E-04	-4.6306222796E-06	-3.2389034513E-04
H6	-7.2168152987E-02	-3.3003693813E-03	-7.5468522368E-02
H7	1.4434545022E-01	6.5983176553E-03	1.5094376788E-01
H8	-7.2167571899E-02	-3.3005912826E-03	-7.5468163182E-02

Total -1.3871800060E-05 -1.3054743326E-05 -2.6926543386E-05

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	1.1222320483E-04	-5.1818971265E-07	1.1170501512E-04
H2	-1.2500676155E-01	-5.7122958022E-03	-1.3071905735E-01
H3	1.2500606824E-01	5.7119995770E-03	1.3071806782E-01
H4	5.4271361725E-07	4.4276425275E-10	5.4315638150E-07
C5	-1.2852477306E-04	-6.7576150408E-07	-1.2920053456E-04
H6	1.2500622129E-01	5.7164065311E-03	1.3072262782E-01
H7	1.6353638089E-06	4.4903118422E-10	1.6358128401E-06
H8	-1.2500721489E-01	-5.7167927047E-03	-1.3072400759E-01

Total -1.5810400804E-05 -1.8754581428E-06 -1.7685858947E-05

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	-5.2023164863E-02	-1.3224511915E-02	-6.5247676778E-02
H2	-6.4785356325E-02	-2.6153906233E-03	-6.7400746948E-02
H3	-6.4785435901E-02	-2.6152551980E-03	-6.7400691099E-02
H4	-6.4787213347E-02	-2.6161558588E-03	-6.7403369206E-02
C5	5.2016325903E-02	1.3233799650E-02	6.5250125553E-02
H6	6.4785596932E-02	2.6172729364E-03	6.7402869868E-02
H7	6.4783311605E-02	2.6163132538E-03	6.7399624859E-02
H8	6.4784645878E-02	2.6174495414E-03	6.7402095419E-02

Total -1.1290118000E-05 1.3521786946E-05 2.2316689455E-06

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	5.2024081266E-02	1.3224512437E-02	6.5248390433E-02
H2	1.5821852880E-01	7.0955875326E-03	1.6530743123E-01

H3	1.5821880167E-01	7.0952201369E-03	1.6530733711E-01
H4	1.5821711353E-01	7.0976636380E-03	1.6530808511E-01
C5	5.2017464431E-02	1.3233800477E-02	6.5251057328E-02
H6	1.5821495263E-01	7.1006942833E-03	1.6530895366E-01
H7	1.5821658088E-01	7.0980906533E-03	1.6530798678E-01
H8	1.5821508319E-01	7.1011734062E-03	1.6530956501E-01

Total	2.3871790359E-05	1.8888684146E-05	3.2292548547E-05

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

C1	C5	1.1986901246E-16	
C1	H2	5.7909499447E-03	
C1	H3	5.7906521407E-03	
C1	H4	-1.1585282509E-02	
C1		-3.6804235021E-06	
H2	C1	3.2979949954E-03	
H2		3.2979949954E-03	
H3	C1	3.2978250215E-03	
H3		3.2978250215E-03	
H4	C1	-6.5979207058E-03	
H4		-6.5979207058E-03	
C5	C1	1.0382644818E-16	
C5	H6	-5.7951099669E-03	
C5	H7	1.1585978088E-02	
C5	H8	-5.7954987435E-03	

C5		-4.6306222796E-06
H6	C5	-3.3003693813E-03
H6		-3.3003693813E-03
H7	C5	6.5983176553E-03
H7		6.5983176553E-03
H8	C5	-3.3005912826E-03
H8		-3.3005912826E-03

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	C5	-1.2107291515E-15	
C1	H2	-1.0030221097E-02	
C1	H3	1.0029702123E-02	
C1	H4	7.8379686865E-10	
C1		-5.1818971265E-07	
H2	C1	-5.7122958022E-03	
H2		-5.7122958022E-03	
H3	C1	5.7119995770E-03	
H3		5.7119995770E-03	
H4	C1	4.4276425275E-10	
H4		4.4276425275E-10	
C5	C1	-1.0486922760E-15	
C5	H6	1.0037423309E-02	
C5	H7	7.7758983550E-10	
C5	H8	-1.0038099848E-02	
C5		-6.7576150408E-07	
H6	C5	5.7164065311E-03	
H6		5.7164065311E-03	
H7	C5	4.4903118422E-10	
H7		4.4903118422E-10	
H8	C5	-5.7167927047E-03	
H8		-5.7167927047E-03	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	C5	1.6130988611E-05	
C1	H2	-4.4131941674E-03	
C1	H3	-4.4129661698E-03	
C1	H4	-4.4144825659E-03	
C1		-1.3224511915E-02	
H2	C1	-2.6153906233E-03	
H2		-2.6153906233E-03	
H3	C1	-2.6152551980E-03	
H3		-2.6152551980E-03	
H4	C1	-2.6161558588E-03	
H4		-2.6161558588E-03	
C5	C1	-1.3972111880E-05	
C5	H6	4.4163634111E-03	
C5	H7	4.4147476120E-03	
C5	H8	4.4166607388E-03	
C5		1.3233799650E-02	
H6	C5	2.6172729364E-03	
H6		2.6172729364E-03	
H7	C5	2.6163132538E-03	
H7		2.6163132538E-03	
H8	C5	2.6174495414E-03	
H8		2.6174495414E-03	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	C5	1.6130988611E-05	
C1	H2	1.2394221205E-02	
C1	H3	1.2393580891E-02	
C1	H4	1.2397839616E-02	

C1		1.3224512437E-02
H2	C1	7.0955875326E-03
H2		7.0955875326E-03
H3	C1	7.0952201369E-03
H3		7.0952201369E-03
H4	C1	7.0976636380E-03
H4		7.0976636380E-03
C5	C1	1.3972111880E-05
C5	H6	1.2403121865E-02
C5	H7	1.2398583981E-02
C5	H8	1.2403956882E-02
C5		1.3233800477E-02
H6	C5	7.1006942833E-03
H6		7.1006942833E-03
H7	C5	7.0980906533E-03
H7		7.0980906533E-03
H8	C5	7.1011734062E-03
H8		7.1011734062E-03

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)

C1 -9.0977421640E-02 -1.4543782208E-03 -1.3087538296E-03 -9.6220371334E-02 -4.0841740506E-04 1.8719779297E-01

H2 -8.9267588719E-02 -2.6413918788E-01 -1.0169050056E-01 2.1573322884E-01 1.7612153458E-01 -1.2646564012E-01

H3 -8.9269576630E-02 2.6413809464E-01 -1.0169556700E-01 2.1573488041E-01 -1.7611844044E-01 -1.2646530378E-01

H4 3.6823671339E-01 6.0110155556E-07 2.0337230958E-01 -2.4176859782E-01 -9.9092031580E-07 -1.2646811558E-01

C5 -9.1001855882E-02 -1.4807605631E-03 -1.3401392257E-03 -9.6122855830E-02 -4.2450050673E-04 1.8712471171E-01

H6 -8.9278695873E-02 -2.6414497404E-01 -1.0168098748E-01 2.1574074209E-01 1.7612790773E-01 -1.2646204622E-01

H7 3.6823869678E-01 -3.3885215697E-06 2.0336929126E-01 -2.4177455694E-01 4.7405535851E-06 -1.2646413983E-01

H8 -8.9283621585E-02 2.6415206439E-01 -1.0168007798E-01 2.1574325286E-01 -1.7612963156E-01 -1.2645963128E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
C1	1	-9.6598631775E-02	2.5103817152E-01	9.6797382727E-01	2.5507175705E-03
C1	2	-9.0605887445E-02	9.6796579109E-01	-2.5104713134E-01	4.1910780892E-03
C1	3	1.8720451922E-01	-4.6972042273E-03	-1.4168867708E-03	9.9998796428E-01
H2	1	-2.4176863185E-01	8.6604498659E-01	4.9996606581E-01	1.1931554822E-04
H2	2	-1.9933709683E-01	1.6854990204E-01	-2.9218807081E-01	9.4139102492E-01
H2	3	4.4110572868E-01	-4.7069842970E-01	8.1526686693E-01	3.3731724529E-01
H3	1	-2.4176876563E-01	8.6607001076E-01	-4.9992266331E-01	2.5915095201E-04
H3	2	-1.9933672662E-01	1.6842130173E-01	2.9226240714E-01	9.4139096580E-01
H3	3	4.4110549224E-01	4.7069841892E-01	8.1526683735E-01	-3.3731733182E-01

H4	1	-2.4176859785E-01	-9.3475769809E-06	9.9999999964E-01	2.5081930085E-05
H4	2	-1.9933986201E-01	-3.3731646692E-01	-2.6765002696E-05	9.4139131100E-01
H4	3	4.4110845986E-01	9.4139131133E-01	3.3917970884E-07	3.3731646705E-01
C5	1	-9.6522218590E-02	2.5968176497E-01	9.6569055115E-01	2.6721454272E-03
C5	2	-9.0609565344E-02	9.6568226699E-01	-2.5969133265E-01	4.2627420561E-03
C5	3	1.8713178393E-01	-4.8104227326E-03	-1.4734870731E-03	9.9998734425E-01
H6	1	-2.4178009457E-01	8.6601518632E-01	5.0001768954E-01	-8.4897112229E-05
H6	2	-1.9933350127E-01	1.6873323926E-01	-2.9208091888E-01	9.4139143335E-01
H6	3	4.4111359583E-01	-4.7068757264E-01	8.1527360252E-01	3.3731611583E-01
H7	1	-2.4177455769E-01	4.6747067635E-05	9.9999999127E-01	-1.2355753992E-04
H7	2	-1.9933419534E-01	-3.3731396674E-01	1.3208454405E-04	9.4139219797E-01
H7	3	4.4110875303E-01	9.4139220607E-01	-2.3296408378E-06	3.3731396997E-01
H8	1	-2.4178930193E-01	8.6600875499E-01	-5.0002882060E-01	-1.2186110959E-04
H8	2	-1.9933124725E-01	1.6876669757E-01	2.9206060249E-01	9.4139173900E-01
H8	3	4.4112054918E-01	4.7068741015E-01	8.1527405395E-01	-3.3731525149E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3754108470E+02	1.4960793264E+01	5.9716461485E+00	6.0370462729E+00	9.1495533192E+00
H2	2.9109956250E+00	1.2789279809E+00	1.0093981914E+00	1.1411310974E+00	1.7204979183E+00
H3	2.9109953233E+00	1.2789276266E+00	1.0093977037E+00	1.1411304222E+00	1.7204974349E+00

H4	2.9109968164E+00	1.2789298519E+00	1.0094009473E+00	1.1411348907E+00
	1.7205026827E+00			
C5	1.3754108302E+02	1.4960788428E+01	5.9716323941E+00	6.0370043965E+00
	9.1494173504E+00			
H6	2.9109993038E+00	1.2789329161E+00	1.0094049704E+00	1.1411406097E+00
	1.7205114374E+00			
H7	2.9109975636E+00	1.2789304644E+00	1.0094015142E+00	1.1411355972E+00
	1.7205036092E+00			
H8	2.9109990679E+00	1.2789329296E+00	1.0094056064E+00	1.1411428257E+00
	1.7205178266E+00			

Atomic Radial Distortion Moments:

$$\text{Dot} = x*(d\rho/dx) + y*(d\rho/dy) + z*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3590491432E+02	-2.7166199978E+01	-1.3079093572E+01	-1.5205812833E+01	-2.8091992586E+01
H2	-2.2478981082E+00	-1.8466690679E+00	-2.1842151193E+00	-3.4162949095E+00	-6.7486501005E+00
H3	-2.2478977057E+00	-1.8466683540E+00	-2.1842139449E+00	-3.4162938500E+00	-6.7486539998E+00
H4	-2.2479014479E+00	-1.8466738136E+00	-2.1842215188E+00	-3.4163029314E+00	-6.7486593009E+00
C5	-1.3590490547E+02	-2.7166173806E+01	-1.3079012194E+01	-1.5205544285E+01	-2.8091057136E+01
H6	-2.2479054654E+00	-1.8466794876E+00	-2.1842301509E+00	-3.4163169257E+00	-6.7486818310E+00
H7	-2.2479015389E+00	-1.8466739668E+00	-2.1842220442E+00	-3.4163038292E+00	-6.7486573232E+00

H8 -2.2479058943E+00 -1.8466810384E+00 -2.1842345826E+00 -3.4163290024E+00 -
6.7487155837E+00

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

C1	2.9858230743E+00	2.9858230743E+00	5.9716461485E+00	0.0000000000E+00

H2	5.0469909570E-01	5.0469909570E-01	1.0093981914E+00	0.0000000000E+00

H3	5.0469885183E-01	5.0469885183E-01	1.0093977037E+00	0.0000000000E+00

H4	5.0470047366E-01	5.0470047366E-01	1.0094009473E+00	0.0000000000E+00

C5	2.9858161970E+00	2.9858161970E+00	5.9716323941E+00	0.0000000000E+00

H6	5.0470248518E-01	5.0470248518E-01	1.0094049704E+00	0.0000000000E+00

H7	5.0470075711E-01	5.0470075711E-01	1.0094015142E+00	0.0000000000E+00

H8	5.0470280319E-01	5.0470280319E-01	1.0094056064E+00	0.0000000000E+00

Total	8.9998437380E+00	8.9998437380E+00	1.7999687476E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions $VeeX(A)$ to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of $VeeX(A)$ into interatomic ($VeeX(A,B)$ and $VeeX(A,A')$) and intraatomic ($VeeX(A,A)$) contributions is ambiguous. Currently, interatomic contributions $VeeX(A,B)$ and $VeeX(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$. For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E\_IQA(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CF3minus

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\cf3\an\cf3pyr.wfn

Sum File: D:\calc\ellipticity\cf3\an\cf3pyr.sum

SumViz File: D:\calc\ellipticity\cf3\an\cf3pyr.sumviz

Wfn Title: cf3pyr.wfn

Total memory allocated for AIMSum = 0.315 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted SCF

Restricted, closed-shell, single-determinant wavefunction.

Number of electrons (from MO Occs)	=	34.0000000000
Number of Alpha electrons (from MO Occs)	=	17.0000000000
Number of Beta electrons (from MO Occs)	=	17.0000000000
Number of electron pairs ($N*(N-1)/2$)	=	561.0000000000
Number of electron pairs (from Muller 2EDM)	=	561.0000000000

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	0.0000000000E+00	0.0000000000E+00	1.0348778900E+00
F2	9.0	0.0000000000E+00	2.3905194700E+00	-2.2997286000E-01
F3	9.0	-2.0702505900E+00	-1.1952597300E+00	-2.2997286000E-01
F4	9.0	2.0702505900E+00	-1.1952597300E+00	-2.2997286000E-01

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol) = \text{Approximation to Virial-Based Total Energy of Atom A.}$

$|Mu\_Intra(A)| = \text{Magnitude of Intraatomic Dipole Moment of Atom A}$

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	Mu_Intra(A)
C1	1.2825824943E+00	-5.5820868606E-04	3.6684239266E+01	-3.6708451964E+01	2.0300965523E+00
F2	-7.6087691530E-01	1.2901170846E-04	9.9779236368E+01	-9.9845093657E+01	1.3431066133E-01
F3	-7.6088231260E-01	1.2003353349E-04	9.9779235006E+01	-9.9845092295E+01	1.3431543383E-01
F4	-7.6087897010E-01	1.2754855045E-04	9.9779237315E+01	-9.9845094605E+01	1.3431374955E-01
Total	-1.0000557037E+00	-1.8161489366E-04	3.3602194795E+02	-3.3624373252E+02	

Molecular charge q(Mol) from the wfn file: -1.0000000000E+00

Molecular energy E(Mol) from the wfn file: -3.3624374360E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0006600300E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	283	1	Proaim(5)	4334	(Very High)	Auto	Auto	Auto	13.00
F2	330	1	Proaim(5)	3074	(Very High)	Auto	Auto	Auto	13.00
F3	359	1	Proaim(5)	3074	(Very High)	Auto	Auto	Auto	13.00
F4	364	1	Proaim(5)	3074	(Very High)	Auto	Auto	Auto	13.00

Total	1336								

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Note: Total time does not include times for diatomic interaction energy calculations (1023 seconds)

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -3.99798066911702E-23 1.22175435033348E-14 1.03484905140791E+00

Type = (3,-3) NACP C1

Rho = 1.2016894626E+02 Rho at Nucleus = 1.2016887048E+02

GradRho = 2.4210076847E-17 7.4424027856E-17 6.3469229872E-12

HessRho_EigVals = -1.8224627378E+05 -1.8224627378E+05 -1.8223785152E+05

HessRho_EigVec1 = 0.0000000000E+00 1.0000000000E+00 3.8312272817E-10

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 -3.8312272817E-10 1.0000000000E+00

DelSqRho = -5.4673039909E+05

Bond Ellipticity = NA

V = -1.3669247398E+05

G = 4.9371059699E+00

K = 1.3668753688E+05

L = 1.3668259977E+05

Vnuc = 2.0806452295E+05

Ven = -2.5002894478E+07

Vrep = 2.4866202004E+07
DelSqV = 4.6324909959E+09
DelSqVen = 1.1375519966E+11
DelSqVrep = -1.0912270866E+11
DelSqG = 2.0730393988E+08
DelSqK = -4.8397949357E+09
Stress_EigVals = -4.5565208673E+04 -4.5563632656E+04 -4.5563632656E+04
Stress_EigVec1 = 0.0000000000E+00 6.4631613265E-11 1.0000000000E+00
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 -6.4631613265E-11
-DivStress = 4.7295941579E-14 -1.8108946972E-05 4.3485210458E+04

CP# 2 Coords = 4.29610152579586E-24 2.39051460345334E+00 -2.29970535677411E-01

Type = (3,-3) NACP F2

Rho = 4.2607215847E+02 Rho at Nucleus = 4.2607213612E+02

GradRho = 9.4503182991E-18 2.4499746676E-10 2.1740387268E-12

HessRho_EigVals = -1.5369674230E+06 -1.5369120344E+06 -1.5369086641E+06

HessRho_EigVec1 = 0.0000000000E+00 8.8656434049E-01 -4.6260530711E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 4.6260530711E-01 8.8656434049E-01

DelSqRho = -4.6107881214E+06

Bond Ellipticity = NA

V = -1.1530155539E+06

G = 1.5926177776E+02

K = 1.1528562921E+06

L = 1.1526970304E+06

Vnuc = 1.6687991533E+06

Ven = -7.1102885731E+08

Vrep = 7.0987584176E+08

DelSqV = 9.7414704629E+10

DelSqVen = 7.6944793252E+12

DelSqVrep = -7.5970646206E+12

DelSqG = 4.1591371018E+09

DelSqK = -1.0157384173E+11

Stress_EigVals = -3.8434368757E+05 -3.8434286052E+05 -3.8432900583E+05

Stress_EigVec1 = 0.0000000000E+00 4.6426023399E-01 8.8569883998E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.8569883998E-01 -4.6426023399E-01

-DivStress = -1.2491520553E-13 1.5439728358E+05 -7.3743295631E+04

CP# 3 Coords = -2.07024637544690E+00 -1.19525729672661E+00 -2.29970535677343E-01

Type = (3,-3) NACP F3

Rho = 4.2607215379E+02 Rho at Nucleus = 4.2607213144E+02

GradRho = 2.4278140609E-10 -6.7972016904E-11 -1.3294920720E-11

HessRho_EigVals = -1.5369674076E+06 -1.5369120191E+06 -1.5369086488E+06

HessRho_EigVec1 = 7.6778725340E-01 4.4328217528E-01 4.6260528162E-01

HessRho_EigVec2 = -4.9999998243E-01 8.6602541393E-01 -3.4854941356E-08

HessRho_EigVec3 = -4.0062794596E-01 -2.3130260592E-01 8.8656435379E-01

DelSqRho = -4.6107880754E+06

Bond Ellipticity = NA

V = -1.1530155424E+06

G = 1.5926177906E+02

K = 1.1528562806E+06

L = 1.1526970189E+06

Vnuc = 1.6687991184E+06

Ven = -7.1102883463E+08

Vrep = 7.0987581908E+08

DelSqV = 9.7414704058E+10

DelSqVen = 7.6944790876E+12

DelSqVrep = -7.5970643836E+12

DelSqG = 4.1591370645E+09

DelSqK = -1.0157384112E+11

Stress_EigVals = -3.8434368374E+05 -3.8434285669E+05 -3.8432900200E+05

Stress_EigVec1 = -4.0206115617E-01 -2.3213006702E-01 8.8569885327E-01

Stress_EigVec2 = -4.9999998122E-01 8.6602541462E-01 -3.7263557398E-08

Stress_EigVec3 = 7.6703770799E-01 4.4284942499E-01 4.6426020863E-01

-DivStress = -1.3371197125E+05 -7.7198643364E+04 -7.3743297314E+04

CP# 4 Coords = 2.07024637544690E+00 -1.19525729672661E+00 -2.29970535677343E-01

Type = (3,-3) NACP F4

Rho = 4.2607215379E+02 Rho at Nucleus = 4.2607213144E+02

GradRho = -2.4278162813E-10 -6.7973626727E-11 -1.3294698675E-11

HessRho_EigVals = -1.5369674076E+06 -1.5369120191E+06 -1.5369086488E+06

HessRho_EigVec1 = 7.6778725340E-01 -4.4328217528E-01 -4.6260528162E-01

HessRho_EigVec2 = 4.9999998248E-01 8.6602541390E-01 -3.4741373639E-08

HessRho_EigVec3 = 4.0062794589E-01 -2.3130260603E-01 8.8656435379E-01

DelSqRho = -4.6107880754E+06

Bond Ellipticity = NA

V = -1.1530155424E+06

G = 1.5926177906E+02

K = 1.1528562806E+06

L = 1.1526970189E+06

Vnuc = 1.6687991184E+06

Ven = -7.1102883463E+08

Vrep = 7.0987581908E+08

DelSqV = 9.7414704058E+10

DelSqVen = 7.6944790876E+12

DelSqVrep = -7.5970643836E+12

DelSqG = 4.1591370645E+09

DelSqK = -1.0157384112E+11

Stress_EigVals = -3.8434368374E+05 -3.8434285669E+05 -3.8432900200E+05

Stress_EigVec1 = 4.0206115619E-01 -2.3213006699E-01 8.8569885327E-01

Stress_EigVec2 = 4.9999998121E-01 8.6602541463E-01 -3.7287188275E-08

Stress_EigVec3 = 7.6703770799E-01 -4.4284942499E-01 -4.6426020863E-01

-DivStress = 1.3371197125E+05 -7.7198643364E+04 -7.3743297314E+04

CP# 5 Coords = 3.65516533488850E-18 7.80947201166175E-01 6.48832310810300E-01

Type = (3,-1) BCP F2 C1

Rho = 2.0142244330E-01

GradRho = 2.2156464672E-19 -4.5970172113E-17 1.0408340856E-17

HessRho_EigVals = -4.1995104225E-01 -2.2657751199E-01 7.1531777713E-01

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 4.6971470746E-01 8.8281826759E-01

HessRho_EigVec3 = 0.0000000000E+00 8.8281826759E-01 -4.6971470746E-01

DelSqRho = 6.8789222888E-02

Bond Ellipticity = 8.5345420457E-01

V = -5.2386735333E-01

G = 2.7053232952E-01

K = 2.5333502380E-01

L = -1.7197305722E-02

Vnuc = 1.7807270752E+01

Ven = -3.5867839834E+00

Vrep = 3.0629166301E+00

DelSqV = -8.9632135863E+00

DelSqVen = -1.2249483168E+00

DelSqVrep = -7.7382652694E+00

DelSqG = 1.3490058824E+01

DelSqK = -4.5268452376E+00

Stress_EigVals = -2.5440658800E-01 -2.0513422021E-01 -6.4326545119E-02

Stress_EigVec1 = 0.0000000000E+00 5.4089637404E-01 8.4108924173E-01

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 8.4108924173E-01 -5.4089637404E-01

-DivStress = 7.4512374894E-19 -8.3103889107E-01 3.8612377863E-01

BPL = 2.7054164481E+00 = 1.8341500517E+00 + 8.7126639639E-01

GBL_I = 2.7045015543E+00

GBL_II = 2.7045204300E+00

GBL_III = 2.7049903333E+00 = 1.8338488666E+00 + 8.7114146672E-01

GBL_IV = 2.7050084977E+00 = 1.8338542518E+00 + 8.7115424594E-01

CP# 6 Coords = -6.76320115115705E-01 -3.90473598479552E-01 6.48832313837312E-01

Type = (3,-1) BCP C1 F3

Rho = 2.0142244400E-01

GradRho = 1.0148132334E-16 7.9580439460E-17 -9.5409791179E-18

HessRho_EigVals = -4.1995104522E-01 -2.2657751185E-01 7.1531779220E-01

HessRho_EigVec1 = -5.0000000026E-01 8.6602540363E-01 2.9999531633E-09

HessRho_EigVec2 = -4.0678486772E-01 -2.3485735610E-01 8.8281826764E-01

HessRho_EigVec3 = 7.6454304727E-01 4.4140913283E-01 4.6971470737E-01

DelSqRho = 6.8789235133E-02

Bond Ellipticity = 8.5345421878E-01

V = -5.2386735884E-01

G = 2.7053233381E-01

K = 2.5333502503E-01

L = -1.7197308783E-02

Vnuc = 1.7807270764E+01

Ven = -3.5867839981E+00

Vrep = 3.0629166393E+00

DelSqV = -8.9632137788E+00

DelSqVen = -1.2249485357E+00

DelSqVrep = -7.7382652431E+00

DelSqG = 1.3490059112E+01

DelSqK = -4.5268453332E+00

Stress_EigVals = -2.5440659007E-01 -2.0513422143E-01 -6.4326547341E-02

Stress_EigVec1 = -4.6843000547E-01 -2.7044818679E-01 8.4108923917E-01

Stress_EigVec2 = -4.9999999852E-01 8.6602540464E-01 -1.9522952472E-09

Stress_EigVec3 = 7.2840464816E-01 4.2054461925E-01 5.4089637802E-01

-DivStress = 7.1970080178E-01 4.1551944911E-01 3.8612378218E-01

BPL = 2.7054164465E+00 = 8.7126639401E-01 + 1.8341500525E+00

GBL_I = 2.7045015527E+00

GBL_II = 2.7045204283E+00

GBL_III = 2.7049903318E+00 = 8.7114146435E-01 + 1.8338488674E+00

$$\text{GBL\_IV} = 2.7050084962\text{E}+00 = 8.7115424357\text{E}-01 + 1.8338542526\text{E}+00$$

CP# 7 Coords = 6.76320115115705E-01 -3.90473598479552E-01 6.48832313837312E-01

Type = (3,-1) BCP F4 C1

Rho = 2.0142244400E-01

GradRho = -7.5026790336E-17 9.3241386834E-18 3.2959746044E-17

HessRho_EigVals = -4.1995104522E-01 -2.2657751185E-01 7.1531779220E-01

HessRho_EigVec1 = 5.0000000026E-01 8.6602540363E-01 2.9999532751E-09

HessRho_EigVec2 = 4.0678486772E-01 -2.3485735610E-01 8.8281826764E-01

HessRho_EigVec3 = 7.6454304727E-01 -4.4140913283E-01 -4.6971470737E-01

DelSqRho = 6.8789235133E-02

Bond Ellipticity = 8.5345421878E-01

V = -5.2386735884E-01

G = 2.7053233381E-01

K = 2.5333502503E-01

L = -1.7197308783E-02

Vnuc = 1.7807270764E+01

Ven = -3.5867839981E+00

Vrep = 3.0629166393E+00

DelSqV = -8.9632137788E+00

DelSqVen = -1.2249485357E+00

DelSqVrep = -7.7382652431E+00

DelSqG = 1.3490059112E+01

DelSqK = -4.5268453332E+00

Stress_EigVals = -2.5440659007E-01 -2.0513422143E-01 -6.4326547341E-02

Stress_EigVec1 = 4.6843000547E-01 -2.7044818679E-01 8.4108923917E-01

Stress_EigVec2 = 4.9999999852E-01 8.6602540464E-01 -1.9522953065E-09

Stress_EigVec3 = 7.2840464816E-01 -4.2054461925E-01 -5.4089637802E-01

-DivStress = -7.1970080178E-01 4.1551944911E-01 3.8612378218E-01

BPL = 2.7054164465E+00 = 1.8341500525E+00 + 8.7126639401E-01

GBL_I = 2.7045015527E+00

GBL_II = 2.7045204283E+00

$$\text{GBL\_III} = 2.7049903318\text{E}+00 = 1.8338488674\text{E}+00 + 8.7114146435\text{E}-01$$

$$\text{GBL\_IV} = 2.7050084962\text{E}+00 = 1.8338542526\text{E}+00 + 8.7115424357\text{E}-01$$

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

F3	C1	F2	99.36418361	99.89972559	99.89905167	101.85714771	101.85507718
F4	C1	F2	99.36418361	99.89972559	99.89905167	101.85714771	101.85507718
F4	C1	F3	99.36418388	99.89972581	99.89905189	101.85714807	101.85507754

Total time for electron density critical point search, analysis and connectivity = 0 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A) = V_{ee}(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.6684239266E+01 3.3259205863E+01	1.9941850888E+01	3.6684239266E+01		-1.2656953528E+02	-8.3314366711E+01
F2	-9.9779236368E+01 7.5321931416E+01	3.2956395421E+01	9.9779236368E+01		-3.0783679957E+02	-2.4353842116E+02
F3	-9.9779235006E+01 7.5321964669E+01	3.2956432607E+01	9.9779235006E+01		-3.0783686729E+02	-2.4353843975E+02
F4	-9.9779237315E+01 7.5321947029E+01	3.2956411428E+01	9.9779237315E+01		-3.0783683309E+02	-2.4353843034E+02
Total	-3.3602194795E+02 2.5922504898E+02	1.1881109034E+02	3.3602194795E+02		-1.0500800352E+03	-8.1392965796E+02

More Virial-Based Atomic Energy Components:

$E(A) = E_e(A) + W(A)$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$E_e(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E(A)$	$E_e(A)$	$W(A)$	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
C1	-3.6684239266E+01				3.7855817347E+01	-4.5966114843E+00
F2	-9.9779236368E+01				8.5649172927E+01	-1.0327241511E+01
F3	-9.9779235006E+01				8.5649207484E+01	-1.0327242815E+01
F4	-9.9779237315E+01				8.5649189321E+01	-1.0327242292E+01
Total	-3.3602194795E+02				2.9480338708E+02	-3.5578338102E+01

Intraatomic and Interatomic Two-Electron Interaction Energy Contributions:

$V_{ee}(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$V_{eeC}(A,A)$ = Coulomb Part of $V_{ee}(A,A)$

$V_{eeX}(A,A)$ = Exchange-Correlation Part of $V_{ee}(A,A)$

$V_{ee}(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule
 $= V_{ee}(A,Mol) - V_{ee}(A,A)$

$V_{eeC}(A,A')$ = Coulomb Part of $V_{ee}(A,A')$

$V_{eeX}(A,A')$ = Exchange-Correlation Part of $V_{ee}(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$V_{ee}(A,A)$	$V_{eeC}(A,A)$	$V_{eeX}(A,A)$	$V_{ee}(A,A')$	$V_{eeC}(A,A')$	$V_{eeX}(A,A')$
C1	9.9472423247E+00	1.4279109989E+01	-4.3318676648E+00	2.3311963538E+01	2.3576707358E+01	-2.6474381949E-01

F2	4.4489613507E+01	5.4696382704E+01	-1.0206769197E+01	3.0832317909E+01
	3.0952790223E+01	-1.2047231354E-01		
F3	4.4489619153E+01	5.4696375578E+01	-1.0206756425E+01	3.0832345516E+01
	3.0952831906E+01	-1.2048639016E-01		
F4	4.4489612432E+01	5.4696373766E+01	-1.0206761334E+01	3.0832334597E+01
	3.0952815555E+01	-1.2048095818E-01		

Total	1.4341608742E+02	1.7836824204E+02	-3.4952154621E+01	1.1580896156E+02
	1.1643514504E+02	-6.2618348137E-01		

Virial-Based Intraatomic and Interatomic Energy Contributions:

$$E\_Intra(A) = T(A) + Ven(A,A) + Vee(A,A)$$

$$= \text{Intraatomic Contribution to } E(A)$$

$$E\_Inter(A) = Ven(A,A') + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic Contribution to } E(A) = E(A) - E\_Intra(A)$$

$$Ee\_Intra(A) = T(A) + Ven(A,A) + Vee(A,A)$$

$$= \text{Intraatomic Contribution to } Ee(A)$$

$$Ee\_Inter(A) = Ven(A,A') + Vee(A,A') + Vnn(A) - W(A)$$

$$= \text{Interatomic Contribution to } Ee(A) = Ee(A) - Ee\_Intra(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E_Intra(A)	E_Inter(A)	Ee_Intra(A)	Ee_Inter(A)

C1	-3.6682885120E+01	-3.6682885120E+01	-1.3541457000E-03	

F2	-9.9269571285E+01	-9.9269571285E+01	-5.0966508300E-01	

F3	-9.9269585591E+01	-9.9269585591E+01	-5.0964941500E-01	

F4	-9.9269580593E+01	-9.9269580593E+01	-5.0965672200E-01	

Total	-3.3449162259E+02	-3.3449162259E+02	-1.5303253657E+00	

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
$VeeC(A)$	$VeeX(A)$					
C1	-3.7728369449E+01	3.6684239266E+01	-7.4336903900E+01	-6.3284767641E+01	3.3259205863E+01	2.9949856963E+01
			3.7855817347E+01	-4.5966114843E+00		
F2	-9.9505147726E+01	9.9779236368E+01	-1.5023405055E+02	-1.5391839979E+02	7.5321931416E+01	2.9546134829E+01
			8.5649172927E+01	-1.0327241511E+01		
F3	-9.9505149729E+01	9.9779235006E+01	-1.5023405058E+02	-1.5391843364E+02	7.5321964669E+01	2.9546134822E+01
			8.5649207484E+01	-1.0327242815E+01		
F4	-9.9505147960E+01	9.9779237315E+01	-1.5023405058E+02	-1.5391841654E+02	7.5321947029E+01	2.9546134822E+01
			8.5649189321E+01	-1.0327242292E+01		
Total	-3.3624381486E+02	3.3602194795E+02	-5.2503905561E+02	-5.2504001761E+02	2.5922504898E+02	1.1858826144E+02
			2.9480338708E+02	-3.5578338102E+01		

IQA Intraatomic ("Self") Energy Components:

$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{ne}(A,A) = (1/2)[V_{ne}(A,A) + V_{en}(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$V_{eeC}(A,A)$ = Coulomb Part of $V_{ee}(A,A)$

$V_{eeX}(A,A)$ = Exchange-Correlation Part of $V_{ee}(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$V_{ne}(A,A)$	$V_{ee}(A,A)$	$V_{eeC}(A,A)$	$V_{eeX}(A,A)$
C1	-3.6682885121E+01 1.4279109989E+01 -4.3318676648E+00		3.6684239266E+01	-8.3314366711E+01		9.9472423247E+00
F2	-9.9269571289E+01 5.4696382704E+01 -1.0206769197E+01		9.9779236368E+01	-2.4353842116E+02		4.4489613507E+01
F3	-9.9269585588E+01 5.4696375578E+01 -1.0206756425E+01		9.9779235006E+01	-2.4353843975E+02		4.4489619153E+01
F4	-9.9269580594E+01 5.4696373766E+01 -1.0206761334E+01		9.9779237315E+01	-2.4353843034E+02		4.4489612432E+01
Total	-3.3449162259E+02 1.7836824204E+02 -3.4952154621E+01		3.3602194795E+02	-8.1392965796E+02		1.4341608742E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= V_{ne}(A,A')/2 + V_{en}(A,A')/2 + V_{ee}(A,A') + V_{nn}(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$V_{ne}(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[V_{ne}(A,Mol) - V_{ne}(A,A)]$$

$V_{en}(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[V_{en}(A,Mol) - V_{en}(A,A)]$$

$V_{ee}(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= V_{ee}(A,Mol) - V_{ee}(A,A)$$

$V_{nn}(A) = V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A, A') =$ Coulomb Part of $V_{ee}(A, A')$

$V_{eeX}(A, A') =$ Exchange-Correlation Part of $V_{ee}(A, A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$V_{ne}(A, A')/2$	$V_{en}(A, A')/2$	$V_{ee}(A, A')$	$V_{nn}(A)$	$V_{eeC}(A, A')$ $V_{eeX}(A, A')$
C1	-1.0454843280E+00	-3.2679720544E+01	-2.1627584285E+01	2.3311963538E+01	2.9949856963E+01	2.3576707358E+01 -2.6474381949E-01
F2	-2.3557643689E-01	-2.8464839970E+01	-3.2149189205E+01	3.0832317909E+01	2.9546134829E+01	3.0952790223E+01 -1.2047231354E-01
F3	-2.3556414163E-01	-2.8464830709E+01	-3.2149213770E+01	3.0832345516E+01	2.9546134822E+01	3.0952831906E+01 -1.2048639016E-01
F4	-2.3556736626E-01	-2.8464835412E+01	-3.2149201374E+01	3.0832334597E+01	2.9546134822E+01	3.0952815555E+01 -1.2048095818E-01
Total	-1.7521922728E+00	-1.1807422664E+02	-1.1807518863E+02	1.1580896156E+02	1.1858826144E+02	1.1643514504E+02 -6.2618348137E-01

IQA Atomic Contributions to Diatomic "Interaction" Energy Components:

$$E\_IQA\_Inter(A, B)/2 = V_{ne}(A, B)/2 + V_{en}(A, B)/2 + V_{ee}(A, B) + V_{nn}(A, B)/2$$

= Contribution to $E\_IQA(A)$ From "Interaction" of Atom A With Atom B

= Half of Total IQA "Interaction" Energy Between Atoms A and B

$V_{ne}(A, B)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Atom B

$V_{en}(A, B)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom B

$V_{ee}(A, B)$ = Half of Two-electron Interaction Energy Between Atom A and Atom B

$V_{nn}(A, B)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Nucleus of Atom B

$V_{eeC}(A, B)$ = Coulomb Part of $V_{ee}(A, B)$

$V_{eeX}(A, B)$ = Exchange-Correlation Part of $V_{ee}(A, B)$

Note that:

$$E\_IQA\_Inter(B,A)/2 = E\_IQA\_Inter(A,B)/2$$

$$Vne(B,A)/2 = Ven(A,B)/2$$

$$Ven(B,A)/2 = Vne(A,B)/2$$

$$Vee(B,A) = Vee(A,B)$$

$$Vnn(B,A)/2 = Vnn(A,B)/2$$

$$VeeC(B,A) = VeeC(A,B)$$

$$VeeX(B,A) = VeeX(A,B)$$

Note that, within numerical integration errors, we should have:

$$E\_IQA\_Inter(A,SumB)/2 = E\_IQA(A) - E\_IQA\_Intra(A)$$

$$Vne(A,SumB)/2 = Vne(A,Mol)/2 - Vne(A,A)/2$$

$$Ven(A,SumB)/2 = Ven(A,Mol)/2 - Ven(A,A)/2$$

$$Vee(A,SumB) = Vee(A,Mol) - Vee(A,A)$$

$$VeeC(A,SumB) = VeeC(A,Mol) - VeeC(A,A)$$

$$VeeX(A,SumB) = VeeX(A,Mol) - VeeX(A,A)$$

See "2EDM Note" and "DFT Note".

Atom A	Atom B	$E\_IQA\_Inter(A,B)/2$	$Vne(A,B)/2$	$Ven(A,B)/2$	$Vee(A,B)$	$Vnn(A,B)/2$
$VeeC(A,B)$	$VeeX(A,B)$					

C1	F2	-3.4861444132E-01	-1.0893299171E+01	-7.2096692722E+00	7.7710683517E+00	
9.9832856504E+00	7.8589789047E+00	-8.7910553000E-02				

C1	F3	-3.4864599831E-01	-1.0893295396E+01	-7.2103419773E+00	7.7717057188E+00	
9.9832856565E+00	7.8597068427E+00	-8.8001123863E-02				

C1	F4	-3.4866512977E-01	-1.0893301437E+01	-7.2105121283E+00	7.7718627787E+00	
9.9832856565E+00	7.8598941158E+00	-8.8031337096E-02				

C1	SumB	-1.0459255694E+00	-3.2679896004E+01	-2.1630523378E+01	2.3314636849E+01	
2.9949856963E+01	2.3578579863E+01	-2.6394301396E-01				

C1	A'=Mol-A	-1.0454843280E+00	-3.2679720544E+01	-2.1627584285E+01	2.3311963538E+01	
2.9949856963E+01	2.3576707358E+01	-2.6474381949E-01				

C1	SumB-A'	-4.4124140000E-04	-1.7546000000E-04	-2.9390928000E-03	2.6733112000E-03	
4.0000358581E-10	1.8725052000E-03	8.0080553100E-04				

Atom A	Atom B	E_IQA_Inter(A,B)/2	Vne(A,B)/2	Ven(A,B)/2	Vee(A,B)	Vnn(A,B)/2
VeeC(A,B)	VeeX(A,B)					

F2	C1	-3.4861444132E-01	-7.2096692722E+00	-1.0893299171E+01	7.7710683517E+00	
9.9832856504E+00	7.8589789047E+00	-8.7910553000E-02				

F2	F3	5.7007428422E-02	-1.0627932085E+01	-1.0627933166E+01	1.1531448090E+01	
9.7814245891E+00	1.1547949859E+01	-1.6501769064E-02				

F2	F4	5.7007642326E-02	-1.0627932900E+01	-1.0627932608E+01	1.1531448561E+01	
9.7814245891E+00	1.1547950155E+01	-1.6501594254E-02				

F2	SumB	-2.3459937057E-01	-2.8465534257E+01	-3.2149164945E+01	3.0833965003E+01	
2.9546134829E+01	3.0954878919E+01	-1.2091391632E-01				

F2	A'=Mol-A	-2.3557643689E-01	-2.8464839970E+01	-3.2149189205E+01	3.0832317909E+01	
2.9546134829E+01	3.0952790223E+01	-1.2047231354E-01				

F2	SumB-A'	9.7706631800E-04	-6.9428720000E-04	2.4259999996E-05	1.6470937000E-03	-
4.0000358581E-10	2.0886957000E-03	-4.4160277800E-04				

Atom A	Atom B	E_IQA_Inter(A,B)/2	Vne(A,B)/2	Ven(A,B)/2	Vee(A,B)	Vnn(A,B)/2
VeeC(A,B)	VeeX(A,B)					

F3	C1	-3.4864599831E-01	-7.2103419773E+00	-1.0893295396E+01	7.7717057188E+00	
9.9832856565E+00	7.8597068427E+00	-8.8001123863E-02				

F3	F2	5.7007428422E-02	-1.0627933166E+01	-1.0627932085E+01	1.1531448090E+01	
9.7814245891E+00	1.1547949859E+01	-1.6501769064E-02				

F3	F4	5.7007901528E-02	-1.0627933585E+01	-1.0627931470E+01	1.1531448380E+01	
9.7814245762E+00	1.1547949673E+01	-1.6501292365E-02				

F3	SumB	-2.3463066836E-01	-2.8466208728E+01	-3.2149158951E+01	3.0834602189E+01	
2.9546134822E+01	3.0955606375E+01	-1.2100418529E-01				

F3	A'=Mol-A	-2.3556414163E-01	-2.8464830709E+01	-3.2149213770E+01	3.0832345516E+01	
2.9546134822E+01	3.0952831906E+01	-1.2048639016E-01				

F3	SumB-A'	9.3347327000E-04	-1.3780193000E-03	5.4819000006E-05	2.2566728000E-03	-
2.0000001655E-10	2.7744687000E-03	-5.1779513200E-04				

Atom A	Atom B	$E\_IQA\_Inter(A,B)/2$	$Vne(A,B)/2$	$Ven(A,B)/2$	$Vee(A,B)$	$Vnn(A,B)/2$
$VeeC(A,B)$	$VeeX(A,B)$					

F4	C1	-3.4866512977E-01	-7.2105121283E+00	-1.0893301437E+01	7.7718627787E+00	
9.9832856565E+00	7.8598941158E+00	-8.8031337096E-02				

F4	F2	5.7007642326E-02	-1.0627932608E+01	-1.0627932900E+01	1.1531448561E+01	
9.7814245891E+00	1.1547950155E+01	-1.6501594254E-02				

F4	F3	5.7007901528E-02	-1.0627931470E+01	-1.0627933585E+01	1.1531448380E+01	
9.7814245762E+00	1.1547949673E+01	-1.6501292365E-02				

F4	SumB	-2.3464958592E-01	-2.8466376206E+01	-3.2149167922E+01	3.0834759720E+01	
2.9546134822E+01	3.0955793944E+01	-1.2103422371E-01				

F4	A'=Mol-A	-2.3556736626E-01	-2.8464835412E+01	-3.2149201374E+01	3.0832334597E+01	
2.9546134822E+01	3.0952815555E+01	-1.2048095818E-01				

F4	SumB-A'	9.1778034400E-04	-1.5407943000E-03	3.3452000004E-05	2.4251227000E-03	-
2.0000001655E-10	2.9783888000E-03	-5.5326553500E-04				

Total Vee(A,A) = 1.4341608742E+02

Total Vee(A,SumB) = 1.1581796376E+02

Total [Vee(A,A) + Vee(A,SumB)] = 2.5923405118E+02

Total Vee(A,Mol) = 2.5922504898E+02

Total [Vee(A,A) + Vee(A,SumB) - Vee(A,Mol)] = 9.0022001000E-03

IQA Diatomic "Interaction" Energy Components:

$E\_IQA\_Inter(A,B) = Vne(A,B) + Ven(A,B) + 2*Vee(A,B) + Vnn(A,B)$

= Total IQA "Interaction" Energy Between Atoms A and B

$Vne(A,B) = Ven(B,A)$ = Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Atom B

$Ven(A,B) = Vne(B,A)$ = Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom B

$2*Vee(A,B)$ = Two-electron Interaction Energy Between Atom A and Atom B

$V_{nn}(A,B)$ = Repulsion Energy Between Nucleus of Atom A and Nucleus of Atom B

$2*V_{eeC}(A,B)$ = Coulomb Part of $2*V_{ee}(A,B)$

$2*V_{eeX}(A,B)$ = Exchange-Correlation Part of $2*V_{ee}(A,B)$

See "2EDM Note" and "DFT Note".

Atom A	Atom B	$E_{IQA\_Inter}(A,B)$	$V_{ne}(A,B)$	$V_{en}(A,B)$	$2*V_{ee}(A,B)$	$V_{nn}(A,B)$
$2*V_{eeC}(A,B)$	$2*V_{eeX}(A,B)$					

F2	C1	-6.9722888264E-01	-1.4419338544E+01	-2.1786598342E+01	1.5542136703E+01	
1.9966571301E+01	1.5717957809E+01	-1.7582110600E-01				

F3	C1	-6.9729199662E-01	-1.4420683955E+01	-2.1786590792E+01	1.5543411438E+01	
1.9966571313E+01	1.5719413685E+01	-1.7600224773E-01				

F3	F2	1.1401485684E-01	-2.1255866332E+01	-2.1255864170E+01	2.3062896180E+01	
1.9562849178E+01	2.3095899718E+01	-3.3003538128E-02				

F4	C1	-6.9733025954E-01	-1.4421024257E+01	-2.1786602874E+01	1.5543725557E+01	
1.9966571313E+01	1.5719788232E+01	-1.7606267419E-01				

F4	F2	1.1401528465E-01	-2.1255865216E+01	-2.1255865800E+01	2.3062897122E+01	
1.9562849178E+01	2.3095900310E+01	-3.3003188508E-02				

F4	F3	1.1401580306E-01	-2.1255862940E+01	-2.1255867170E+01	2.3062896760E+01	
1.9562849152E+01	2.3095899346E+01	-3.3002584730E-02				

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other

Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1	4.7174175062E+00	3.7599894144E+00	7.9704402026E+01	9.5742809181E-01	2.0295597974E+01
F2	9.7608769154E+00	9.2783220189E+00	9.5056234182E+01	4.8255489646E-01	4.9437658178E+00
F3	9.7608823122E+00	9.2783266110E+00	9.5056228671E+01	4.8255570117E-01	4.9437713287E+00
F4	9.7608789696E+00	9.2783244058E+00	9.5056238630E+01	4.8255456382E-01	4.9437613695E+00
Total	3.4000055703E+01	3.1594962450E+01	9.2926207903E+01	2.4050932533E+00	7.0737920969E+00

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	4.7174175062E+00	3.7599894144E+00	9.5742809181E-01	9.5736384866E-01	6.4243150189E-05
F2	9.7608769154E+00	9.2783220189E+00	4.8255489646E-01	3.1908242934E-01	1.6347246712E-01
F3	9.7608823122E+00	9.2783266110E+00	4.8255570117E-01	3.1918880430E-01	1.6336689688E-01
F4	9.7608789696E+00	9.2783244058E+00	4.8255456382E-01	3.1909261502E-01	1.6346194880E-01
Total	3.4000055703E+01	3.1594962450E+01	2.4050932533E+00	1.9147276973E+00	4.9036555595E-01

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	9.2470192567E+00	6.8590369596E+01	7.7837388852E+01
F2	4.2998198069E+01	1.1805627103E+02	1.6105446910E+02
F3	4.2998248451E+01	1.1805630970E+02	1.6105455815E+02
F4	4.2998216927E+01	1.1805628607E+02	1.6105450300E+02
Total	1.3824168270E+02	4.2275923640E+02	5.6100091911E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A)$ = Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A)$ = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$

C1	F2	4.5727049207E+01	6.3816485868E-01	6.7639217627E+00	3.2689934737E+00 (Bonded)
C1	F3	4.5726968291E+01	6.3837760859E-01	6.7661767032E+00	3.2700814751E+00 (Bonded)
F2	F3	9.5193032709E+01	1.6347625298E-01	8.3740556505E-01	8.3740510205E-01
C1	F4	4.5727048712E+01	6.3818523005E-01	6.7641376792E+00	3.2690971378E+00 (Bonded)
F2	F4	9.5193002159E+01	1.6347209947E-01	8.3738428878E-01	8.3738411255E-01
F3	F4	9.5193054416E+01	1.6347293980E-01	8.3738813037E-01	8.3738841713E-01

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
C1	F2	5.2782391847E+01	4.2089725676E+01	3.4679497859E+01
C1	F3	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
C1	F4	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
C1	Total	1.5834717558E+02	1.2626917700E+02	1.0403849351E+02
F2	C1	5.2782391847E+01	4.2089725676E+01	3.4679497859E+01
F2	Total	5.2782391847E+01	4.2089725676E+01	3.4679497859E+01
F3	C1	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
F3	Total	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
F4	C1	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
F4	Total	5.2782391867E+01	4.2089725660E+01	3.4679497828E+01
Total	Total	3.1669435116E+02	2.5253835399E+02	2.0807698703E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\text{DelSqRho\_IAS}(A|B)$ = Integral of Laplacian of Electron Density $\text{DelSqRho}(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	N_IAS(A B)	G_IAS(A B)	K_IAS(A B)	L_IAS(A B)	DelSqRho_IAS(A B)	V_IAS(A B)
C1	F2	1.0692980183E+00	1.1930868990E+00	4.1300136048E-01	-7.8008553851E-01	3.1203421540E+00	-1.6060882595E+00
C1	F3	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00
C1	F4	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00
C1	Total	3.2078940601E+00	3.5792607088E+00	1.2390040939E+00	-2.3402566148E+00	9.3610264592E+00	-4.8182648027E+00
F2	C1	1.0692980183E+00	1.1930868990E+00	4.1300136048E-01	-7.8008553851E-01	3.1203421540E+00	-1.6060882595E+00
F2	Total	1.0692980183E+00	1.1930868990E+00	4.1300136048E-01	-7.8008553851E-01	3.1203421540E+00	-1.6060882595E+00
F3	C1	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00
F3	Total	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00
F4	C1	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00
F4	Total	1.0692980209E+00	1.1930869049E+00	4.1300136670E-01	-7.8008553815E-01	3.1203421526E+00	-1.6060882716E+00

Total Total 6.4157881202E+00 7.1585214176E+00 2.4780081878E+00 -4.6805132296E+00
1.8722052918E+01 -9.6365296054E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)
C1	7.4309243513E+01	-1.4363389838E+01	-1.9056786998E-01	-2.0001976044E-01	-1.9329210148E-01	1.7704220600E-03	4.7077772849E-06
F2	8.8123028465E+01	-1.7073351189E+01	-1.8258727591E-01	-2.1215900423E-01	-1.9374448979E-01	5.8342335986E-03	4.8290270593E-05
F3	8.8154900285E+01	-1.7078976099E+01	-1.8258755110E-01	-2.1207217671E-01	-1.9373824987E-01	5.8263375349E-03	4.8075786348E-05
F4	8.7926417562E+01	-1.7032801934E+01	-1.8258849668E-01	-2.1221145033E-01	-1.9371654624E-01	5.8193992611E-03	4.7972892673E-05
Total	3.3851358982E+02	-6.5548519060E+01	-1.8258727591E-01	-2.1221145033E-01	-1.9363630008E-01		3.8618344404E-05

0.0004 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)	ESP-_Int_IDS(A)
C1	1.4363389838E+01	2.7766796376E+00	0.0000000000E+00	NULL	7.4309243513E+01	-1.4363389838E+01
F2	1.7073351189E+01	3.3121231999E+00	0.0000000000E+00	NULL	8.8123028465E+01	-1.7073351189E+01
F3	1.7078976099E+01	3.3130890552E+00	0.0000000000E+00	NULL	8.8154900285E+01	-1.7078976099E+01
F4	1.7032801934E+01	3.3037536481E+00	0.0000000000E+00	NULL	8.7926417562E+01	-1.7032801934E+01
Total	6.5548519060E+01	1.2705645541E+01	0.0000000000E+00	NULL	3.3851358982E+02	-6.5548519060E+01

0.0004 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

C1	NULL	NULL	NULL	NULL	NULL
F2	NULL	NULL	NULL	NULL	NULL
F3	NULL	NULL	NULL	NULL	NULL
F4	NULL	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL	NULL

0.0004 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-1.9056786998E-01	-1.9329210148E-01	1.7704220600E-03	4.7077772849E-06	2.7766796376E+00
F2	-1.8258727591E-01	-1.9374448979E-01	5.8342335986E-03	4.8290270593E-05	3.3121231999E+00
F3	-1.8258755110E-01	-1.9373824987E-01	5.8263375349E-03	4.8075786348E-05	3.3130890552E+00
F4	-1.8258849668E-01	-1.9371654624E-01	5.8193992611E-03	4.7972892673E-05	3.3037536481E+00

Total	-1.8258727591E-01	-1.9363630008E-01	3.8618344404E-05	1.2705645541E+01	

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	5.8378660655E+01	-1.2392910954E+01	-2.0503584891E-01	-2.1667755864E-01	-2.1228494822E-01	2.5221627956E-03	9.1277495271E-06
F2	7.7757335310E+01	-1.6039840266E+01	-1.9426370739E-01	-2.2186337268E-01	-2.0628073483E-01	5.7578271579E-03	4.9341901226E-05

F3 7.7571685988E+01 -1.5998277103E+01 -1.9426264350E-01 -2.2181252122E-01 -2.0623861528E-01 5.7276751655E-03 4.8762262464E-05

F4 7.7476681000E+01 -1.5977054653E+01 -1.9426691238E-01 -2.2186787464E-01 -2.0621759279E-01 5.7150785695E-03 4.8628688919E-05

Total 2.9118436295E+02 -6.0408082976E+01 -1.9426264350E-01 -2.2186787464E-01 -
2.0745648002E-01 4.6782132520E-05

0.001 IsoDensity Surface:

Atom A |ESP|_Int_IDS(A) ESP*ESP_Int_IDS(A) Area_ESP+_IDS(A) ESP+_Int_IDS(A) Area_ESP-
_IDS(A) ESP-_Int_IDS(A)

C1 1.2392910954E+01 2.6313613260E+00 0.0000000000E+00 NULL 5.8378660655E+01
-1.2392910954E+01

F2 1.6039840266E+01 3.3125467314E+00 0.0000000000E+00 NULL 7.7757335310E+01
-1.6039840266E+01

F3 1.5998277103E+01 3.3032450874E+00 0.0000000000E+00 NULL 7.7571685988E+01
-1.5998277103E+01

F4 1.5977054653E+01 3.2985173398E+00 0.0000000000E+00 NULL 7.7476681000E+01
-1.5977054653E+01

Total 6.0408082976E+01 1.2545670485E+01 0.0000000000E+00 NULL 2.9118436295E+02
-6.0408082976E+01

0.001 IsoDensity Surface:

Atom A ESP+_Min_IDS(A) ESP+_Avg_IDS(A) ESP+_MAD_IDS(A) ESP+_Var_IDS(A)
ESP*ESP+_Int_IDS(A)

C1 NULL NULL NULL NULL NULL

F2 NULL NULL NULL NULL NULL

F3 NULL NULL NULL NULL NULL

F4 NULL NULL NULL NULL NULL

Total NULL NULL NULL NULL NULL

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
C1	-2.0503584891E-01	-2.1228494822E-01	2.5221627956E-03	9.1277495271E-06	2.6313613260E+00
F2	-1.9426370739E-01	-2.0628073483E-01	5.7578271579E-03	4.9341901226E-05	3.3125467314E+00
F3	-1.9426264350E-01	-2.0623861528E-01	5.7276751655E-03	4.8762262464E-05	3.3032450874E+00
F4	-1.9426691238E-01	-2.0621759279E-01	5.7150785695E-03	4.8628688919E-05	3.2985173398E+00
Total	-1.9426264350E-01	-2.0745648002E-01	4.6782132520E-05	1.2545670485E+01	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)
C1	4.8008643936E+01	-1.0909827434E+01	-2.0594200073E-01	-2.3879384081E-01	-2.2724714842E-01	6.2182860599E-03	6.1147092589E-05
F2	6.9571108050E+01	-1.5020398600E+01	-2.0376294466E-01	-2.3120478809E-01	-2.1589994785E-01	5.3803723315E-03	4.3641779427E-05
F3	6.9511883921E+01	-1.5005813384E+01	-2.0376739865E-01	-2.3121915605E-01	-2.1587407127E-01	5.3600332008E-03	4.3210443257E-05
F4	6.9767719934E+01	-1.5063022331E+01	-2.0376160115E-01	-2.3122012303E-01	-2.1590245955E-01	5.3758689353E-03	4.3502750326E-05
Total	2.5685935584E+02	-5.5999061749E+01	-2.0376160115E-01	-2.3879384081E-01	-2.1801449110E-01	6.6353897172E-05	

0.002 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)

C1	1.0909827434E+01	2.4821627632E+00	0.0000000000E+00	NULL	4.8008643936E+01

F2	1.5020398600E+01	3.2459394813E+00	0.0000000000E+00	NULL	6.9571108050E+01

F3	1.5005813384E+01	3.2423696672E+00	0.0000000000E+00	NULL	6.9511883921E+01

F4	1.5063022331E+01	3.2551786571E+00	0.0000000000E+00	NULL	6.9767719934E+01

Total	5.5999061749E+01	1.2225650569E+01	0.0000000000E+00	NULL	2.5685935584E+02

0.002 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)

C1	NULL	NULL	NULL	NULL

F2	NULL	NULL	NULL	NULL

F3	NULL	NULL	NULL	NULL

F4	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL

0.002 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-2.0594200073E-01	-2.2724714842E-01	6.2182860599E-03	6.1147092589E-05	2.4821627632E+00

F2	-2.0376294466E-01	-2.1589994785E-01	5.3803723315E-03	4.3641779427E-05	3.2459394813E+00

F3	-2.0376739865E-01	-2.1587407127E-01	5.3600332008E-03	4.3210443257E-05
	3.2423696672E+00			
F4	-2.0376160115E-01	-2.1590245955E-01	5.3758689353E-03	4.3502750326E-05
	3.2551786571E+00			

Total	-2.0376160115E-01	-2.1801449110E-01	6.6353897172E-05	1.2225650569E+01

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A) = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$

$\text{Isosurface of the Electron Density Distribution (IsoDensity Surface)}$

$N(\text{Vol}(A)) = \text{Average Number of Electrons in Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A) = \text{Average Electron Density in Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

$= \text{Percentage of Atom A's Electron Population in Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.3265641909E+02	1.2756478854E+02	4.6919168191E+00	3.6780657677E-02	
	9.9459435452E+01				
F2	1.4090542031E+02	1.3877109239E+02	9.7433732325E+00	7.0211836377E-02	
	9.9820675100E+01				
F3	1.4093729215E+02	1.3883006315E+02	9.7434023630E+00	7.0182222368E-02	
	9.9820918345E+01				
F4	1.4070880943E+02	1.3878902206E+02	9.7433834562E+00	7.0202839614E-02	
	9.9820758828E+01				
Total	6.5520794099E+02	5.4395496614E+02	3.3922075871E+01	6.2361919612E-02	
	9.9770647927E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.8464783765E+02	9.2494123737E+01	4.6692791130E+00	5.0481900086E-02	9.8979560477E+01
F2	1.1984706099E+02	1.1094225304E+02	9.7254523416E+00	8.7662293448E-02	9.9637075910E+01
F3	1.1966141165E+02	1.1096588955E+02	9.7254819811E+00	8.7643887872E-02	9.9637324472E+01
F4	1.1956640666E+02	1.1101738389E+02	9.7255311828E+00	8.7603678286E-02	9.9637862662E+01
Total	5.4372271695E+02	4.2541965022E+02	3.3845744618E+01	7.9558489132E-02	9.9546144612E+01

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.5204713745E+02	7.1406229905E+01	4.6390615230E+00	6.4967181844E-02	9.8339006827E+01
F2	1.0425060591E+02	9.1397486315E+01	9.6976458433E+00	1.0610407610E-01	9.9352198859E+01
F3	1.0419138175E+02	9.1426424938E+01	9.6977061439E+00	1.0607115121E-01	9.9352761700E+01
F4	1.0444721776E+02	9.1411204669E+01	9.6976766672E+00	1.0608848994E-01	9.9352493734E+01
Total	4.6493634287E+02	3.4564134583E+02	3.3732090177E+01	9.7592752096E-02	9.9211867391E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	q(A B)	q(A)*	q(A)
C1	F2	4.7514671424E-01		
C1	F3	4.7515211154E-01		
C1	F4	4.7514876904E-01		
C1		1.4254475948E+00	1.2825824943E+00	
F2	C1	-6.1801181477E-01		
F2		-6.1801181477E-01	-7.6087691530E-01	
F3	C1	-6.1801721207E-01		
F3		-6.1801721207E-01	-7.6088231260E-01	
F4	C1	-6.1801386957E-01		
F4		-6.1801386957E-01	-7.6087897010E-01	

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)
C1	2.4053302625E-04	2.2605999847E-06	2.4279362623E-04
F2	3.1287708824E-06	2.2589353619E-18	3.1287708824E-06
F3	-9.4897232772E-02	8.6147302591E-01	7.6657579314E-01
F4	9.4891710337E-02	-8.6146836670E-01	-7.6657665636E-01
Total	2.3813936213E-04	6.9198125974E-06	2.4505917473E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	3.1478953210E-04	2.9078493264E-06	3.1769738143E-04
F2	1.0956309322E-01	-9.9473467887E-01	-8.8517158565E-01
F3	-5.4786874145E-02	4.9737168132E-01	4.4258480717E-01
F4	-5.4778895133E-02	4.9736899132E-01	4.4259009619E-01

Total	3.1211347410E-04	8.9016159575E-06	3.2101509006E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	-2.0300965137E+00	5.5028773947E-01	-1.4798087742E+00
F2	-7.7687079624E-02	5.4311197844E-01	4.6542489882E-01
F3	-7.7675925483E-02	5.4311672349E-01	4.6544079801E-01
F4	-7.7685386496E-02	5.4311378608E-01	4.6542839959E-01

Total	-2.2631449053E+00	2.1796302275E+00	-8.3514677815E-02

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	2.0300965523E+00	5.5028773949E-01	1.4798088282E+00
F2	1.3431066133E-01	1.1333435942E+00	1.0000745335E+00
F3	1.3431543383E-01	1.1333534926E+00	1.0000774443E+00
F4	1.3431374955E-01	1.1333473629E+00	1.0000746764E+00

Total	2.2631449394E+00	2.1796302275E+00	8.3515654312E-02

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	F2	-1.7367397989E-18
C1	F3	3.2135493078E-01
C1	F4	-3.2135267018E-01
C1		2.2605999847E-06
F2	C1	2.2589353619E-18
F2		2.2589353619E-18
F3	C1	8.6147302591E-01
F3		8.6147302591E-01
F4	C1	-8.6146836670E-01
F4		-8.6146836670E-01

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	F2	-3.7106449663E-01
C1	F3	1.8553435482E-01
C1	F4	1.8553304966E-01
C1		2.9078493264E-06
F2	C1	-9.9473467887E-01
F2		-9.9473467887E-01
F3	C1	4.9737168132E-01
F3		4.9737168132E-01
F4	C1	4.9736899132E-01
F4		4.9736899132E-01

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	F2	1.8342828850E-01
C1	F3	1.8343037067E-01
C1	F4	1.8342908031E-01
C1		5.5028773947E-01
F2	C1	5.4311197844E-01

F2		5.4311197844E-01
F3	C1	5.4311672349E-01
F3		5.4311672349E-01
F4	C1	5.4311378608E-01
F4		5.4311378608E-01

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	F2	4.1392607756E-01	
C1	F3	4.1393077831E-01	
C1	F4	4.1392786648E-01	
C1		5.5028773949E-01	
F2	C1	1.1333435942E+00	
F2		1.1333435942E+00	
F3	C1	1.1333534926E+00	
F3		1.1333534926E+00	
F4	C1	1.1333473629E+00	
F4		1.1333473629E+00	

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)

C1 2.2309855017E+00 1.2408242327E-03 -1.5328100435E-03 2.2367156167E+00 2.5963425202E-03 -4.4677011184E+00

F2 -1.3511885715E-01 -7.1699849010E-06 1.8352811487E-05 2.8310207994E-01 -1.5084398077E-01 -1.4798322278E-01

F3 1.7852124828E-01 1.8104341393E-01 1.3067689547E-01 -3.0546168155E-02 7.5482105679E-02 -1.4797508012E-01

F4 1.7851839706E-01 -1.8108567708E-01 -1.3062892591E-01 -3.0541036041E-02 7.5447258888E-02 -1.4797736102E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)

C1	1	-4.4677024748E+00	2.2889414552E-04	-3.8730076786E-04	9.999989880E-01
C1	2	2.2307289624E+00	9.7921480270E-01	-2.0282573446E-01	-3.0269112888E-04
C1	3	2.2369735125E+00	2.0282583116E-01	9.7921477289E-01	3.3282502180E-04
F2	1	-1.9552334004E-01	-2.5410169603E-04	3.0058609596E-01	9.5375465102E-01
F2	2	-1.3511885358E-01	9.999996736E-01	1.0167920621E-04	2.3437718690E-04
F2	3	3.3064219362E-01	-2.6526492241E-05	9.5375467945E-01	-3.0058611199E-01
F3	1	-1.9555950810E-01	-2.6016932721E-01	-1.5081368298E-01	9.5371230159E-01
F3	2	-1.3506749312E-01	-5.0014079233E-01	8.6594395886E-01	4.9795335242E-04
F3	3	3.3062700122E-01	8.2593650424E-01	4.7686087398E-01	3.0072013208E-01
F4	1	-1.9552452272E-01	2.6018614283E-01	-1.5056994521E-01	9.5374622551E-01
F4	2	-1.3510097003E-01	5.0012192884E-01	8.6595495312E-01	2.7470014748E-04
F4	3	3.3062549275E-01	8.2594262959E-01	-4.7691792876E-01	-3.0061281054E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r*r) \rangle(A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle(A)$$

$$R0(A) = \langle \text{Rho} \rangle(A) = N(A)$$

$$R+1(A) = \langle \text{Rho}*r \rangle(A)$$

$$R+2(A) = \langle \text{Rho}*r*r \rangle(A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3713104051E+02 8.5406278882E+00		1.3885727785E+01	4.7174175057E+00	4.6784051857E+00
F2	3.3040624121E+02 1.2201684108E+01		2.7059824574E+01	9.7608769153E+00	8.9398536870E+00
F3	3.3040624020E+02 1.2201722057E+01		2.7059826639E+01	9.7608823126E+00	8.9398677868E+00
F4	3.3040623992E+02 1.2201692829E+01		2.7059825593E+01	9.7608789701E+00	8.9398577643E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x*(d\text{Rho}/dx) + y*(d\text{Rho}/dy) + z*(d\text{Rho}/dz)$$

$$GR-2(A) = \langle \text{Dot}/(r*r) \rangle(A)$$

$$GR-1(A) = \langle \text{Dot}/r \rangle(A)$$

$$GR0(A) = \langle \text{Dot} \rangle(A)$$

$$GR+1(A) = \langle \text{Dot}*r \rangle(A)$$

$$GR+2(A) = \langle \text{Dot}*r*r \rangle(A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3597730671E+02 3.8087380279E+01	-2.6347813308E+01	-1.2245687201E+01	-1.5898528678E+01	-
F2	-3.2993302631E+02 5.1282495934E+01	-5.3144995332E+01	-2.7239396824E+01	-3.1373731239E+01	-
F3	-3.2993302649E+02 5.1282604256E+01	-5.3145000985E+01	-2.7239411656E+01	-3.1373770009E+01	-

F4 -3.2993302466E+02 -5.3144996170E+01 -2.7239398981E+01 -3.1373736792E+01 -
5.1282520284E+01

Atomic Basin-Integrated Ehrenfest Forces and Basin and Surface Electronic Virial Energies:

EhF(A) = Electronic Ehrenfest Force on Basin of Atom A, Calculated as Minus Basin

Integral of Divergence of Stress Tensor

Vb(A) = Basin Electronic Virial Energy of Atom A = $-\langle \mathbf{r} \cdot \text{DivStress} \rangle(\text{A})$

Vs(A) = Surface Electronic Virial Energy of Atom A = $V(\text{A}) - Vb(\text{A})$

V(A) = Total Electronic Virial Energy of Atom A = $-K(\text{A}) - G(\text{A}) = -2T(\text{A})$

Atom A	EhF_X(A)	EhF_Y(A)	EhF_Z(A)	Vb(A)	Vs(A)	V(A)
C1	5.5557642510E-05	2.9296096879E-05	-4.1984482472E-01	-7.3017620532E+01	-3.5141620854E-01	-7.3369036740E+01
F2	-6.8045634130E-06	-2.8981095356E-01	1.3998477412E-01	-1.9880548895E+02	-7.5285477058E-01	-1.9955834372E+02
F3	2.5098142689E-01	1.4490333426E-01	1.3999232079E-01	-1.9880548405E+02	-7.5286593334E-01	-1.9955834998E+02
F4	-2.5098291776E-01	1.4490637753E-01	1.3999096394E-01	-1.9880547877E+02	-7.5286830928E-01	-1.9955834708E+02
Total	4.7262209097E-05	2.8054326879E-05	1.2323413000E-04	-6.6943407230E+02	-2.6100052217E+00	-6.7204407752E+02

Atomic Surface-Integrated Ehrenfest Forces and Basin and Surface Electronic Virial Energies:

EhFs(A) = Electronic Ehrenfest Force on Surface of Atom A, Calculated as Minus Flux of

Stress Tensor

Vb(A) = Basin Electronic Virial Energy of Atom A = $V(\text{A}) - Vs(\text{A})$

Vs(A) = Surface Electronic Virial Energy of Atom A

V(A) = Total Electronic Virial Energy of Atom A = $-K(\text{A}) - G(\text{A}) = -2T(\text{A})$

Atom A	EhFs_X(A)	EhFs_Y(A)	EhFs_Z(A)	Vb(A)	Vs(A)	V(A)

C1 7.0247371364E-07 1.2133210666E-06 -4.1995266746E-01 -7.3017653917E+01 -3.5138282308E-01 -7.3369036740E+01

F2 -7.0247371630E-07 -2.8981195698E-01 1.3998422186E-01 -1.9880561105E+02 -7.5273266722E-01 -1.9955834372E+02

F3 2.5098487476E-01 1.4490537183E-01 1.3998422280E-01 -1.9880561730E+02 -7.5273268162E-01 -1.9955834998E+02

F4 -2.5098487476E-01 1.4490537183E-01 1.3998422280E-01 -1.9880561440E+02 -7.5273268162E-01 -1.9955834708E+02

Total -2.6645352591E-15 1.0665912598E-12 0.0000000000E+00 -6.6943449667E+02 -2.6095808535E+00 -6.7204407752E+02

Bond Contributions to Atomic Basin-Integrated Ehrenfest Forces:

EhF(A|B) = Contribution of Bond Between Atom A and Atom B to

Basin-Integrated Ehrenfest Force on Atom A

EhF(A)* = Sum of EhF(A|B) Over all B

EhF(A) = Total Basin-Integrated Ehrenfest Force on Atom A

Atom A	Atom B	EhF_X(A B)	EhF_X(A)*	EhF_X(A)

C1	F2	2.0308051726E-05		

C1	F3	-2.5096792340E-01		

C1	F4	2.5099642125E-01		

C1		4.8805898353E-05	5.5557642510E-05	

F2	C1	-1.3556307570E-05		

F2		-1.3556307570E-05	-6.8045634130E-06	

F3	C1	2.5097467515E-01		

F3		2.5097467515E-01	2.5098142689E-01	

F4	C1	-2.5098966950E-01		

F4		-2.5098966950E-01	-2.5098291776E-01	

Atom A	Atom B	EhF_Y(A B)	EhF_Y(A)*	EhF_Y(A)

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C1    F2    2.8981896908E-01
C1    F3    -1.4489531874E-01
C1    F4    -1.4489836201E-01
C1                                2.5288335896E-05 2.9296096879E-05
F2    C1    -2.8981496132E-01
F2                                -2.8981496132E-01 -2.8981095356E-01
F3    C1    1.4489932650E-01
F3                                1.4489932650E-01 1.4490333426E-01
F4    C1    1.4490236977E-01
F4                                1.4490236977E-01 1.4490637753E-01

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Atom A  Atom B  EhF_Z(A|B)  EhF_Z(A)*  EhF_Z(A)
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C1    F2    -1.3994956437E-01
C1    F3    -1.3995711104E-01
C1    F4    -1.3995575419E-01
C1                                -4.1986242960E-01 -4.1984482472E-01
F2    C1    1.3996716924E-01
F2                                1.3996716924E-01 1.3998477412E-01
F3    C1    1.3997471591E-01
F3                                1.3997471591E-01 1.3999232079E-01
F4    C1    1.3997335906E-01
F4                                1.3997335906E-01 1.3999096394E-01

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Interatomic Surface Contributions to Atomic Surface-Integrated Ehrenfest Forces:

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EhFs(A|B) = Contribution of Interatomic Surface (IAS) Between Atom A and Atom B
           to Ehrenfest Force on Atom A
EhFs(A) = Total Ehrenfest Force on Surface of Atom A

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Atom A  Atom B  EhFs_X(A|B)  EhFs_X(A)

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C1	F2	7.0247371636E-07
C1	F3	-2.5098487476E-01
C1	F4	2.5098487476E-01
C1		7.0247371364E-07
F2	C1	-7.0247371630E-07
F2		-7.0247371630E-07
F3	C1	2.5098487476E-01
F3		2.5098487476E-01
F4	C1	-2.5098487476E-01
F4		-2.5098487476E-01

Atom A	Atom B	EhFs_Y(A B)	EhFs_Y(A)

C1	F2	2.8981195698E-01
C1	F3	-1.4490537183E-01
C1	F4	-1.4490537183E-01
C1		1.2133210666E-06
F2	C1	-2.8981195698E-01
F2		-2.8981195698E-01
F3	C1	1.4490537183E-01
F3		1.4490537183E-01
F4	C1	1.4490537183E-01
F4		1.4490537183E-01

Atom A	Atom B	EhFs_Z(A B)	EhFs_Z(A)

C1	F2	-1.3998422186E-01
C1	F3	-1.3998422280E-01
C1	F4	-1.3998422280E-01
C1		-4.1995266746E-01
F2	C1	1.3998422186E-01

F2		1.3998422186E-01
F3	C1	1.3998422280E-01
F3		1.3998422280E-01
F4	C1	1.3998422280E-01
F4		1.3998422280E-01

Interatomic Surface Contributions to Atomic Surface Electronic Virial Energies:

$V_s(A|B)$ = Contribution of Interatomic Surface (IAS) Between Atom A and Atom B
to Surface Electronic Virial Energy of Atom A

$V_s(A)$ = Total Surface Electronic Virial Energy of Atom A

Atom A	Atom B	$V_s(A B)$	$V_s(A)$

C1	F2	-1.1712760659E-01	
C1	F3	-1.1712760824E-01	
C1	F4	-1.1712760824E-01	
C1		-3.5138282308E-01	
F2	C1	-7.5273266722E-01	
F2		-7.5273266722E-01	
F3	C1	-7.5273268162E-01	
F3		-7.5273268162E-01	
F4	C1	-7.5273268162E-01	
F4		-7.5273268162E-01	

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)

C1	2.3587087528E+00	2.3587087528E+00	4.7174175057E+00	0.0000000000E+00
F2	4.8804384577E+00	4.8804384577E+00	9.7608769153E+00	0.0000000000E+00
F3	4.8804411563E+00	4.8804411563E+00	9.7608823126E+00	0.0000000000E+00
F4	4.8804394850E+00	4.8804394850E+00	9.7608789701E+00	0.0000000000E+00

Total	1.7000027852E+01	1.7000027852E+01	3.4000055704E+01	0.0000000000E+00

Atomic Sources of Electron Density at Electron Density CPs:

r = Position of Electron Density Critical Point

Rho(r,A) = Source Contribution of Atom A to Electron Density at r

%Rho(r,A) = Percentage of Total Source Electron Density at r from Atom A's Source Contribution

%Rho(r,A)* = Percentage of Analytic Electron Density at r from Atom A's Source Contribution

CP# 1 (3,-3) NACP C1

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	1.2008951174E+02	9.9933867921E+01	9.9933897631E+01
F2	2.6490513932E-02	2.2044385743E-02	2.2044392296E-02
F3	2.6489456133E-02	2.2043505483E-02	2.2043512037E-02
F4	2.6490276480E-02	2.2044188144E-02	2.2044194698E-02

Total	1.2016898199E+02	1.0000000000E+02	1.0000002973E+02
Analytic	1.2016894626E+02		
Error	3.5726545022E-05		

CP# 2 (3,-3) NACP F2

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	8.9669660883E-03	2.1045650746E-03	2.1045651329E-03
F2	4.2605368673E+02	9.9995661872E+01	9.9995664645E+01
F3	4.7577712581E-03	1.1166585358E-03	1.1166585668E-03
F4	4.7588172276E-03	1.1169040269E-03	1.1169040579E-03

Total	4.2607217028E+02	1.0000000000E+02	1.0000000277E+02
Analytic	4.2607215847E+02		
Error	1.1814573952E-05		

CP# 3 (3,-3) NACP F3

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	8.9552031099E-03	2.1018043608E-03	2.1018043611E-03
F2	4.7589065622E-03	1.1169250370E-03	1.1169250372E-03
F3	4.2605368111E+02	9.9995664409E+01	9.9995664424E+01
F4	4.7586360371E-03	1.1168615442E-03	1.1168615444E-03

Total	4.2607215386E+02	1.0000000000E+02	1.0000000002E+02
Analytic	4.2607215379E+02		
Error	6.5709173214E-08		

CP# 4 (3,-3) NACP F4

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	8.9723704342E-03	2.1058334805E-03	2.1058335670E-03
F2	4.7589559465E-03	1.1169365819E-03	1.1169366278E-03
F3	4.7579336628E-03	1.1166966499E-03	1.1166966957E-03
F4	4.2605368203E+02	9.9995660533E+01	9.9995664640E+01

Total	4.2607217129E+02	1.0000000000E+02	1.0000000411E+02
Analytic	4.2607215379E+02		
Error	1.7500043498E-05		

CP# 5 (3,-1) BCP F2 C1

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	7.9503123296E-02	3.9478569836E+01	3.9470836513E+01
F2	8.6797737920E-02	4.3100829452E+01	4.3092386577E+01
F3	1.7540512606E-02	8.7100270174E+00	8.7083208398E+00
F4	1.7541613520E-02	8.7105736942E+00	8.7088674095E+00

Total	2.0138298734E-01	1.0000000000E+02	9.9980411340E+01

Analytic	2.0142244330E-01		

Error	-3.9455958000E-05		

CP# 6 (3,-1) BCP C1 F3

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	7.9488821214E-02	3.9472593769E+01	3.9463735836E+01
F2	1.7541745929E-02	8.7108879020E+00	8.7089331162E+00
F3	8.6805260897E-02	4.3105794602E+01	4.3096121352E+01
F4	1.7541415317E-02	8.7107237266E+00	8.7087689776E+00

Total	2.0137724336E-01	1.0000000000E+02	9.9977559282E+01

Analytic	2.0142244400E-01		

Error	-4.5200643000E-05		

CP# 7 (3,-1) BCP F4 C1

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	7.9500002437E-02	3.9474937922E+01	3.9469286966E+01
F2	1.7541827874E-02	8.7102206936E+00	8.7089737994E+00
F3	1.7540615076E-02	8.7096184908E+00	8.7083716828E+00
F4	8.6811164386E-02	4.3105222894E+01	4.3099052252E+01

Total 2.0139360977E-01 1.0000000000E+02 9.9985684700E+01
Analytic 2.0142244400E-01
Error -2.8834227000E-05

Atomic Sources of Electron Density at Nuclei:

r = Position of Nucleus

$\text{Rho}(r,A)$ = Source Contribution of Atom A to Electron Density at r

$\%\text{Rho}(r,A)$ = Percentage of Total Source Electron Density at r from Atom A's Source Contribution

$\%\text{Rho}(r,A)^*$ = Percentage of Analytic Electron Density at r from Atom A's Source Contribution

Nucleus C1

Atom A	$\text{Rho}(r,A)$	$\%\text{Rho}(r,A)$	$\%\text{Rho}(r,A)^*$
C1	1.2008936131E+02	9.9933868774E+01	9.9933835465E+01
F2	2.6490138624E-02	2.2044101227E-02	2.2044093880E-02
F3	2.6489080840E-02	2.2043220979E-02	2.2043213632E-02
F4	2.6489901176E-02	2.2043903632E-02	2.2043896285E-02

Total 1.2016883043E+02 1.0000000000E+02 9.9999966669E+01
Analytic 1.2016887048E+02
Error -4.0053492185E-05

Nucleus F2

Atom A	$\text{Rho}(r,A)$	$\%\text{Rho}(r,A)$	$\%\text{Rho}(r,A)^*$
C1	8.9669258939E-03	2.1045558617E-03	2.1045558096E-03
F2	4.2605364210E+02	9.9995661889E+01	9.9995659415E+01
F3	4.7577541077E-03	1.1166546277E-03	1.1166546001E-03
F4	4.7588000758E-03	1.1169001186E-03	1.1169000909E-03

Total 4.2607212558E+02 1.0000000000E+02 9.999997526E+01

Analytic 4.2607213612E+02

Error -1.0541099527E-05

Nucleus F3

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	8.9551629367E-03	2.1017951525E-03	2.1017950426E-03

F2	4.7588894103E-03	1.1169211286E-03	1.1169210702E-03

F3	4.2605363649E+02	9.9995664426E+01	9.9995659198E+01

F4	4.7586188857E-03	1.1168576359E-03	1.1168575775E-03

Total 4.2607210916E+02 1.0000000000E+02 9.9999994771E+01

Analytic 4.2607213144E+02

Error -2.2278434699E-05

Nucleus F4

Atom A	Rho(r,A)	%Rho(r,A)	%Rho(r,A)*

C1	8.9723302303E-03	2.1058242655E-03	2.1058242415E-03

F2	4.7589387946E-03	1.1169326735E-03	1.1169326608E-03

F3	4.7579165119E-03	1.1166927417E-03	1.1166927290E-03

F4	4.2605363740E+02	9.9995660550E+01	9.9995659411E+01

Total 4.2607212659E+02 1.0000000000E+02 9.9999998861E+01

Analytic 4.2607213144E+02

Error -4.8541304523E-06

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CF3plus

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\cf3\cat\cf3.wfn

Sum File: D:\calc\ellipticity\cf3\cat\cf3.sum

SumViz File: D:\calc\ellipticity\cf3\cat\cf3.sumviz

Wfn Title: cf3.wfn

Total memory allocated for AIMSum = 0.313 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted SCF

Restricted, closed-shell, single-determinant wavefunction.

Number of electrons (from MO Occs)	=	32.0000000000
Number of Alpha electrons (from MO Occs)	=	16.0000000000
Number of Beta electrons (from MO Occs)	=	16.0000000000
Number of electron pairs ($N*(N-1)/2$)	=	496.0000000000
Number of electron pairs (from Muller 2EDM)	=	496.0000000000

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
F2	9.0	0.0000000000E+00	2.3296521100E+00	0.0000000000E+00
F3	9.0	2.0175379100E+00	-1.1648260500E+00	0.0000000000E+00
F4	9.0	-2.0175379100E+00	-1.1648260500E+00	0.0000000000E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

C1	2.8773324837E+00	-5.8173016378E-04	3.5768602300E+01	-3.5798975924E+01	8.5625150415E-04
F2	-6.2587740760E-01	2.1218289040E-05	9.9948366648E+01	-1.0003323980E+02	5.8538726790E-01
F3	-6.2587817730E-01	2.1617004740E-05	9.9948367787E+01	-1.0003324094E+02	5.8538864335E-01
F4	-6.2587707330E-01	2.1159607279E-05	9.9948365699E+01	-1.0003323885E+02	5.8538685590E-01

Total	9.9969982550E-01	-5.1773526272E-04	3.3561370243E+02	-3.3589869551E+02	

Molecular charge $q(Mol)$ from the wfn file: 1.0000000000E+00

Molecular energy $E(Mol)$ from the wfn file: -3.3589876760E+02

Molecular virial ratio $(-V(Mol)/T(Mol))$ from the wfn file: 2.0008491700E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	12	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
F2	7	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00
F3	7	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00
F4	6	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00

Total 32

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = $(-1/4)\text{DelSqRho}$

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -5.81996974893904E-24 2.23698535621703E-14 0.00000000000000E+00

Type = (3,-3) NACP C1

Rho = 1.1953177495E+02 Rho at Nucleus = 1.1953177495E+02

GradRho = 3.0163853615E-17 -8.9239214061E-18 0.0000000000E+00

HessRho_EigVals = -1.8123685572E+05 -1.8123228381E+05 -1.8123228381E+05

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

DelSqRho = -5.4370142334E+05

Bond Ellipticity = NA

V = -1.3593712447E+05

G = 5.8843163274E+00
K = 1.3593124015E+05
L = 1.3592535584E+05
Vnuc = 6.0000001159E+08
Ven = -7.1719066355E+10
Vrep = 7.1718930418E+10
DelSqV = 4.6069449766E+09
DelSqVen = 2.1515719491E+27
DelSqVrep = -2.1515719491E+27
DelSqG = 2.0610777396E+08
DelSqK = -4.8130527506E+09
Stress_EigVals = -4.5312890917E+04 -4.5312890917E+04 -4.5311342633E+04
Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
-DivStress = -7.6434369445E-15 -3.0850818482E-05 0.0000000000E+00

CP# 2 Coords = 7.37334153978044E-25 2.32964167925568E+00 0.00000000000000E+00

Type = (3,-3) NACP F2

Rho = 4.2642911450E+02 Rho at Nucleus = 4.2642903082E+02

GradRho = -8.2737602167E-18 -1.0651213245E-10 0.0000000000E+00

HessRho_EigVals = -1.5382723505E+06 -1.5382219948E+06 -1.5381982308E+06

HessRho_EigVec1 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

DelSqRho = -4.6146925761E+06

Bond Ellipticity = NA

V = -1.1539891860E+06

G = 1.5802099310E+02

K = 1.1538311650E+06

L = 1.1536731440E+06

Vnuc = 8.6284095514E+05

Ven = -3.6794050445E+08
Vrep = 3.6678651527E+08
DelSqV = 9.7496581142E+10
DelSqVen = 3.9817457490E+12
DelSqVrep = -3.8842491678E+12
DelSqG = 4.1626876671E+09
DelSqK = -1.0165926881E+11
Stress_EigVals = -3.8467152693E+05 -3.8466560845E+05 -3.8465205064E+05
Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00
-DivStress = -2.1935607808E-14 3.3118736452E+05 0.0000000000E+00

CP# 3 Coords = 2.01752887671044E+00 -1.16482083462785E+00 0.00000000000000E+00

Type = (3,-3) NACP F3

Rho = 4.2642911404E+02 Rho at Nucleus = 4.2642903036E+02

GradRho = -2.7947244519E-10 1.2906475888E-10 0.0000000000E+00

HessRho_EigVals = -1.5382723554E+06 -1.5382219998E+06 -1.5381982358E+06

HessRho_EigVec1 = 8.6602540294E-01 -5.0000000147E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 5.0000000147E-01 8.6602540294E-01 0.0000000000E+00

DelSqRho = -4.6146925910E+06

Bond Ellipticity = NA

V = -1.1539891897E+06

G = 1.5802099362E+02

K = 1.1538311687E+06

L = 1.1536731477E+06

Vnuc = 8.6284095578E+05

Ven = -3.6794050433E+08

Vrep = 3.6678651514E+08

DelSqV = 9.7496581459E+10

DelSqVen = 3.9817457690E+12

DelSqVrep = -3.8842491875E+12

DelSqG = 4.1626876982E+09

DelSqK = -1.0165926916E+11

Stress_EigVals = -3.8467152817E+05 -3.8466560968E+05 -3.8465205188E+05

Stress_EigVec1 = 5.0000000129E-01 8.6602540304E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540304E-01 -5.0000000129E-01 0.0000000000E+00

-DivStress = 2.8681667201E+05 -1.6559368241E+05 0.0000000000E+00

CP# 4 Coords = -2.01752887671044E+00 -1.16482083462785E+00 0.00000000000000E+00

Type = (3,-3) NACP F4

Rho = 4.2642911404E+02 Rho at Nucleus = 4.2642903036E+02

GradRho = 2.7947244519E-10 1.2906298252E-10 0.0000000000E+00

HessRho_EigVals = -1.5382723554E+06 -1.5382219998E+06 -1.5381982358E+06

HessRho_EigVec1 = 8.6602540294E-01 5.0000000147E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = -5.0000000147E-01 8.6602540294E-01 0.0000000000E+00

DelSqRho = -4.6146925910E+06

Bond Ellipticity = NA

V = -1.1539891897E+06

G = 1.5802099362E+02

K = 1.1538311687E+06

L = 1.1536731477E+06

Vnuc = 8.6284095578E+05

Ven = -3.6794050433E+08

Vrep = 3.6678651514E+08

DelSqV = 9.7496581459E+10

DelSqVen = 3.9817457690E+12

DelSqVrep = -3.8842491875E+12

DelSqG = 4.1626876982E+09

DelSqK = -1.0165926916E+11

Stress_EigVals = -3.8467152817E+05 -3.8466560968E+05 -3.8465205188E+05

Stress_EigVec1 = -5.0000000129E-01 8.6602540304E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602540304E-01 5.0000000129E-01 0.0000000000E+00
-DivStress = -2.8681667201E+05 -1.6559368241E+05 0.0000000000E+00

CP# 5 Coords = 4.46506910959273E-18 7.65696488424601E-01 0.00000000000000E+00

Type = (3,-1) BCP F2 C1

Rho = 3.6370035019E-01

GradRho = -1.1137029685E-18 1.3877787808E-16 0.0000000000E+00

HessRho_EigVals = -1.1316617412E+00 -1.0770888821E+00 2.4152732753E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

DelSqRho = 2.0652265197E-01

Bond Ellipticity = 5.0666997020E-02

V = -1.1987582807E+00

G = 6.2519447187E-01

K = 5.7356380888E-01

L = -5.1630662992E-02

Vnuc = 2.0036760042E+01

Ven = -7.2873766438E+00

Vrep = 6.0886183631E+00

DelSqV = -2.3910184115E+01

DelSqVen = -4.1380448207E+00

DelSqVrep = -1.9772139294E+01

DelSqG = 3.5330364808E+01

DelSqK = -1.1420180694E+01

Stress_EigVals = -5.2155613240E-01 -4.8393510177E-01 -1.9326704658E-01

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

-DivStress = -1.2841430205E-17 -2.2972835498E+00 0.0000000000E+00

BPL = 2.3296416793E+00 = 1.5639451908E+00 + 7.6569648842E-01

GBL_I = 2.3296416793E+00

GBL_II = 2.3296521100E+00

GBL_III = 2.3296416793E+00 = 1.5639451908E+00 + 7.6569648842E-01

GBL_IV = 2.3296521100E+00 = 1.5639556216E+00 + 7.6569648842E-01

CP# 6 Coords = 6.63112610354503E-01 -3.82848241930470E-01 0.00000000000000E+00

Type = (3,-1) BCP F3 C1

Rho = 3.6370034977E-01

GradRho = -3.7470027081E-16 1.3877787808E-16 0.0000000000E+00

HessRho_EigVals = -1.1316617461E+00 -1.0770888869E+00 2.4152733125E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 4.9999999867E-01 8.6602540455E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540455E-01 -4.9999999867E-01 0.0000000000E+00

DelSqRho = 2.0652267940E-01

Bond Ellipticity = 5.0666996790E-02

V = -1.1987582856E+00

G = 6.2519447773E-01

K = 5.7356380788E-01

L = -5.1630669850E-02

Vnuc = 2.0036760053E+01

Ven = -7.2873766396E+00

Vrep = 6.0886183540E+00

DelSqV = -2.3910184401E+01

DelSqVen = -4.1380453727E+00

DelSqVrep = -1.9772139029E+01

DelSqG = 3.5330365252E+01

DelSqK = -1.1420180851E+01

Stress_EigVals = -5.2155613406E-01 -4.8393510300E-01 -1.9326704856E-01

Stress_EigVec1 = 4.9999999775E-01 8.6602540508E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540508E-01 -4.9999999775E-01 0.0000000000E+00

-DivStress = -1.9895059295E+00 1.1486417767E+00 0.0000000000E+00

BPL = 2.3296416774E+00 = 1.5639451903E+00 + 7.6569648710E-01

GBL_I = 2.3296416774E+00

GBL_II = 2.3296521082E+00

GBL_III = 2.3296416774E+00 = 1.5639451903E+00 + 7.6569648710E-01

GBL_IV = 2.3296521082E+00 = 1.5639556211E+00 + 7.6569648710E-01

CP# 7 Coords = -6.63112610354503E-01 -3.82848241930471E-01 0.00000000000000E+00

Type = (3,-1) BCP C1 F4

Rho = 3.6370034977E-01

GradRho = 3.1918911958E-16 2.2204460493E-16 0.0000000000E+00

HessRho_EigVals = -1.1316617461E+00 -1.0770888869E+00 2.4152733125E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -4.9999999867E-01 8.6602540455E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540455E-01 4.9999999867E-01 0.0000000000E+00

DelSqRho = 2.0652267940E-01

Bond Ellipticity = 5.0666996790E-02

V = -1.1987582856E+00

G = 6.2519447773E-01

K = 5.7356380788E-01

L = -5.1630669850E-02

Vnuc = 2.0036760053E+01

Ven = -7.2873766396E+00

Vrep = 6.0886183540E+00

DelSqV = -2.3910184401E+01

DelSqVen = -4.1380453727E+00

DelSqVrep = -1.9772139029E+01

DelSqG = 3.5330365252E+01

DelSqK = -1.1420180851E+01

Stress_EigVals = -5.2155613406E-01 -4.8393510300E-01 -1.9326704856E-01

Stress_EigVec1 = -4.9999999775E-01 8.6602540508E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540508E-01 4.9999999775E-01 0.0000000000E+00

-DivStress = 1.9895059295E+00 1.1486417767E+00 0.0000000000E+00

BPL = 2.3296416774E+00 = 7.6569648710E-01 + 1.5639451903E+00

GBL_I = 2.3296416774E+00

GBL_II = 2.3296521082E+00

GBL_III = 2.3296416774E+00 = 7.6569648710E-01 + 1.5639451903E+00

GBL_IV = 2.3296521082E+00 = 7.6569648710E-01 + 1.5639556211E+00

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

F3	C1	F2	119.99999984	119.99999988	119.99999988	119.99999986	119.99999986
F4	C1	F2	119.99999984	119.99999988	119.99999988	119.99999986	119.99999986
F4	C1	F3	120.00000032	120.00000023	120.00000023	120.00000028	120.00000028

Total time for electron density critical point search, analysis and connectivity = 1 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.5768602300E+01	3.5768602300E+01	-1.1303683702E+02	-7.7363317616E+01		
F2	-9.9948366648E+01	9.9948366648E+01	-3.1210495734E+02	-2.4323978428E+02		
F3	-9.9948367787E+01	9.9948367787E+01	-3.1210497307E+02	-2.4323978750E+02		
F4	-9.9948365699E+01	9.9948365699E+01	-3.1210494963E+02	-2.4323978085E+02		
Total	-3.3561370243E+02	3.3561370243E+02	-1.0493517171E+03	-8.0708267025E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$E_e(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E(A)$	$E_e(A)$	$W(A)$	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
C1	-3.5768602300E+01					
F2	-9.9948366648E+01					
F3	-9.9948367787E+01					
F4	-9.9948365699E+01					
Total	-3.3561370243E+02					

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	E_IQA(A) VeeX(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2
C1			3.5768602300E+01	-7.6760364901E+01	-5.6518418511E+01	
3.4769139862E+01						
F2			9.9948366648E+01	-1.4930452037E+02	-1.5605247867E+02	
3.1663685549E+01						
F3			9.9948367787E+01	-1.4930451950E+02	-1.5605248653E+02	
3.1663685545E+01						
F4			9.9948365699E+01	-1.4930451950E+02	-1.5605247482E+02	
3.1663685545E+01						
Total			3.3561370243E+02	-5.2467392427E+02	-5.2467585853E+02	
1.2976019650E+02						

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)
C1	3.5768602300E+01	-7.7363317616E+01				

F2	9.9948366648E+01 -2.4323978428E+02
F3	9.9948367787E+01 -2.4323978750E+02
F4	9.9948365699E+01 -2.4323978085E+02

Total 3.3561370243E+02 -8.0708267025E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$ $VeeX(A,A')$
C1	-3.8078706093E+01	-1.7836759703E+01		3.4769139862E+01		
F2	-2.7684628230E+01	-3.4432586531E+01		3.1663685549E+01		
F3	-2.7684625747E+01	-3.4432592787E+01		3.1663685545E+01		
F4	-2.7684629073E+01	-3.4432584393E+01		3.1663685545E+01		

Total -1.2113258914E+02 -1.2113452341E+02 1.2976019650E+02

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$

C1	3.1226675162E+00	2.1448598007E+00	6.8686781081E+01	9.7780771545E-01	
	3.1313218919E+01				
F2	9.6258774078E+00	9.1011135556E+00	9.4548404992E+01	5.2476385223E-01	
	5.4515950079E+00				
F3	9.6258781774E+00	9.1011148265E+00	9.4548410637E+01	5.2476335086E-01	
	5.4515893634E+00				
F4	9.6258770732E+00	9.1011130955E+00	9.4548403499E+01	5.2476397768E-01	
	5.4515965006E+00				

Total	3.2000300175E+01	2.9448201278E+01	9.2024765761E+01	2.5520988962E+00	
	7.9752342393E+00				

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= \text{LI}(\text{A}) + \text{DI}(\text{A}, \text{A}')/2 = \text{LI}(\text{A}) + \text{DI\_Bond}(\text{A}, \text{A}')/2 + \text{DI\_NonBond}(\text{A}, \text{A}')/2$$

$\text{LI}(\text{A})$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\text{DI}(\text{A}, \text{A}')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= \text{N}(\text{A}) - \text{LI}(\text{A}) = \text{DI\_Bond}(\text{A}, \text{A}')/2 + \text{DI\_NonBond}(\text{A}, \text{A}')/2$$

$\text{DI\_Bond}(\text{A}, \text{A}')/2$ = Bonding Contribution to $\text{DI}(\text{A}, \text{A}')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$\text{DI\_NonBond}(\text{A}, \text{A}')/2$ = Non-Bonding Contribution to $\text{DI}(\text{A}, \text{A}')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= \text{DI}(\text{A}, \text{A}')/2 - \text{DI\_Bond}(\text{A}, \text{A}')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	3.1226675162E+00	2.1448598007E+00	9.7780771545E-01	9.7783527483E-01	- 2.7559378798E-05
F2	9.6258774078E+00	9.1011135556E+00	5.2476385223E-01	3.2600183159E-01	1.9876202064E-01
F3	9.6258781774E+00	9.1011148265E+00	5.2476335086E-01	3.2583926292E-01	1.9892408793E-01
F4	9.6258770732E+00	9.1011130955E+00	5.2476397768E-01	3.2599418031E-01	1.9876979737E-01
Total	3.2000300175E+01	2.9448201278E+01	2.5520988962E+00	1.9556705497E+00	5.9642834656E-01

Atomic Electron Pair Contributions:

$\text{D2}(\text{A}, \text{A})$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[\text{N}(\text{A}) * \text{N}(\text{A}) - \text{LI}(\text{A})]$$

$\text{D2}(\text{A}, \text{A}')$ = Half of Average Number of Electron Pairs Formed Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	3.8030963080E+00	4.4598250193E+01	4.8401346501E+01
F2	4.1778201157E+01	1.0742289866E+02	1.4920109982E+02
F3	4.1778207930E+01	1.0742290382E+02	1.4920111175E+02
F4	4.1778198166E+01	1.0742289647E+02	1.4920109463E+02
Total	1.2913770356E+02	3.6686694914E+02	4.9600465271E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$$2 * D2(A,B) = 2 * D2(B,A) = \text{Average Number of Electron Pairs Formed Between Atoms A and B}$$

$$= N(A) * N(B) - DI(A,B) / 2$$

DI(A,B) = DI(B,A) = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
C1	F2	2.9732412865E+01	6.5200366319E-01	1.0439850862E+01	3.3867232854E+00 (Bonded)
C1	F3	2.9732577837E+01	6.5167852585E-01	1.0434644778E+01	3.3850341436E+00 (Bonded)
F2	F3	9.2558068437E+01	1.9890968287E-01	1.0332028678E+00	1.0332027852E+00

C1	F4	2.9732419471E+01	6.5198836062E-01	1.0439605838E+01	3.3866439165E+00 (Bonded)
F2	F4	9.2558057857E+01	1.9890958507E-01	1.0332023599E+00	1.0332023958E+00
F3	F4	9.2558065401E+01	1.9890931338E-01	1.0332008660E+00	1.0332009846E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A Atom B Area_IAS(A|B),0.0004 Area_IAS(A|B),0.001 Area_IAS(A|B),0.002

C1 F2 3.8742500331E+01 3.1990514505E+01 2.7007019925E+01
C1 F3 3.8742500309E+01 3.1990514489E+01 2.7007019913E+01
C1 F4 3.8742500309E+01 3.1990514489E+01 2.7007019913E+01

C1 Total 1.1622750095E+02 9.5971543483E+01 8.1021059751E+01

F2 C1 3.8742500331E+01 3.1990514505E+01 2.7007019925E+01

F2 Total 3.8742500331E+01 3.1990514505E+01 2.7007019925E+01

F3 C1 3.8742500309E+01 3.1990514489E+01 2.7007019913E+01

F3 Total 3.8742500309E+01 3.1990514489E+01 2.7007019913E+01

F4 C1 3.8742500309E+01 3.1990514489E+01 2.7007019913E+01

F4	Total	3.8742500309E+01	3.1990514489E+01	2.7007019913E+01

Total	Total	2.3245500190E+02	1.9194308697E+02	1.6204211950E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta^2\rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta^2\rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta^2\rho\_IAS(A B)$	$V\_IAS(A B)$

C1	F2	1.2690595804E+00	1.7032919725E+00	9.4579318748E-01	-7.5749878503E-01
		3.0299951401E+00	-2.6490851600E+00		

C1	F3	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

C1	F4	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

C1	Total	3.8071787302E+00	5.1098759243E+00	2.8373795574E+00	-2.2724963669E+00
		9.0899854677E+00	-7.9472554818E+00		

F2	C1	1.2690595804E+00	1.7032919725E+00	9.4579318748E-01	-7.5749878503E-01
		3.0299951401E+00	-2.6490851600E+00		

F2	Total	1.2690595804E+00	1.7032919725E+00	9.4579318748E-01	-7.5749878503E-01
		3.0299951401E+00	-2.6490851600E+00		

F3	C1	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

F3	Total	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

F4	C1	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

F4	Total	1.2690595749E+00	1.7032919759E+00	9.4579318497E-01	-7.5749879095E-01
		3.0299951638E+00	-2.6490851609E+00		

Total	Total	7.6143574604E+00	1.0219751849E+01	5.6747591148E+00	-4.5449927339E+00
		1.8179970935E+01	-1.5894510964E+01		

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_{Int_IDS}(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_{Min_IDS}(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_{Avg_IDS}(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_{MAD_IDS}(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_{Var_IDS}(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_{Int_IDS}(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_{Min_IDS}(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{Avg_IDS}(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{MAD_IDS}(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{Var_IDS}(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP*ESP-_{Int_IDS}(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	4.5739899601E+00						

F2	8.7732306509E+01						

F3	8.7787168399E+01						

F4	8.7704337873E+01						

Total	2.6779780274E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	4.7449037592E+00	1.6865108767E+00	3.7287261697E-01	2.9551263516E-01	3.5543626643E-01	1.3630623384E-02	3.1197448726E-04

F2	7.7550340960E+01	1.8617778264E+01	3.6159574764E-01	2.0063317278E-01	2.4007345466E-01	3.2175886214E-02	1.5545181547E-03

F3 7.7513611390E+01 1.8586708977E+01 3.6406680790E-01 2.0063161507E-01 2.3978638904E-01 3.1847892425E-02 1.5172582569E-03

F4 7.7091720758E+01 1.8472925276E+01 3.6406561461E-01 2.0063187008E-01 2.3962268704E-01 3.1823143360E-02 1.5230210847E-03

Total 2.3690057687E+02 5.7363923394E+01 3.7287261697E-01 2.0063161507E-01
2.4214345171E-01 1.7695569739E-03

0.001 IsoDensity Surface:

Atom A |ESP|_Int_IDS(A) ESP*ESP_Int_IDS(A) Area_ESP+_IDS(A) ESP+_Int_IDS(A) Area_ESP-
_IDS(A) ESP-_Int_IDS(A)

C1 1.6865108767E+00 6.0092741825E-01 4.7449037592E+00 1.6865108767E+00
0.0000000000E+00 NULL

F2 1.8617778264E+01 4.5901877588E+00 7.7550340960E+01 1.8617778264E+01
0.0000000000E+00 NULL

F3 1.8586708977E+01 4.5744479965E+00 7.7513611390E+01 1.8586708977E+01
0.0000000000E+00 NULL

F4 1.8472925276E+01 4.5439443083E+00 7.7091720758E+01 1.8472925276E+01
0.0000000000E+00 NULL

Total 5.7363923394E+01 1.4309507482E+01 2.3690057687E+02 5.7363923394E+01
0.0000000000E+00 NULL

0.001 IsoDensity Surface:

Atom A ESP+_Min_IDS(A) ESP+_Avg_IDS(A) ESP+_MAD_IDS(A) ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)

C1 2.9551263516E-01 3.5543626643E-01 1.3630623384E-02 3.1197448726E-04
6.0092741825E-01

F2 2.0063317278E-01 2.4007345466E-01 3.2175886214E-02 1.5545181547E-03
4.5901877588E+00

F3 2.0063161507E-01 2.3978638904E-01 3.1847892425E-02 1.5172582569E-03
4.5744479965E+00

F4	2.0063187008E-01	2.3962268704E-01	3.1823143360E-02	1.5230210847E-03
	4.5439443083E+00			

Total	2.0063161507E-01	2.4214345171E-01	1.7695569739E-03	1.4309507482E+01

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	NULL	NULL	NULL	NULL	NULL
F2	NULL	NULL	NULL	NULL	NULL
F3	NULL	NULL	NULL	NULL	NULL
F4	NULL	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL	NULL

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	4.8208690592E+00
F2	6.9125094198E+01
F3	6.9168621111E+01
F4	6.9156477827E+01

Total	2.1227106220E+02

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A | \text{Total}) + \text{Area\_IDS}(A)$

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an

Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(\text{A}))$ = Average Number of Electrons in Vol(A)

$N(\text{Vol}(\text{A}))/\text{Vol}(\text{A})$ = Average Electron Density in Vol(A)

$\%N(\text{Vol}(\text{A})) = 100 * N(\text{Vol}(\text{A})) / N(\text{A})$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1 9.9977245595E+01	1.2080149091E+02		1.6130759251E+01	3.1219569719E+00	1.9354060918E-01
F2 9.9887032815E+01	1.2647480684E+02		1.1949250210E+02	9.6150033249E+00	8.0465327582E-02
F3 9.9887158281E+01	1.2652966871E+02		1.1952320184E+02	9.6150161709E+00	8.0444767403E-02
F4 9.9887097189E+01	1.2644683818E+02		1.1950780124E+02	9.6150091875E+00	8.0455075636E-02
Total 9.9895893103E+01	5.0025280464E+02		3.7465426443E+02	3.1966985655E+01	8.5323960489E-02

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1 9.9946710190E+01	1.0071644724E+02		1.4681734979E+01	3.1210034527E+00	2.1257729125E-01
F2 9.9736962315E+01	1.0954085546E+02		9.7115842864E+01	9.6005577225E+00	9.8856761569E-02
F3 9.9736610393E+01	1.0950412588E+02		9.7080209856E+01	9.6005246146E+00	9.8892705617E-02
F4 9.9737125082E+01	1.0908223525E+02		9.7129141967E+01	9.6005730568E+00	9.8843383792E-02

Total	4.2884366383E+02	3.0600692967E+02	3.1922658847E+01	1.0432005210E-01
	9.9757373126E+01			

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	8.5841928811E+01	1.3525066462E+01	3.1193478469E+00	2.3063456699E-01	
	9.9893691231E+01				
F2	9.6132114123E+01	8.0663034906E+01	9.5771661121E+00	1.1873054520E-01	
	9.9493954749E+01				
F3	9.6175641024E+01	8.0631238115E+01	9.5771018463E+00	1.1877656936E-01	
	9.9493279157E+01				
F4	9.6163497740E+01	8.0654442155E+01	9.5771475913E+00	1.1874296487E-01	
	9.9493765798E+01				

Total	3.7431318170E+02	2.5547378164E+02	3.1850763397E+01	1.2467331556E-01	
	9.9532701952E+01				

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	F2	9.1150592917E-01		
C1	F3	9.1150669887E-01		
C1	F4	9.1150559487E-01		
C1		2.7345182229E+00	2.8773324837E+00	
F2	C1	-7.6869166839E-01		
F2		-7.6869166839E-01	-6.2587740760E-01	

F3 C1 -7.6869243809E-01
F3 -7.6869243809E-01 -6.2587817730E-01
F4 C1 -7.6869133409E-01
F4 -7.6869133409E-01 -6.2587707330E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A Mu_Intra_X(A) Mu_Bond_X(A) Mu_X(A)

C1 7.3101201791E-04 -7.3207632267E-07 7.3027994159E-04
F2 -2.9721355689E-07 3.4322614233E-18 -2.9721355689E-07
F3 5.0696128345E-01 -1.0411364858E+00 -5.3417520234E-01
F4 -5.0695971379E-01 1.0411349905E+00 5.3417527671E-01

Total 7.3228446435E-04 -2.2273618554E-06 7.3005710250E-04

Atom A Mu_Intra_Y(A) Mu_Bond_Y(A) Mu_Y(A)

C1 -4.3926898645E-04 1.6253232105E-07 -4.3910645413E-04
F2 5.8538726790E-01 -1.2021996560E+00 -6.1681238813E-01
F3 -2.9269458628E-01 6.0110042781E-01 3.0840584153E-01
F4 -2.9269373012E-01 6.0109956451E-01 3.0840583439E-01

Total -4.4031748645E-04 4.9882658881E-07 -4.3981865986E-04

Atom A Mu_Intra_Z(A) Mu_Bond_Z(A) Mu_Z(A)

C1	-7.6359842795E-05	0.0000000000E+00	-7.6359842795E-05
F2	5.9432766268E-07	0.0000000000E+00	5.9432766268E-07
F3	2.9432406514E-07	0.0000000000E+00	2.9432406514E-07
F4	1.1861164890E-06	0.0000000000E+00	1.1861164890E-06

Total	-7.4285074578E-05	0.0000000000E+00	-7.4285074578E-05

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	8.5625150415E-04	7.4990165862E-07	8.5554315890E-04
F2	5.8538726790E-01	1.2021996560E+00	6.1681238813E-01
F3	5.8538864335E-01	1.2022008594E+00	6.1681221606E-01
F4	5.8538685590E-01	1.2021991328E+00	6.1681227690E-01

Total	8.5769359209E-04	2.2825356077E-06	8.5553614697E-04

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

C1	F2	-4.0699369676E-18	
C1	F3	-6.0443158644E-01	
C1	F4	6.0443085437E-01	
C1			-7.3207632267E-07
F2	C1	3.4322614233E-18	
F2			3.4322614233E-18
F3	C1	-1.0411364858E+00	
F3			-1.0411364858E+00

F4	C1	1.0411349905E+00
F4		1.0411349905E+00

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	F2	-6.9793688914E-01	
C1	F3	3.4896873717E-01	
C1	F4	3.4896831451E-01	
C1		1.6253232105E-07	
F2	C1	-1.2021996560E+00	
F2		-1.2021996560E+00	
F3	C1	6.0110042781E-01	
F3		6.0110042781E-01	
F4	C1	6.0109956451E-01	
F4		6.0109956451E-01	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	F2	0.0000000000E+00	
C1	F3	0.0000000000E+00	
C1	F4	0.0000000000E+00	
C1		0.0000000000E+00	
F2	C1	0.0000000000E+00	
F2		0.0000000000E+00	
F3	C1	0.0000000000E+00	
F3		0.0000000000E+00	
F4	C1	0.0000000000E+00	
F4		0.0000000000E+00	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	F2	6.9793688914E-01	

C1	F3	6.9793747730E-01
C1	F4	6.9793663197E-01
C1		7.4990165862E-07
F2	C1	1.2021996560E+00
F2		1.2021996560E+00
F3	C1	1.2022008594E+00
F3		1.2022008594E+00
F4	C1	1.2021991328E+00
F4		1.2021991328E+00

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	3.6888032566E-01	2.6765197243E-03	-5.9383144782E-04	3.7193533740E-01	8.8458345099E-04	-7.4081566307E-01
F2	2.5624306905E-01	1.1775504931E-06	-1.6845111534E-05	-9.2221999372E-02	-2.7199660108E-06	-1.6402106968E-01
F3	-5.1084117140E-03	1.5089403198E-01	-9.7361862830E-06	1.6912559596E-01	-1.4095561581E-05	-1.6401718425E-01
F4	-5.1033741903E-03	-1.5089023917E-01	1.3242445337E-05	1.6912573212E-01	-1.1586281845E-05	-1.6402235793E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$

C1	1	-7.4081668633E-01	5.3704959668E-04	-7.9624251222E-04	9.9999953879E-01
C1	2	3.6732693375E-01	8.6480586321E-01	-5.0210563833E-01	-8.6424189350E-04
C1	3	3.7348975257E-01	5.0210609490E-01	8.6480592849E-01	4.1893956255E-04
F2	1	-1.6402107046E-01	4.0082094370E-05	3.7882367708E-05	9.999999848E-01
F2	2	-9.2221999273E-02	-3.3810810030E-06	9.999999928E-01	-3.7882232218E-05
F2	3	2.5624306973E-01	9.999999919E-01	3.3795625987E-06	-4.008222424E-05
F3	1	-1.6401718497E-01	3.7010039281E-05	2.5547506964E-05	9.999999899E-01
F3	2	-9.2227974747E-02	8.6602328309E-01	-5.0000367276E-01	-1.9277708433E-05
F3	3	2.5624515972E-01	5.0000367176E-01	8.6602328293E-01	-4.0629891425E-05
F4	1	-1.6402235904E-01	-8.8264372594E-05	-5.1987405522E-06	9.999999609E-01
F4	2	-9.2220877477E-02	8.6602295486E-01	5.0000423538E-01	7.9038365367E-05
F4	3	2.5624323652E-01	-5.0000423384E-01	8.6602295845E-01	-3.9630331476E-05

Atomic Radial Moments:

$R-2(A) = \langle \text{Rho}/(r^2) \rangle(A)$

$R-1(A) = \langle \text{Rho}/r \rangle(A)$

$R0(A) = \langle \text{Rho} \rangle(A) = N(A)$

$R+1(A) = \langle \text{Rho} \cdot r \rangle(A)$

$R+2(A) = \langle \text{Rho} \cdot r^2 \rangle(A)$

Atom A	$R-2(A)$	$R-1(A)$	$R0(A)$	$R+1(A)$	$R+2(A)$

C1	1.3593588981E+02 1.4954521360E+00	1.2893886269E+01	3.1226675163E+00	1.6328008152E+00
F2	3.3061296178E+02 1.1080234118E+01	2.7026642698E+01	9.6258774076E+00	8.5486652852E+00
F3	3.3061296042E+02 1.1080234893E+01	2.7026643055E+01	9.6258781773E+00	8.5486662987E+00
F4	3.3061295995E+02 1.1080233335E+01	2.7026642316E+01	9.6258770733E+00	8.5486648080E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3383421232E+02 4.2196973353E+00	-2.3707690252E+01	-7.1715183104E+00	-4.0009477683E+00	-
F2	-3.3004053968E+02 4.6585344256E+01	-5.2960350858E+01	-2.6744459642E+01	-2.9923020102E+01	-
F3	-3.3004053802E+02 4.6585333449E+01	-5.2960350352E+01	-2.6744458715E+01	-2.9923016843E+01	-
F4	-3.3004053794E+02 4.6585342737E+01	-5.2960350445E+01	-2.6744459515E+01	-2.9923019892E+01	-

Atomic Electronic Spin Populations:

$$N\_alpha(A) = \text{Average number of Alpha electrons in Atom A}$$

$$N\_beta(A) = \text{Average number of Beta electrons in Atom A}$$

$$N\_total(A) = N\_alpha(A) + N\_beta(A)$$

$$N\_spin(A) = N\_alpha(A) - N\_beta(A)$$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)
C1	1.5613337581E+00	1.5613337581E+00	3.1226675163E+00	0.0000000000E+00
F2	4.8129387038E+00	4.8129387038E+00	9.6258774076E+00	0.0000000000E+00
F3	4.8129390887E+00	4.8129390887E+00	9.6258781773E+00	0.0000000000E+00
F4	4.8129385367E+00	4.8129385367E+00	9.6258770733E+00	0.0000000000E+00
Total	1.6000150087E+01	1.6000150087E+01	3.2000300174E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while

the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$.

For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E_{IQA}(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CH3F

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\ch3f\ch3f.wfx

Sum File: D:\calc\ellipticity\ch3f\ch3f.sum

SumViz File: D:\calc\ellipticity\ch3f\ch3f.sumviz

Wfx Title: nh3_as_pyr_mp2

Total memory allocated for AIMSum = 0.405 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs) = 18.0000000083

Number of Alpha electrons (from MO Occs) = 9.0000000042
 Number of Beta electrons (from MO Occs) = 9.0000000042
 Number of electron pairs ($N*(N-1)/2$) = 153.0000001459
 Number of electron pairs (from Muller 2EDM) = 152.9997685488
 Number of electron pairs (from Muller 2EDM, no SOSI) = 153.1732763304

Nuclear Charges and Cartesian Coordinates:

```
-----
Atom   Charge      X           Y           Z
-----
C1      6.0    -1.6653345400E-16  2.7755575600E-16 -1.2018781300E+00
H2      1.0    -6.6613381500E-16  1.9527660400E+00 -1.8639333900E+00
H3      1.0     1.6911450000E+00 -9.7638302200E-01 -1.8639333900E+00
H4      1.0    -1.6911450000E+00 -9.7638302200E-01 -1.8639333900E+00
F5      9.0     4.4408921000E-16  0.0000000000E+00  1.4225632200E+00
```

Some Atomic Properties:

q(A) = Net Charge of Atom A

L(A) = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

K(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

K_Scaled(A) = $K(A) * E(\text{Mol})/K(\text{Mol})$ = Approximation to Virial-Based Total Energy of Atom A.

|Mu_Intra(A)| = Magnitude of Intraatomic Dipole Moment of Atom A

```
-----
Atom A    q(A)      L(A)      K(A)      K_Scaled(A)  |Mu_Intra(A)|
-----
C1      5.5156830060E-01  1.9834786528E-04  3.7558140206E+01 -3.7584529517E+01  6.2369670071E-01
H2      2.7788628600E-02  1.8567219523E-05  6.1942223177E-01 -6.1985745369E-01  1.4488753315E-01
H3      2.7791355660E-02  2.0759846819E-05  6.1942219095E-01 -6.1985741284E-01  1.4488823329E-01
```

H4 2.7791205720E-02 2.1076696943E-05 6.1942254739E-01 -6.1985776954E-01 1.4488790683E-01

F5 -6.3473761550E-01 3.9502958169E-05 9.9933154276E+01 -1.0000336987E+02 1.1263874557E-01

Total 2.0187508000E-04 2.9825458673E-04 1.3934956145E+02 -1.3944747202E+02

Molecular charge q(Mol) from the wfx file: -8.3367838361E-09

Molecular energy E(Mol) from the wfx file: -1.3944740141E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0007026256E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0006966494E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR
C1	15	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00 13.00
H2	4	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H3	5	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H4	4	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
F5	12	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00 13.00

Total 40

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -1.66533444622003E-16 4.54741019152550E-13 -1.20187048677145E+00

Type = (3,-3) NACP C1

Rho = 1.1943366038E+02 Rho at Nucleus = 1.1943365509E+02

GradRho = -2.3388060185E-17 6.2074174265E-17 1.6741052988E-11

HessRho_EigVals = -1.8107968765E+05 -1.8107511206E+05 -1.8107511206E+05

HessRho_EigVec1 = 0.0000000000E+00 -6.2761003827E-09 1.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 1.0000000000E+00 6.2761003827E-09

HessRho_EigVec3 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

DelSqRho = -5.4322991176E+05

Bond Ellipticity = NA

V = -1.3582200644E+05

G = 7.2642512820E+00

K = 1.3581474219E+05

L = 1.3580747794E+05

Vnuc = 7.8501346567E+05

Ven = -9.3757031655E+07

Vrep = 9.3621209649E+07

DelSqV = 4.6029954000E+09

DelSqVen = 4.2644279552E+11

DelSqVrep = -4.2183980012E+11

DelSqG = 2.0592560334E+08

DelSqK = -4.8089210034E+09

Stress_EigVals = -4.5274406011E+04 -4.5274406011E+04 -4.5273194420E+04

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 1.0000000000E+00 -5.1582391911E-09

Stress_EigVec3 = 0.0000000000E+00 5.1582391911E-09 1.0000000000E+00

-DivStress = -7.0933804143E-14 -6.8899194104E-04 -1.1454089212E+04

CP# 2 Coords = -6.58559130693051E-16 1.92561687771774E+00 -1.85477462747042E+00

Type = (3,-3) NACP H2

Rho = 4.3573301229E-01 Rho at Nucleus = 4.3235289111E-01

GradRho = -1.2580517078E-18 -9.2946483843E-15 3.5262591458E-15

HessRho_EigVals = -8.6844231601E+00 -8.6745347027E+00 -7.9828483308E+00

HessRho_EigVec1 = 0.0000000000E+00 3.2511013406E-01 9.4567616060E-01

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 9.4567616060E-01 -3.2511013406E-01

DelSqRho = -2.5341806194E+01

Bond Ellipticity = NA

V = -6.3530335866E+00

G = 8.7910191273E-03

K = 6.3442425675E+00

L = 6.3354515484E+00

Vnuc = 4.0815107965E+01

Ven = -1.7784489941E+01

Vrep = 1.1431456354E+01

DelSqV = 1.6355681849E+03

DelSqVen = 1.0343285558E+03

DelSqVrep = 6.0123962908E+02

DelSqG = 1.2401005557E+02

DelSqK = -1.7595782405E+03

Stress_EigVals = -2.1756820928E+00 -2.1752926914E+00 -2.0020588025E+00

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 3.2661765776E-01 9.4515655086E-01

Stress_EigVec3 = 0.0000000000E+00 9.4515655086E-01 -3.2661765776E-01

-DivStress = -4.0602464081E-15 1.4402775585E+01 -4.8646025513E+00

CP# 3 Coords = 1.66763313571525E+00 -9.62808440743038E-01 -1.85477462771842E+00

Type = (3,-3) NACP H3

Rho = 4.3573302724E-01 Rho at Nucleus = 4.3235290587E-01

GradRho = 3.2959746044E-17 -4.1633363423E-17 3.4694469520E-17

HessRho_EigVals = -8.6844236161E+00 -8.6745351585E+00 -7.9828487711E+00

HessRho_EigVec1 = 2.8155363875E-01 -1.6255505106E-01 9.4567616227E-01

HessRho_EigVec2 = 4.9999999688E-01 8.6602540559E-01 -1.5301766897E-08

HessRho_EigVec3 = 8.1897957950E-01 -4.7283808249E-01 -3.2511012921E-01

DelSqRho = -2.5341807546E+01

Bond Ellipticity = NA

V = -6.3530339241E+00

G = 8.7910188526E-03

K = 6.3442429053E+00

L = 6.3354518864E+00

Vnuc = 4.0815107934E+01

Ven = -1.7784490537E+01

Vrep = 1.1431456613E+01

DelSqV = 1.6355682742E+03

DelSqVen = 1.0343286102E+03

DelSqVrep = 6.0123966401E+02

DelSqG = 1.2401006443E+02

DelSqK = -1.7595783387E+03

Stress_EigVals = -2.1756822072E+00 -2.1752928053E+00 -2.0020589116E+00

Stress_EigVec1 = 4.9999993321E-01 8.6602544235E-01 -2.2742385593E-07

Stress_EigVec2 = 2.8285930391E-01 -1.6330861797E-01 9.4515655290E-01

Stress_EigVec3 = 8.1852958467E-01 -4.7257827765E-01 -3.2661765187E-01

-DivStress = 1.2473170236E+01 -7.2013882445E+00 -4.8646026812E+00

CP# 4 Coords = -1.66763313571525E+00 -9.62808440743038E-01 -1.85477462771842E+00

Type = (3,-3) NACP H4

Rho = 4.3573302724E-01 Rho at Nucleus = 4.3235290587E-01

GradRho = 1.7347234760E-17 3.4694469520E-17 8.8470897275E-17

HessRho_EigVals = -8.6844236161E+00 -8.6745351585E+00 -7.9828487711E+00

HessRho_EigVec1 = -2.8155363875E-01 -1.6255505106E-01 9.4567616227E-01

HessRho_EigVec2 = -4.9999999688E-01 8.6602540559E-01 -1.5301880695E-08

HessRho_EigVec3 = 8.1897957950E-01 4.7283808249E-01 3.2511012921E-01

DelSqRho = -2.5341807546E+01

Bond Ellipticity = NA

V = -6.3530339241E+00

G = 8.7910188526E-03

K = 6.3442429053E+00

L = 6.3354518864E+00

Vnuc = 4.0815107934E+01

Ven = -1.7784490537E+01

Vrep = 1.1431456613E+01

DelSqV = 1.6355682742E+03

DelSqVen = 1.0343286102E+03

DelSqVrep = 6.0123966401E+02

DelSqG = 1.2401006443E+02

DelSqK = -1.7595783387E+03

Stress_EigVals = -2.1756822072E+00 -2.1752928053E+00 -2.0020589116E+00

Stress_EigVec1 = -4.9999993321E-01 8.6602544235E-01 -2.2742436654E-07

Stress_EigVec2 = -2.8285930391E-01 -1.6330861796E-01 9.4515655290E-01

Stress_EigVec3 = 8.1852958467E-01 4.7257827765E-01 3.2661765187E-01

-DivStress = -1.2473170236E+01 -7.2013882445E+00 -4.8646026812E+00

CP# 5 Coords = 4.44089236930802E-16 -1.03488957055258E-14 1.42255644753566E+00

Type = (3,-3) NACP F5

Rho = 4.2599104360E+02 Rho at Nucleus = 4.2599100836E+02

GradRho = -7.9939843694E-18 2.2917905756E-17 3.7332359426E-11

HessRho_EigVals = -1.5366896777E+06 -1.5366238436E+06 -1.5366238436E+06

HessRho_EigVec1 = 0.0000000000E+00 2.3549892370E-10 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 -2.3549892370E-10

DelSqRho = -4.6099373649E+06

Bond Ellipticity = NA

V = -1.1528146048E+06

G = 1.6513180624E+02

K = 1.1526494730E+06

L = 1.1524843412E+06

Vnuc = 1.3289137231E+06

Ven = -5.6610534374E+08

Vrep = 5.6495252913E+08

DelSqV = 9.7397291501E+10

DelSqVen = 6.1262090199E+12

DelSqVrep = -6.0288117284E+12

DelSqG = 4.1584742433E+09

DelSqK = -1.0155576574E+11

Stress_EigVals = -3.8427711046E+05 -3.8427711046E+05 -3.8426038391E+05

Stress_EigVec1 = 0.0000000000E+00 1.0000000000E+00 2.8148372920E-11

Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 -2.8148372920E-11 1.0000000000E+00

-DivStress = -8.2125096091E-13 3.3330571346E-04 2.1484312527E+05

CP# 6 Coords = 5.17741781809694E-17 3.21979274375086E-09 -3.30639501757248E-01

Type = (3,-1) BCP F5 C1

Rho = 2.2900673296E-01

GradRho = -5.9475825473E-18 -2.5071844366E-18 -5.5511151231E-17

HessRho_EigVals = -3.5722213941E-01 -3.5722213666E-01 8.0086229054E-01

HessRho_EigVec1 = 0.0000000000E+00 1.0000000000E+00 3.8762347574E-09

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 -3.8762347574E-09 1.0000000000E+00

DelSqRho = 8.6418014470E-02

Bond Ellipticity = 7.6713990715E-09

V = -6.2640583816E-01

G = 3.2400517089E-01

K = 3.0240066727E-01
L = -2.1604503617E-02
Vnuc = 1.3228523468E+01
Ven = -3.0294209412E+00
Vrep = 2.4030151030E+00
DelSqV = -1.0177264931E+01
DelSqVen = -1.1431827324E+00
DelSqVrep = -9.0340821988E+00
DelSqG = 1.4176682110E+01
DelSqK = -3.9994171792E+00
Stress_EigVals = -2.8859207208E-01 -2.8859207188E-01 -4.9221694200E-02
Stress_EigVec1 = 0.0000000000E+00 1.0000000000E+00 -4.7292778974E-11
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 4.7292778974E-11 1.0000000000E+00
-DivStress = -3.1232449392E-16 -1.7723001399E-09 -9.8151807269E-01
BPL = 2.6244269343E+00 = 1.7531959493E+00 + 8.7123098501E-01
GBL_I = 2.6244269343E+00
GBL_II = 2.6244413500E+00
GBL_III = 2.6244269343E+00 = 1.7531959493E+00 + 8.7123098501E-01
GBL_IV = 2.6244413500E+00 = 1.7532027218E+00 + 8.7123862824E-01

CP# 7 Coords = -4.61194785151952E-16 1.26467703473368E+00 -1.62470015752216E+00

Type = (3,-1) BCP H2 C1
Rho = 2.8448237699E-01
GradRho = -1.6143284768E-18 -9.7144514655E-17 7.1123662515E-17
HessRho_EigVals = -7.7407313039E-01 -7.3702232225E-01 5.0723820542E-01
HessRho_EigVec1 = 0.0000000000E+00 3.3336437793E-01 9.4279806508E-01
HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
HessRho_EigVec3 = 0.0000000000E+00 9.4279806508E-01 -3.3336437793E-01
DelSqRho = -1.0038572472E+00
Bond Ellipticity = 5.0270944349E-02
V = -3.3207605699E-01

G = 4.0555872592E-02
K = 2.9152018440E-01
L = 2.5096431181E-01
Vnuc = 9.3098481272E+00
Ven = -2.6484877247E+00
Vrep = 2.3164116677E+00
DelSqV = -2.6990028695E+00
DelSqVen = 9.3457585130E+00
DelSqVrep = -1.2044761383E+01
DelSqG = 1.6352144683E+00
DelSqK = 1.0637884012E+00
Stress_EigVals = -2.2310827720E-01 -2.1746543352E-01 1.0849765373E-01
Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 3.3245450094E-01 9.4311929511E-01
Stress_EigVec3 = 0.0000000000E+00 9.4311929511E-01 -3.3245450094E-01
-DivStress = 4.5441114232E-18 -9.0121090306E-02 2.8051520358E-02
BPL = 2.0338110319E+00 = 6.9984222941E-01 + 1.3339688025E+00
GBL_I = 2.0332939228E+00
GBL_II = 2.0619438339E+00
GBL_III = 2.0333288017E+00 = 6.9983979436E-01 + 1.3334890073E+00
GBL_IV = 2.0619775025E+00 = 7.2849091874E-01 + 1.3334865838E+00

CP# 8 Coords = 1.09524242538130E+00 -6.32338508845221E-01 -1.62470015270048E+00

Type = (3,-1) BCP H3 C1
Rho = 2.8448238050E-01
GradRho = 3.9551695252E-16 -8.3266726847E-17 5.2041704279E-17
HessRho_EigVals = -7.7407313932E-01 -7.3702232899E-01 5.0723819608E-01
HessRho_EigVec1 = 2.8870202711E-01 -1.6668217777E-01 9.4279806489E-01
HessRho_EigVec2 = 4.9999999847E-01 8.6602540467E-01 -1.3427788618E-08
HessRho_EigVec3 = 8.1648707343E-01 -4.7139903487E-01 -3.3336437848E-01
DelSqRho = -1.0038572722E+00
Bond Ellipticity = 5.0270946848E-02

V = -3.3207606788E-01
G = 4.0555874911E-02
K = 2.9152019297E-01
L = 2.5096431806E-01
Vnuc = 9.3098481612E+00
Ven = -2.6484877670E+00
Vrep = 2.3164116991E+00
DelSqV = -2.6990025843E+00
DelSqVen = 9.3457587800E+00
DelSqVrep = -1.2044761364E+01
DelSqG = 1.6352145015E+00
DelSqK = 1.0637880828E+00
Stress_EigVals = -2.2310828254E-01 -2.1746543703E-01 1.0849765169E-01
Stress_EigVec1 = 4.9999998574E-01 8.6602541202E-01 -5.3128145460E-08
Stress_EigVec2 = 2.8791407098E-01 -1.6622720220E-01 9.4311929520E-01
Stress_EigVec3 = 8.1676526738E-01 -4.7155964945E-01 -3.3245450068E-01
-DivStress = -7.8047196221E-02 4.5060568650E-02 2.8051535846E-02
BPL = 2.0338110343E+00 = 6.9984224902E-01 + 1.3339687852E+00
GBL_I = 2.0332939252E+00
GBL_II = 2.0619438363E+00
GBL_III = 2.0333288040E+00 = 6.9983981397E-01 + 1.3334889900E+00
GBL_IV = 2.0619775049E+00 = 7.2849093838E-01 + 1.3334865665E+00

CP# 9 Coords = -1.09524242538130E+00 -6.32338508845221E-01 -1.62470015270048E+00

Type = (3,-1) BCP C1 H4
Rho = 2.8448238050E-01
GradRho = -1.5265566589E-16 -6.9388939039E-17 -5.5511151231E-17
HessRho_EigVals = -7.7407313932E-01 -7.3702232899E-01 5.0723819608E-01
HessRho_EigVec1 = -2.8870202711E-01 -1.6668217777E-01 9.4279806489E-01
HessRho_EigVec2 = -4.9999999847E-01 8.6602540467E-01 -1.3427787187E-08
HessRho_EigVec3 = 8.1648707343E-01 4.7139903487E-01 3.3336437848E-01
DelSqRho = -1.0038572722E+00

Bond Ellipticity = 5.0270946848E-02

V = -3.3207606788E-01

G = 4.0555874911E-02

K = 2.9152019297E-01

L = 2.5096431806E-01

Vnuc = 9.3098481612E+00

Ven = -2.6484877670E+00

Vrep = 2.3164116991E+00

DelSqV = -2.6990025843E+00

DelSqVen = 9.3457587800E+00

DelSqVrep = -1.2044761364E+01

DelSqG = 1.6352145015E+00

DelSqK = 1.0637880828E+00

Stress_EigVals = -2.2310828254E-01 -2.1746543703E-01 1.0849765169E-01

Stress_EigVec1 = -4.9999998574E-01 8.6602541202E-01 -5.3128147665E-08

Stress_EigVec2 = -2.8791407098E-01 -1.6622720220E-01 9.4311929520E-01

Stress_EigVec3 = 8.1676526738E-01 4.7155964945E-01 3.3245450068E-01

-DivStress = 7.8047196221E-02 4.5060568650E-02 2.8051535846E-02

BPL = 2.0338110343E+00 = 1.3339687852E+00 + 6.9984224902E-01

GBL_I = 2.0332939252E+00

GBL_II = 2.0619438363E+00

GBL_III = 2.0333288040E+00 = 1.3334889900E+00 + 6.9983981397E-01

GBL_IV = 2.0619775049E+00 = 1.3334865665E+00 + 7.2849093838E-01

Number of NACPs = 5

Number of NNACPs = 0

Number of BCPs = 4

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H2	C1	F5	106.16952998	108.72986182	108.72843712	108.48674310	108.48643164
H3	C1	F5	106.16953033	108.72986181	108.72843710	108.48674345	108.48643199
H3	C1	H2	112.56138337	110.20229605	110.20368099	110.43750068	110.43780055
H4	C1	F5	106.16953033	108.72986181	108.72843710	108.48674345	108.48643199
H4	C1	H2	112.56138337	110.20229605	110.20368099	110.43750068	110.43780055
H4	C1	H3	112.56138522	110.20229600	110.20368093	110.43750070	110.43780056

Total time for electron density critical point search, analysis and connectivity = 2 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$$V_{nn}(A) - W(A) = \text{Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus}$$

the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
C1	-3.7558140206E+01	3.7558140206E+01	-1.1289288839E+02	-8.7623028535E+01		
H2	-6.1942223177E-01	6.1942223177E-01	-6.5677220871E+00	-1.2601675294E+00		
H3	-6.1942219095E-01	6.1942219095E-01	-6.5677062287E+00	-1.2601658468E+00		
H4	-6.1942254739E-01	6.1942254739E-01	-6.5677085444E+00	-1.2601662131E+00		
F5	-9.9933154276E+01	9.9933154276E+01	-2.7251504262E+02	-2.4286725354E+02		
Total	-1.3934956145E+02	1.3934956145E+02	-4.0511106787E+02	-3.3427078166E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$$V_{nn}(A) = \text{Contribution of Atom A to Nuclear Repulsion Energy of Molecule}$$

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$$V_{eeC}(A) = \text{Coulomb Part of } V_{ee}(A)$$

$$V_{eeX}(A) = \text{Exchange-Correlation Part of } V_{ee}(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

C1	-3.7558625577E+01	-3.7558140206E+01	-4.8537115862E-04
H2	-6.1950055640E-01	-6.1942223177E-01	-7.8324626351E-05
H3	-6.1950051558E-01	-6.1942219095E-01	-7.8324628427E-05
H4	-6.1950087202E-01	-6.1942254739E-01	-7.8324628426E-05
F5	-9.9933266717E+01	-9.9933154276E+01	-1.1244060746E-04

Total -1.3935039424E+02 -1.3934956145E+02 -8.3278564929E-04

IQA Atomic Energy Components:

E_IQA(A) = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E_IQA(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2
VeeC(A)	VeeX(A)					

C1	3.7558140206E+01	-5.8679951467E+01	-5.6446444194E+01
	1.4652717107E+01		

H2	6.1942223177E-01	-3.4735694900E+00	-3.2838610435E+00
2.9277207383E+00			

H3	6.1942219095E-01	-3.4735694940E+00	-3.2838531144E+00
2.9277207363E+00			

H4	6.1942254739E-01	-3.4735694940E+00	-3.2838542722E+00
2.9277207363E+00			
F5	9.9933154276E+01	-1.3345540186E+02	-1.3625752131E+02
1.3819279572E+01			

Total	1.3934956145E+02	-2.0255606181E+02	-2.0255553393E+02
3.7255158890E+01			

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

C1	3.7558140206E+01	-8.7623028535E+01				
H2	6.1942223177E-01	-1.2601675294E+00				
H3	6.1942219095E-01	-1.2601658468E+00				
H4	6.1942254739E-01	-1.2601662131E+00				
F5	9.9933154276E+01	-2.4286725354E+02				

Total	1.3934956145E+02	-3.3427078166E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$ $VeeX(A,A')$
C1	-1.4868437199E+01	-1.2634929926E+01		1.4652717107E+01		
H2	-2.8434857254E+00	-2.6537772789E+00		2.9277207383E+00		
H3	-2.8434865706E+00	-2.6537701910E+00		2.9277207363E+00		
H4	-2.8434863874E+00	-2.6537711657E+00		2.9277207363E+00		
F5	-1.2021775093E+01	-1.4823894542E+01		1.3819279572E+01		
Total	-3.5420670975E+01	-3.5420143104E+01		3.7255158890E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$$\%Loc(A) = 100 * LI(A) / N(A)$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A)$$

$$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1	5.4484316995E+00	3.8412350582E+00	7.0501664885E+01	1.6071966412E+00	2.9498335115E+01
H2	9.7221137107E-01	4.9881097991E-01	5.1306844865E+01	4.7340039115E-01	4.8693155135E+01
H3	9.7220864426E-01	4.9880867493E-01	5.1306751681E+01	4.7339996933E-01	4.8693248319E+01
H4	9.7220879429E-01	4.9880888359E-01	5.1306765226E+01	4.7339991070E-01	4.8693234774E+01
F5	9.6347376155E+00	9.1844462166E+00	9.5326376110E+01	4.5029139894E-01	4.6736238900E+00
Total	1.7999798125E+01	1.4522109813E+01	8.0679292694E+01	3.4776883114E+00	1.9320707306E+01

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that
are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	5.4484316995E+00	3.8412350582E+00	1.6071966412E+00	1.6071617780E+00	3.4863238457E-05
H2	9.7221137107E-01	4.9881097991E-01	4.7340039115E-01	4.1387318426E-01	5.9527206897E-02
H3	9.7220864426E-01	4.9880867493E-01	4.7339996933E-01	4.1391238365E-01	5.9487585677E-02
H4	9.7220879429E-01	4.9880888359E-01	4.7339991070E-01	4.1392180807E-01	5.9478102627E-02
F5	9.6347376155E+00	9.1844462166E+00	4.5029139894E-01	3.6545440200E-01	8.4836996938E-02
Total	1.7999798125E+01	1.4522109813E+01	3.4776883114E+00	3.2143235560E+00	2.6336475538E-01

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A')$ = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.2922086463E+01	3.3389568802E+01	4.6311655264E+01
H2	2.2319198506E-01	8.0405907764E+00	8.2637827614E+00
H3	2.2319048652E-01	8.0405690979E+00	8.2637595845E+00
H4	2.2319052805E-01	8.0405703319E+00	8.2637608599E+00
F5	4.1821861352E+01	4.0073232825E+01	8.1895094176E+01
Total	5.5413520814E+01	9.7584531833E+01	1.5299805265E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) = \text{Average Number of Electron Pairs Formed Between Atoms A and B}$
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) = \text{Electron Delocalization Index. Average Number of Electrons Delocalized}$
 (Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
C1	H2	4.8831540684E+00	8.2774636851E-01	7.5961892722E+00	4.2570288373E+01 (Bonded)
C1	H3	4.8831000122E+00	8.2782476730E-01	7.5969087342E+00	4.2574439766E+01 (Bonded)
H2	H3	9.2962693939E-01	3.1130719210E-02	1.6010262858E+00	1.6010307763E+00
C1	H4	4.8830914052E+00	8.2784361615E-01	7.5970817091E+00	4.2575402579E+01 (Bonded)
H2	H4	9.2962708764E-01	3.1130714443E-02	1.6010260407E+00	1.6010302841E+00
H3	H4	9.2962448391E-01	3.1130619854E-02	1.6010256665E+00	1.6010254195E+00

C1	F5	5.2128755438E+01	7.3090880401E-01	6.7075155231E+00	3.7930913802E+00 (Bonded)
H2	F5	9.3386290932E+00	5.6744747753E-02	2.9183338851E+00	2.9447998491E-01
H3	F5	9.3386029484E+00	5.6744493176E-02	2.9183289776E+00	2.9447866377E-01
H4	F5	9.3386044573E+00	5.6744366475E-02	2.9183220111E+00	2.9447800625E-01

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	F5	4.5041297667E+01	3.5932112101E+01	2.9558193542E+01
C1	H2	3.8115122552E+01	2.9745700845E+01	2.4029617468E+01
C1	H3	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01
C1	H4	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01

C1	Total	1.5938666549E+02	1.2516921476E+02	1.0164704604E+02

H2	C1	3.8115122552E+01	2.9745700845E+01	2.4029617468E+01

H2	Total	3.8115122552E+01	2.9745700845E+01	2.4029617468E+01

H3	C1	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01

H3	Total	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01

H4	C1	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01

H4	Total	3.8115122636E+01	2.9745700907E+01	2.4029617517E+01
F5	C1	4.5041297667E+01	3.5932112101E+01	2.9558193542E+01

F5	Total	4.5041297667E+01	3.5932112101E+01	2.9558193542E+01
Total	Total	3.1877333098E+02	2.5033842952E+02	2.0329409209E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta \rho\_IAS(A B)$ $V\_IAS(A B)$

C1	F5	1.0780658078E+00	1.1919457837E+00	4.6929835204E-01	-7.2264743170E-01	2.8905897268E+00 -1.6612441358E+00
C1	H2	9.3837503070E-01	5.3566738452E-01	4.0880536616E-01	-1.2686201836E-01	5.0744807343E-01 -9.4447275068E-01
C1	H3	9.3837504258E-01	5.3566740307E-01	4.0880537808E-01	-1.2686202500E-01	5.0744809999E-01 -9.4447278115E-01
C1	H4	9.3837504258E-01	5.3566740307E-01	4.0880537808E-01	-1.2686202500E-01	5.0744809999E-01 -9.4447278115E-01

C1 Total 3.8931909237E+00 2.7989479744E+00 1.6957144744E+00 -1.1032335001E+00
4.4129340002E+00 -4.4946624488E+00

H2 C1 9.3837503070E-01 5.3566738452E-01 4.0880536616E-01 -1.2686201836E-01
5.0744807343E-01 -9.4447275068E-01

H2 Total 9.3837503070E-01 5.3566738452E-01 4.0880536616E-01 -1.2686201836E-01
5.0744807343E-01 -9.4447275068E-01

H3 C1 9.3837504258E-01 5.3566740307E-01 4.0880537808E-01 -1.2686202500E-01
5.0744809999E-01 -9.4447278115E-01

H3 Total 9.3837504258E-01 5.3566740307E-01 4.0880537808E-01 -1.2686202500E-01
5.0744809999E-01 -9.4447278115E-01

H4 C1 9.3837504258E-01 5.3566740307E-01 4.0880537808E-01 -1.2686202500E-01
5.0744809999E-01 -9.4447278115E-01

H4 Total 9.3837504258E-01 5.3566740307E-01 4.0880537808E-01 -1.2686202500E-01
5.0744809999E-01 -9.4447278115E-01

F5 C1 1.0780658078E+00 1.1919457837E+00 4.6929835204E-01 -7.2264743170E-01
2.8905897268E+00 -1.6612441358E+00

F5 Total 1.0780658078E+00 1.1919457837E+00 4.6929835204E-01 -7.2264743170E-01
2.8905897268E+00 -1.6612441358E+00

Total Total 7.7863818473E+00 5.5978959487E+00 3.3914289487E+00 -2.2064670001E+00
8.8258680004E+00 -8.9893248976E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

$\text{Area\_IDS}(A)$ = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

$\text{ESP\_Int\_IDS}(A)$ = Surface Integral of ESP Over Atom A's Part of IDS

$\text{ESP\_Max\_IDS}(A)$ = Maximum Value of ESP on Atom A's Part of IDS

$\text{ESP\_Min\_IDS}(A)$ = Minimum Value of ESP on Atom A's Part of IDS

$\text{ESP\_Avg\_IDS}(A)$ = Average Value of ESP on Atom A's Part of IDS

$\text{ESP\_MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Atom A's Part of IDS

$\text{ESP\_Var\_IDS}(A)$ = Variance of ESP on Atom A's Part of IDS

$|\text{ESP}|\_Int\_IDS(A)$ = Surface Integral of $|\text{ESP}|$ Over Atom A's Part of IDS

$\text{ESP*ESP\_Int\_IDS}(A)$ = Surface Integral of ESP*ESP Over Atom A's Part of IDS

$\text{Area\_ESP+\_IDS}(A)$ = Surface Area of Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Int\_IDS}(A)$ = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

$\text{Area\_ESP-\_IDS}(A)$ = Surface Area of Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Int\_IDS}(A)$ = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Min\_IDS}(A)$ = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Avg\_IDS}(A)$ = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Var\_IDS}(A)$ = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+*ESP+\_Int\_IDS}(A)$ = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

$\text{ESP-\_Min\_IDS}(A)$ = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Avg\_IDS}(A)$ = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Var\_IDS}(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-*ESP-\_Int\_IDS}(A)$ = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	$\text{Area\_IDS}(A)$	$\text{ESP\_Int\_IDS}(A)$	$\text{ESP\_Max\_IDS}(A)$	$\text{ESP\_Min\_IDS}(A)$	$\text{ESP\_Avg\_IDS}(A)$	$\text{ESP\_MAD\_IDS}(A)$	$\text{ESP\_Var\_IDS}(A)$

C1 2.3881910686E+01

H2 5.2757124077E+01

H3 5.2797339748E+01
H4 5.2801850211E+01
F5 9.7759312929E+01

Total 2.7999753765E+02

0.001 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 2.3227077280E+01 4.1078536240E-01 3.5784419660E-02 -1.3185138866E-03 1.7685624301E-02 8.5404426892E-03 1.0132047759E-04

H2 4.3152502660E+01 9.0907233963E-01 3.2316005866E-02 1.6931196983E-03 2.1066503298E-02 5.5605887927E-03 4.4840134784E-05

H3 4.3044663616E+01 9.0943250242E-01 3.2275522205E-02 3.1483883905E-04 2.1127648029E-02 5.5233602695E-03 4.4289446857E-05

H4 4.2894979641E+01 9.0596155448E-01 3.2295647276E-02 5.5881201369E-04 2.1120456568E-02 5.5151006510E-03 4.4228333389E-05

F5 8.5082097189E+01 -2.4328788608E+00 3.8976509595E-03 -4.0873711413E-02 -2.8594486280E-02 1.0663263175E-02 1.5858761142E-04

Total 2.3740132039E+02 7.0237289813E-01 3.5784419660E-02 -4.0873711413E-02 2.9585888444E-03 6.4800927735E-04

0.001 IsoDensity Surface:

Atom A |ESP|_Int_IDS(A) ESP*ESP_Int_IDS(A) Area_ESP+_IDS(A) ESP+_Int_IDS(A) Area_ESP-_IDS(A) ESP-_Int_IDS(A)

C1 4.1125612634E-01 9.6183741511E-03 2.2817894547E+01 4.1102074437E-01 4.0918273312E-01 -2.3538196769E-04

H2 9.0907233963E-01 2.1085939477E-02 4.3152502660E+01 9.0907233963E-01 0.0000000000E+00 NULL

H3 9.0943250242E-01 2.1120594159E-02 4.3044663616E+01 9.0943250242E-01 0.0000000000E+00 NULL

H4	9.0596155448E-01	2.1031495124E-02	4.2894979641E+01	9.0596155448E-01
	0.0000000000E+00	NULL		
F5	2.4386692783E+00	8.3059887774E-02	1.6664191880E+00	2.8952087409E-03
	8.3415678001E+01	-2.4357740695E+00		

Total	5.5743918012E+00	1.5591629069E-01	1.5357645965E+02	3.1383823496E+00
	8.3824860734E+01	-2.4360094515E+00		

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

C1	2.6680848563E-05	1.8013088084E-02	8.4110924268E-03	9.7046418506E-05
	9.6181478163E-03			
H2	1.6931196983E-03	2.1066503298E-02	5.5605887927E-03	4.4840134784E-05
	2.1085939477E-02			
H3	3.1483883905E-04	2.1127648029E-02	5.5233602695E-03	4.4289446857E-05
	2.1120594159E-02			
H4	5.5881201369E-04	2.1120456568E-02	5.5151006510E-03	4.4228333389E-05
	2.1031495124E-02			
F5	9.0451828325E-06	1.7373832237E-03	9.8578603240E-04	1.2769003165E-06
	7.1579382842E-06			

Total	9.0451828325E-06	2.0435308619E-02	5.6841541042E-05	7.2863334515E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-6.6978865436E-06	-5.7524902359E-04	4.3169320697E-04	2.2222739187E-07	
	2.2633485866E-07				
H2	NULL	NULL	NULL	NULL	NULL
H3	NULL	NULL	NULL	NULL	NULL
H4	NULL	NULL	NULL	NULL	NULL

F5	-5.9231322650E-05	-2.9200434833E-02	1.0136143495E-02	1.4298352704E-04
	8.3052729836E-02			

Total	-6.6978865436E-06	-2.9060703831E-02	1.4626695308E-04	8.3052956171E-02

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	2.3161701872E+01

H2	3.6180555247E+01

H3	3.6102644971E+01

H4	3.6053418257E+01

F5	7.5425971779E+01

Total	2.0692429213E+02

Atomic Surface Area and Volume Data:

$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$

$\text{Vol(A)} = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$
 Isosurface of the Electron Density Distribution (IsoDensity Surface)

$\text{N(Vol(A))} = \text{Average Number of Electrons in Vol(A)}$

$\text{N(Vol(A))}/\text{Vol(A)} = \text{Average Electron Density in Vol(A)}$

$\% \text{N(Vol(A))} = 100 * \text{N(Vol(A))} / \text{N(A)}$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.8326857618E+02	7.2226450816E+01	5.4437869918E+00	7.5371099235E-02
9.9914751476E+01				
H2	9.0872246629E+01	6.7251801165E+01	9.6081436478E-01	1.4286819805E-02
9.8827723378E+01				
H3	9.0912462384E+01	6.7217904444E+01	9.6079411654E-01	1.4293723146E-02
9.8825917886E+01				
H4	9.0916972847E+01	6.7260988075E+01	9.6081154234E-01	1.4284826462E-02
9.8827695038E+01				
F5	1.4280061060E+02	1.4269183918E+02	9.6171775180E+00	6.7398230852E-02
9.9817741819E+01				

Total	5.9877086863E+02	4.1664898368E+02	1.7943384533E+01	4.3065950563E-02
9.9686587645E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.4839629204E+02	6.2240848189E+01	5.4372908238E+00	8.7358880575E-02	
9.9795521423E+01					
H2	7.2898203505E+01	4.8304362543E+01	9.4857181606E-01	1.9637394350E-02	
9.7568475741E+01					
H3	7.2790364523E+01	4.8403312071E+01	9.4867023822E-01	1.9599283554E-02	
9.7578872986E+01					
H4	7.2640680548E+01	4.8361169502E+01	9.4863262320E-01	1.9615584838E-02	
9.7574988910E+01					
F5	1.2101420929E+02	1.1225195830E+02	9.5973610947E+00	8.5498384530E-02	
9.9612064985E+01					

Total	4.8773974991E+02	3.1956165061E+02	1.7880526596E+01	5.5953292775E-02
9.9337372965E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.2480874791E+02	5.4764008517E+01	5.4265789934E+00	9.9090244493E-02
	9.9598917501E+01			
H2	6.0210172715E+01	3.6182419643E+01	9.3120192005E-01	2.5736308662E-02
	9.5781837926E+01			
H3	6.0132262488E+01	3.6192521171E+01	9.3122321116E-01	2.5729713793E-02
	9.5784296569E+01			
H4	6.0083035774E+01	3.6231603244E+01	9.3129725075E-01	2.5704003339E-02
	9.5791897402E+01			
F5	1.0498416532E+02	9.1057421341E+01	9.5665233663E+00	1.0506033693E-01
	9.9291996815E+01			

Total	4.1021838421E+02	2.5442797392E+02	1.7786824742E+01	6.9909076694E-02
	9.8816801269E+01			

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	F5	6.3478247663E-01		
C1	H2	-2.7743767471E-02		
C1	H3	-2.7746494531E-02		
C1	H4	-2.7746344591E-02		
C1		5.5154587004E-01	5.5156830060E-01	
H2	C1	2.7766198036E-02		
H2		2.7766198036E-02	2.7788628600E-02	
H3	C1	2.7768925096E-02		
H3		2.7768925096E-02	2.7791355660E-02	
H4	C1	2.7768775156E-02		
H4		2.7768775156E-02	2.7791205720E-02	
F5	C1	-6.3476004606E-01		

F5 -6.3476004606E-01 -6.3473761550E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	2.9550831167E-05	1.6422064907E-07	2.9715051816E-05
H2	5.5516311536E-07	-5.6903776880E-18	5.5516311535E-07
H3	-1.1487706700E-01	1.6547573959E-02	-9.8329493041E-02
H4	1.1487708893E-01	-1.6547484609E-02	9.8329604321E-02
F5	-1.9673755746E-08	-2.4902590767E-16	-1.9673755995E-08

Total 3.0108250527E-05 2.5357028080E-07 3.0361820807E-05

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	4.9299495003E-04	-3.3556082962E-06	4.8963934173E-04
H2	-1.3264626721E-01	1.9105615586E-02	-1.1354065162E-01
H3	6.6325429772E-02	-9.5537463153E-03	5.6771683457E-02
H4	6.6324020728E-02	-9.5536947293E-03	5.6770325999E-02
F5	4.4905461824E-07	2.0437957903E-09	4.5109841403E-07

Total 4.9662729465E-04 -5.1790228169E-06 4.9144827183E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	6.2369650517E-01	-5.8824128467E-01	3.5455220503E-02

H2	5.8286920114E-02	-6.6425973097E-03	5.1644322804E-02
H3	5.8282046887E-02	-6.6432498469E-03	5.1638797040E-02
H4	5.8282795549E-02	-6.6432139763E-03	5.1639581573E-02
F5	1.1263874557E-01	-1.1128630404E+00	-1.0002242949E+00

Total	9.1118701329E-01	-1.7210333862E+00	-8.0984637293E-01

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	6.2369670071E-01	5.8824128468E-01	3.5458613771E-02
H2	1.4488753315E-01	2.0227423117E-02	1.2473417996E-01
H3	1.4488823329E-01	2.0229410301E-02	1.2473282889E-01
H4	1.4488790683E-01	2.0229301071E-02	1.2473262358E-01
F5	1.1263874557E-01	1.1128630404E+00	1.0002242949E+00

Total	9.1118714913E-01	1.7210333862E+00	8.0984652262E-01

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	F5	-1.3857785942E-16	
C1	H2	-8.1750154542E-18	
C1	H3	3.0389137966E-02	
C1	H4	-3.0388973745E-02	
C1		1.6422064907E-07	
H2	C1	-5.6903776880E-18	
H2		-5.6903776880E-18	

H3	C1	1.6547573959E-02
H3		1.6547573959E-02
H4	C1	-1.6547484609E-02
H4		-1.6547484609E-02
F5	C1	-2.4902590767E-16
F5		-2.4902590767E-16

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	F5	-2.0438678359E-09	
C1	H2	3.5086905578E-02	
C1	H3	-1.7545176977E-02	
C1	H4	-1.7545082165E-02	
C1		-3.3556082962E-06	
H2	C1	1.9105615586E-02	
H2		1.9105615586E-02	
H3	C1	-9.5537463153E-03	
H3		-9.5537463153E-03	
H4	C1	-9.5536947293E-03	
H4		-9.5536947293E-03	
F5	C1	2.0437957903E-09	
F5		2.0437957903E-09	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	F5	-5.5304701417E-01	
C1	H2	-1.1730676013E-02	
C1	H3	-1.1731828940E-02	
C1	H4	-1.1731765543E-02	
C1		-5.8824128467E-01	
H2	C1	-6.6425973097E-03	
H2		-6.6425973097E-03	

H3	C1	-6.6432498469E-03
H3		-6.6432498469E-03
H4	C1	-6.6432139763E-03
H4		-6.6432139763E-03
F5	C1	-1.1128630404E+00
F5		-1.1128630404E+00

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	F5	5.5304701417E-01	
C1	H2	3.6995941706E-02	
C1	H3	3.6999577724E-02	
C1	H4	3.6999377781E-02	
C1		5.8824128468E-01	
H2	C1	2.0227423117E-02	
H2		2.0227423117E-02	
H3	C1	2.0229410301E-02	
H3		2.0229410301E-02	
H4	C1	2.0229301071E-02	
H4		2.0229301071E-02	
F5	C1	1.1128630404E+00	
F5		1.1128630404E+00	

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$Q_{XX}(A) = -[3\langle Rho * x * x \rangle(A) - \langle Rho * r * r \rangle(A)]$

$Q_{XY}(A) = -3\langle Rho * x * y \rangle(A)$

$Q_{XZ}(A) = -3\langle Rho * x * z \rangle(A)$

$Q_{YY}(A) = -[3\langle Rho * y * y \rangle(A) - \langle Rho * r * r \rangle(A)]$

$Q_{YZ}(A) = -3\langle Rho * y * z \rangle(A)$

$$Q\_ZZ(A) = -[3\langle Rho*z*z\rangle(A) - \langle Rho*r*r\rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	-6.2006295553E-01	-6.0885057287E-04	2.6445809649E-04	-6.1540000772E-01	2.5537000777E-03	1.2354629632E+00
H2	-2.3150060928E-01	-1.1441683862E-07	-1.0509307420E-07	3.5893474557E-01	-1.7819685168E-01	-1.2743413630E-01
H3	2.1132532915E-01	-2.5567603361E-01	-1.5430557262E-01	-8.3904048145E-02	8.9091161144E-02	-1.2742128100E-01
H4	2.1132433657E-01	2.5567093856E-01	1.5430615839E-01	-8.3899416063E-02	8.9089978191E-02	-1.2742492051E-01
F5	-3.3897718222E-01	1.9864298976E-06	-6.9060185911E-08	-3.3897993720E-01	-2.0971839443E-06	6.7795711942E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
C1	1	-6.2014132952E-01	9.9183392862E-01	1.2753571118E-01	-3.1687061226E-04
C1	2	-6.1532519460E-01	-1.2753602569E-01	9.9183301964E-01	-1.3502983116E-03
C1	3	1.2354665241E+00	1.4207148071E-04	1.3796840978E-03	9.9999903814E-01
H2	1	-2.3150060928E-01	1.0000000000E+00	1.0317882083E-06	2.7766337824E-06
H2	2	-1.8573400716E-01	-2.9598198723E-06	3.1094704905E-01	9.5042723692E-01
H2	3	4.1723461644E-01	-1.1725353500E-07	9.5042723692E-01	-3.1094704905E-01
H3	1	-2.3151864418E-01	4.9998725837E-01	8.6603275869E-01	-4.8453231599E-05
H3	2	-1.8571082633E-01	2.6929583374E-01	-1.5541956428E-01	9.5043385513E-01
H3	3	4.1722947051E-01	8.2309932292E-01	-4.7521786574E-01	-3.1092681564E-01
H4	1	-2.3151100573E-01	-4.9999375782E-01	8.6602900737E-01	-2.2955909602E-05

H4	2	-1.8571445091E-01	-2.6928260282E-01	-1.5544260213E-01	9.5043383634E-01
H4	3	4.1722545664E-01	8.2309970354E-01	4.7521716702E-01	3.1092687599E-01
F5	1	-3.3898097702E-01	-4.6376470339E-01	8.8595840754E-01	1.7955764243E-06
F5	2	-3.3897614240E-01	8.8595840754E-01	4.6376470339E-01	1.0165704880E-06
F5	3	6.7795711942E-01	-6.7914202840E-08	-2.0622555403E-06	1.0000000000E+00

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r*r) \rangle(A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle(A)$$

$$R0(A) = \langle \text{Rho} \rangle(A) = N(A)$$

$$R+1(A) = \langle \text{Rho}*r \rangle(A)$$

$$R+2(A) = \langle \text{Rho}*r*r \rangle(A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3730721811E+02	1.4603838089E+01	5.4484316994E+00	5.1783944213E+00	7.5678121467E+00
H2	2.9229218372E+00	1.2601675294E+00	9.7221137140E-01	1.0720383791E+00	1.5744969182E+00
H3	2.9229207963E+00	1.2601658468E+00	9.7220864434E-01	1.0720336007E+00	1.5744860534E+00
H4	2.9229212193E+00	1.2601662131E+00	9.7220879428E-01	1.0720329595E+00	1.5744823520E+00
F5	3.3039629744E+02	2.6985250393E+01	9.6347376155E+00	8.7476358797E+00	1.1886389688E+01

Atomic Radial Distortion Moments:

$$\text{Dot} = x*(d\text{Rho}/dx) + y*(d\text{Rho}/dy) + z*(d\text{Rho}/dz)$$

$$GR-2(A) = \langle \text{Dot}/(r*r) \rangle(A)$$

$$GR-1(A) = \langle \text{Dot}/r \rangle(A)$$

$$GR0(A) = \langle \text{Dot} \rangle(A)$$

$$GR+1(A) = \langle \text{Dot}*r \rangle(A)$$

$$GR+2(A) = \langle \text{Dot} * r * r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3569719414E+02	-2.6720709649E+01	-1.2268682510E+01	-1.3587273403E+01	-2.4445226604E+01
H2	-2.2599840815E+00	-1.8353212539E+00	-2.1373058037E+00	-3.2805194774E+00	-6.3447099955E+00
H3	-2.2599810226E+00	-1.8353162124E+00	-2.1372971318E+00	-3.2805019867E+00	-6.3446489135E+00
H4	-2.2599813352E+00	-1.8353160774E+00	-2.1372953259E+00	-3.2804938307E+00	-6.3446127670E+00
F5	-3.2990158453E+02	-5.3001520226E+01	-2.6972345836E+01	-3.1047240400E+01	-5.1123401618E+01

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
C1	2.7242158497E+00	2.7242158497E+00	5.4484316994E+00	0.0000000000E+00
H2	4.8610568570E-01	4.8610568570E-01	9.7221137140E-01	0.0000000000E+00
H3	4.8610432217E-01	4.8610432217E-01	9.7220864434E-01	0.0000000000E+00
H4	4.8610439714E-01	4.8610439714E-01	9.7220879428E-01	0.0000000000E+00
F5	4.8173688078E+00	4.8173688078E+00	9.6347376155E+00	0.0000000000E+00
Total	8.9998990625E+00	8.9998990625E+00	1.7999798125E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions $VeeX(A)$ to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of $VeeX(A)$ into interatomic ($VeeX(A,B)$ and $VeeX(A,A')$) and intraatomic ($VeeX(A,A)$) contributions is ambiguous. Currently, interatomic contributions $VeeX(A,B)$ and $VeeX(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $VeeX(A,A)$ is calculated as $VeeX(A) - VeeX(A,A')$. For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E\_IQA(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CH3plus

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\ch3\an\ch3cation.wfn

Sum File: D:\calc\ellipticity\ch3\an\ch3cation.sum

SumViz File: D:\calc\ellipticity\ch3\an\ch3cation.sumviz

Wfn Title: ch3_as_plane_mp2

Total memory allocated for AIMSum = 0.328 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	8.0000001000
Number of Alpha electrons (from MO Occs)	=	4.0000000500
Number of Beta electrons (from MO Occs)	=	4.0000000500
Number of electron pairs ($N*(N-1)/2$)	=	28.0000007500
Number of electron pairs (from Muller 2EDM)	=	28.0000006500
Number of electron pairs (from Muller 2EDM, no SOSI)	=	28.0694490226

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
H2	1.0	0.0000000000E+00	2.0620331000E+00	0.0000000000E+00

H3	1.0	1.7857730500E+00	-1.0310165500E+00	0.0000000000E+00
H4	1.0	-1.7857730500E+00	-1.0310165500E+00	0.0000000000E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
C1	1.7557591640E-01	-5.6614164524E-05	3.7797573082E+01	-3.7848356011E+01	2.4783497737E-06
H2	2.7480760681E-01	1.8708567127E-05	5.0235806681E-01	-5.0303300999E-01	1.0729530169E-01
H3	2.7480922781E-01	1.8992675424E-05	5.0235740199E-01	-5.0303234428E-01	1.0729603907E-01
H4	2.7480776643E-01	1.8004599184E-05	5.0235744893E-01	-5.0303239128E-01	1.0729575949E-01
Total	1.0000005174E+00	-9.0832278900E-07	3.9304646000E+01	-3.9357453757E+01	

Molecular charge $q(Mol)$ from the wfn file: 9.9999990000E-01

Molecular energy $E(Mol)$ from the wfn file: -3.9243647387E+01

Molecular virial ratio $(-V(Mol)/T(Mol))$ from the wfn file: 2.0013435500E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use $K\_Scaled(A)$ with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	11	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 20

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = $(-1/4)\text{DelSqRho}$

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -7.61151727416618E-17 1.37218077296279E-15 -8.20843315720818E-20

Type = (3,-3) NACP C1

Rho = 1.2005306652E+02 Rho at Nucleus = 1.2005306652E+02

GradRho = -9.2049174696E-18 1.2564027471E-17 9.7324108603E-30

HessRho_EigVals = -1.8204647884E+05 -1.8203377922E+05 -1.8203377922E+05

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -6.5070974552E-01 7.5932656156E-01 0.0000000000E+00

HessRho_EigVec3 = 7.5932656156E-01 6.5070974552E-01 0.0000000000E+00

DelSqRho = -5.4611403728E+05

Bond Ellipticity = NA

V = -1.3654177303E+05

G = 6.6318562110E+00

K = 1.3653514118E+05

L = 1.3652850932E+05

Vnuc = 6.0000000145E+08

Ven = -7.2031840087E+10

Vrep = 7.2031703545E+10

DelSqV = 4.6273280473E+09

DelSqVen = 2.1609551974E+27

DelSqVrep = -2.1609551974E+27

DelSqG = 2.0704289508E+08

DelSqK = -4.8343709424E+09

Stress_EigVals = -4.5515060551E+04 -4.5515060551E+04 -4.5511651930E+04

Stress_EigVec1 = 5.4013946428E-01 8.4157552194E-01 0.0000000000E+00

Stress_EigVec2 = 8.4157552194E-01 -5.4013946428E-01 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

-DivStress = 1.0632062878E-07 -1.6963185025E-06 1.2361449656E-10

CP# 2 Coords = 3.36442562675706E-11 2.02695697134568E+00 -1.48783747296871E-17

Type = (3,-3) NACP H2

Rho = 4.0331808065E-01 Rho at Nucleus = 3.9872225065E-01

GradRho = 2.2554956280E-17 -1.9577798593E-15 -1.2485244294E-30

HessRho_EigVals = -7.9860122613E+00 -7.9803056658E+00 -7.1259511297E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 4.0273293486E-10 0.0000000000E+00

HessRho_EigVec3 = -4.0273293486E-10 1.0000000000E+00 0.0000000000E+00

DelSqRho = -2.3092269057E+01

Bond Ellipticity = NA

V = -5.7857156078E+00

G = 6.3241717944E-03

K = 5.7793914360E+00

L = 5.7730672642E+00
Vnuc = 3.2034298189E+01
Ven = -1.2920011660E+01
Vrep = 7.1342960527E+00
DelSqV = 1.4701163366E+03
DelSqVen = 7.3974463282E+02
DelSqVrep = 7.3037170378E+02
DelSqG = 1.1120715943E+02
DelSqK = -1.5813234960E+03
Stress_EigVals = -2.0012723148E+00 -1.9978055307E+00 -1.7866377623E+00
Stress_EigVec1 = 1.0000000000E+00 1.8943154599E-10 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = -1.8943154599E-10 1.0000000000E+00 0.0000000000E+00
-DivStress = -1.4721954241E-08 1.6954671302E+01 6.9756812600E-15

CP# 3 Coords = 1.75539623178777E+00 -1.01347848584378E+00 2.95338471565410E-17

Type = (3,-3) NACP H3

Rho = 4.0331807400E-01 Rho at Nucleus = 3.9872224411E-01

GradRho = -5.0929618467E-12 2.9412359383E-12 4.1966066634E-27

HessRho_EigVals = -7.9860122285E+00 -7.9803056328E+00 -7.1259511098E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 4.9999999996E-01 8.6602540380E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540380E-01 -4.9999999996E-01 0.0000000000E+00

DelSqRho = -2.3092268971E+01

Bond Ellipticity = NA

V = -5.7857155863E+00

G = 6.3241717930E-03

K = 5.7793914146E+00

L = 5.7730672428E+00

Vnuc = 3.2034298444E+01

Ven = -1.2920011551E+01

Vrep = 7.1342959642E+00

DelSqV = 1.4701163384E+03
DelSqVen = 7.3974463598E+02
DelSqVrep = 7.3037170246E+02
DelSqG = 1.1120716040E+02
DelSqK = -1.5813234988E+03
Stress_EigVals = -2.0012723065E+00 -1.9978055225E+00 -1.7866377573E+00
Stress_EigVec1 = 5.0000000028E-01 8.6602540362E-01 0.0000000000E+00
Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec3 = 8.6602540362E-01 -5.0000000028E-01 0.0000000000E+00
-DivStress = 1.4683175934E+01 -8.4773355714E+00 -1.4104007501E-14

CP# 4 Coords = -1.75539623175532E+00 -1.01347848592898E+00 -1.86379754070587E-17

Type = (3,-3) NACP H4

Rho = 4.0331807735E-01 Rho at Nucleus = 3.9872224744E-01

GradRho = 5.0927837155E-12 2.9405174221E-12 -2.7363128393E-27

HessRho_EigVals = -7.9860122590E+00 -7.9803056636E+00 -7.1259511373E+00

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -4.9999999818E-01 8.6602540484E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540484E-01 4.9999999818E-01 0.0000000000E+00

DelSqRho = -2.3092269060E+01

Bond Ellipticity = NA

V = -5.7857156085E+00

G = 6.3241717556E-03

K = 5.7793914367E+00

L = 5.7730672650E+00

Vnuc = 3.2034298456E+01

Ven = -1.2920011663E+01

Vrep = 7.1342960541E+00

DelSqV = 1.4701163436E+03

DelSqVen = 7.3974463910E+02

DelSqVrep = 7.3037170446E+02

DelSqG = 1.1120716034E+02

DelSqK = -1.5813235039E+03

Stress_EigVals = -2.0012723142E+00 -1.9978055302E+00 -1.7866377642E+00

Stress_EigVec1 = -4.9999999847E-01 8.6602540467E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540467E-01 4.9999999847E-01 0.0000000000E+00

-DivStress = -1.4683176002E+01 -8.4773355633E+00 8.8042566292E-15

CP# 5 Coords = 2.26318853095290E-10 1.43051760552871E+00 -7.53632806232515E-17

Type = (3,-1) BCP H2 C1

Rho = 2.9341655278E-01

GradRho = 9.4713060329E-18 -1.9182802580E-16 3.8499038662E-32

HessRho_EigVals = -9.0634607773E-01 -8.6370422255E-01 6.0413741328E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 5.1849200315E-11 0.0000000000E+00

HessRho_EigVec3 = -5.1849200315E-11 1.0000000000E+00 0.0000000000E+00

DelSqRho = -1.1659128870E+00

Bond Ellipticity = 4.9370900436E-02

V = -3.3471102457E-01

G = 2.1616401410E-02

K = 3.1309462316E-01

L = 2.9147822175E-01

Vnuc = 6.4354406704E+00

Ven = -1.8882648171E+00

Vrep = 1.5535537925E+00

DelSqV = -4.1264461490E+00

DelSqVen = 7.5031632111E+00

DelSqVrep = -1.1629609360E+01

DelSqG = 1.7944557661E+00

DelSqK = 2.3319903829E+00

Stress_EigVals = -2.4404767105E-01 -2.2853479811E-01 1.3787144459E-01

Stress_EigVec1 = 1.0000000000E+00 -1.4054864220E-11 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 1.4054864220E-11 1.0000000000E+00 0.0000000000E+00

-DivStress = -6.9741989310E-10 3.1696637051E-01 -2.2395378723E-17

BPL = 2.0269569713E+00 = 5.9643936582E-01 + 1.4305176055E+00

GBL_I = 2.0269569713E+00

GBL_II = 2.0620331000E+00

GBL_III = 2.0269569713E+00 = 5.9643936582E-01 + 1.4305176055E+00

GBL_IV = 2.0620331000E+00 = 6.3151549447E-01 + 1.4305176055E+00

CP# 6 Coords = 1.23886459583733E+00 -7.15258806644452E-01 4.97692934366004E-17

Type = (3,-1) BCP H3 C1

Rho = 2.9341654813E-01

GradRho = -5.2718655175E-17 6.9197556208E-17 -7.2676795521E-32

HessRho_EigVals = -9.0634606793E-01 -8.6370421394E-01 6.0413741616E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 5.0000000029E-01 8.6602540362E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540362E-01 -5.0000000029E-01 0.0000000000E+00

DelSqRho = -1.1659128657E+00

Bond Ellipticity = 4.9370899553E-02

V = -3.3471101814E-01

G = 2.1616400856E-02

K = 3.1309461728E-01

L = 2.9147821643E-01

Vnuc = 6.4354406604E+00

Ven = -1.8882647843E+00

Vrep = 1.5535537661E+00

DelSqV = -4.1264462370E+00

DelSqVen = 7.5031630624E+00

DelSqVrep = -1.1629609299E+01

DelSqG = 1.7944557548E+00

DelSqK = 2.3319904821E+00

Stress_EigVals = -2.4404766795E-01 -2.2853479563E-01 1.3787144544E-01

Stress_EigVec1 = 5.0000000065E-01 8.6602540341E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.6602540341E-01 -5.0000000065E-01 0.0000000000E+00

-DivStress = 2.7450095987E-01 -1.5848320357E-01 2.4403516709E-18

BPL = 2.0269569734E+00 = 5.9643935819E-01 + 1.4305176152E+00

GBL_I = 2.0269569734E+00

GBL_II = 2.0620331017E+00

GBL_III = 2.0269569734E+00 = 5.9643935819E-01 + 1.4305176152E+00

GBL_IV = 2.0620331017E+00 = 6.3151548653E-01 + 1.4305176152E+00

CP# 7 Coords = -1.23886459191697E+00 -7.15258805692945E-01 -4.71624426416156E-17

Type = (3,-1) BCP C1 H4

Rho = 2.9341655043E-01

GradRho = -8.8951117509E-17 -7.9742131570E-17 -3.0369883969E-32

HessRho_EigVals = -9.0634607139E-01 -8.6370421728E-01 6.0413741268E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = -4.9999999916E-01 8.6602540427E-01 0.0000000000E+00

HessRho_EigVec3 = 8.6602540427E-01 4.9999999916E-01 0.0000000000E+00

DelSqRho = -1.1659128760E+00

Bond Ellipticity = 4.9370899500E-02

V = -3.3471102103E-01

G = 2.1616401014E-02

K = 3.1309462001E-01

L = 2.9147821900E-01

Vnuc = 6.4354406627E+00

Ven = -1.8882647998E+00

Vrep = 1.5535537787E+00

DelSqV = -4.1264461688E+00

DelSqVen = 7.5031631313E+00

DelSqVrep = -1.1629609300E+01

DelSqG = 1.7944557537E+00

DelSqK = 2.3319904151E+00

Stress_EigVals = -2.4404766904E-01 -2.2853479651E-01 1.3787144452E-01

$\text{Stress\_EigVec1} = -4.9999999887\text{E-}01 \ 8.6602540444\text{E-}01 \ 0.0000000000\text{E+}00$
 $\text{Stress\_EigVec2} = 0.0000000000\text{E+}00 \ 0.0000000000\text{E+}00 \ 1.0000000000\text{E+}00$
 $\text{Stress\_EigVec3} = 8.6602540444\text{E-}01 \ 4.9999999887\text{E-}01 \ 0.0000000000\text{E+}00$
 $-\text{DivStress} = -2.7450094506\text{E-}01 \ -1.5848319367\text{E-}01 \ -2.2945747528\text{E-}17$
 $\text{BPL} = 2.0269569734\text{E+}00 = 1.4305176113\text{E+}00 + 5.9643936208\text{E-}01$
 $\text{GBL\_I} = 2.0269569734\text{E+}00$
 $\text{GBL\_II} = 2.0620331017\text{E+}00$
 $\text{GBL\_III} = 2.0269569734\text{E+}00 = 1.4305176113\text{E+}00 + 5.9643936208\text{E-}01$
 $\text{GBL\_IV} = 2.0620331017\text{E+}00 = 1.4305176113\text{E+}00 + 6.3151549040\text{E-}01$

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

 BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H3	C1	H2	119.99999988	119.99999997	119.99999997	119.99999995	119.99999995
H4	C1	H2	120.00000004	119.99999998	119.99999997	120.00000001	120.00000001
H4	C1	H3	120.00000007	120.00000005	120.00000005	120.00000004	120.00000004

Total time for electron density critical point search, analysis and connectivity = 1 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7797573082E+01	3.7797573082E+01	-9.7200919952E+01	-8.8864763943E+01		
H2	-5.0235806681E-01	5.0235806681E-01	-3.3190558360E+00	-1.0271437698E+00		
H3	-5.0235740199E-01	5.0235740199E-01	-3.3190482799E+00	-1.0271422582E+00		
H4	-5.0235744893E-01	5.0235744893E-01	-3.3190537411E+00	-1.0271432677E+00		
Total	-3.9304646000E+01	3.9304646000E+01	-1.0715807781E+02	-9.1946193239E+01		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$$V_{nn}(A) = \text{Contribution of Atom A to Nuclear Repulsion Energy of Molecule}$$

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$$V_{eeC}(A) = \text{Coulomb Part of } V_{ee}(A)$$

$$V_{eeX}(A) = \text{Exchange-Correlation Part of } V_{ee}(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	$E_e(A)$	W(A)	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
C1	-3.7797573082E+01					
H2	-5.0235806681E-01					
H3	-5.0235740199E-01					
H4	-5.0235744893E-01					
Total	-3.9304646000E+01					

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, \text{Mol})/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, \text{Mol})/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{ee}(A) = V_{ee}(A, \text{Mol}) = (1/2)[V_{ee}(A, \text{Mol}) + V_{ee}(\text{Mol}, A)]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, \text{Mol})/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$ $VeeC(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
C1	4.3646244064E+00		3.7797573082E+01	-4.7288450819E+01	-4.8600459976E+01	
H2	1.7348655892E+00		5.0235806681E-01	-2.0968621411E+00	-1.6595279180E+00	
H3	1.7348655879E+00		5.0235740199E-01	-2.0968621318E+00	-1.6595241400E+00	
H4	1.7348655879E+00		5.0235744893E-01	-2.0968621369E+00	-1.6595268706E+00	
Total	9.5692211714E+00		3.9304646000E+01	-5.3579037229E+01	-5.3579038905E+01	

IQA Intraatomic ("Self") Energy Components:

$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$

C1	3.7797573082E+01 -8.8864763943E+01
H2	5.0235806681E-01 -1.0271437698E+00
H3	5.0235740199E-01 -1.0271422582E+00
H4	5.0235744893E-01 -1.0271432677E+00

Total	3.9304646000E+01 -9.1946193239E+01

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$	$VeeX(A,A')$

C1	-2.8560688476E+00	-4.1680780045E+00		4.3646244064E+00			
H2	-1.5832902562E+00	-1.1459560331E+00		1.7348655892E+00			
H3	-1.5832910027E+00	-1.1459530109E+00		1.7348655879E+00			

H4	-1.5832905031E+00 -1.1459552367E+00	1.7348655879E+00

Total	-7.6059406096E+00 -7.6059422852E+00	9.5692211714E+00

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$\%Loc(A)$	$DI(A,A')/2$	$\%Deloc(A,A')$

C1	5.8244240837E+00	4.6123036612E+00	7.9189008130E+01	1.2121204226E+00	
	2.0810991870E+01				
H2	7.2519239318E-01	3.0328871317E-01	4.1821827700E+01	4.2190368001E-01	
	5.8178172300E+01				
H3	7.2519077209E-01	3.0328747687E-01	4.1821750710E+01	4.2190329521E-01	
	5.8178249290E+01				
H4	7.2519223384E-01	3.0328855720E-01	4.1821815382E+01	4.2190367664E-01	
	5.8178184618E+01				

Total	7.9999994828E+00	5.5221684084E+00	6.9027109567E+01	2.4778310744E+00	
	3.0972890433E+01				

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$N(A)$	$LI(A)$	$DI(A,A')/2$	$DI\_Bond(A,A')/2$	$DI\_NonBond(A,A')/2$

C1	5.8244240837E+00	4.6123036612E+00	1.2121204226E+00	1.2121200886E+00	3.3393517418E-07
H2	7.2519239318E-01	3.0328871317E-01	4.2190368001E-01	4.0404035774E-01	1.7863322267E-02
H3	7.2519077209E-01	3.0328747687E-01	4.2190329521E-01	4.0403939527E-01	1.7863899946E-02
H4	7.2519223384E-01	3.0328855720E-01	4.2190367664E-01	4.0404033561E-01	1.7863341031E-02

Total	7.9999994828E+00	5.5221684084E+00	2.4778310744E+00	2.4242401772E+00	5.3590897179E-02

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A') = \text{Half of Average Number of Electron Pairs Formed}$

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.4655806123E+01	5.7296784553E+00	2.0385484578E+01
H2	1.1130764698E-01	2.4268657343E+00	2.5381733813E+00
H3	1.1130708952E-01	2.4268606180E+00	2.5381677075E+00
H4	1.1130760941E-01	2.4268652142E+00	2.5381728236E+00
Total	1.4989728469E+01	1.3010270022E+01	2.7999998491E+01

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) = \text{Average Number of Electron Pairs Formed Between Atoms A and B}$

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A) = \text{Electron Delocalization Index. Average Number of Electrons Delocalized}$

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
C1	H2	3.8197876824E+00	8.0808071548E-01	6.9370010139E+00	5.5714919454E+01 (Bonded)

C1	H3	3.8197792030E+00	8.0807879053E-01	6.9369844891E+00	5.5714911278E+01 (Bonded)
H2	H3	5.1697109823E-01	1.7863466569E-02	1.2316363725E+00	1.2316391257E+00
C1	H4	3.8197867765E+00	8.0808067122E-01	6.9370006339E+00	5.5714928643E+01 (Bonded)
H2	H4	5.1697214739E-01	1.7863488366E-02	1.2316378753E+00	1.2316381459E+00
H3	H4	5.1697095469E-01	1.7863522569E-02	1.2316429867E+00	1.2316405041E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	H2	3.1163623248E+01	2.4563480432E+01	2.0030252640E+01
C1	H3	3.1163623186E+01	2.4563480385E+01	2.0030252602E+01
C1	H4	3.1163623227E+01	2.4563480415E+01	2.0030252626E+01

C1	Total	9.3490869661E+01	7.3690441232E+01	6.0090757868E+01
H2	C1	3.1163623248E+01	2.4563480432E+01	2.0030252640E+01

H2	Total	3.1163623248E+01	2.4563480432E+01	2.0030252640E+01
H3	C1	3.1163623186E+01	2.4563480385E+01	2.0030252602E+01

H3	Total	3.1163623186E+01	2.4563480385E+01	2.0030252602E+01

H4	C1	3.1163623227E+01	2.4563480415E+01	2.0030252626E+01

H4	Total	3.1163623227E+01	2.4563480415E+01	2.0030252626E+01

Total	Total	1.8698173932E+02	1.4738088246E+02	1.2018151574E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta^2 \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta^2 \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N_{IAS}(A B)$	$G_{IAS}(A B)$	$K_{IAS}(A B)$	$L_{IAS}(A B)$	$\Delta^2 \rho_{IAS}(A B)$	$V_{IAS}(A B)$

C1	H2	8.3651328998E-01	4.3674994078E-01	3.9083176043E-01	-4.5918180350E-02	1.8367272140E-01	-8.2758170120E-01

C1	H3	8.3651327570E-01	4.3674993036E-01	3.9083175098E-01	-4.5918179378E-02	1.8367271751E-01	-8.2758168134E-01

C1	H4	8.3651328405E-01	4.3674993548E-01	3.9083175590E-01	-4.5918179575E-02	1.8367271830E-01	-8.2758169138E-01

C1	Total	2.5095398497E+00	1.3102498066E+00	1.1724952673E+00	-1.3775453930E-01	5.5101815721E-01	-2.4827450739E+00

H2	C1	8.3651328998E-01	4.3674994078E-01	3.9083176043E-01	-4.5918180350E-02	1.8367272140E-01	-8.2758170120E-01

H2	Total	8.3651328998E-01	4.3674994078E-01	3.9083176043E-01	-4.5918180350E-02
		1.8367272140E-01	-8.2758170120E-01		

H3 C1 8.3651327570E-01 4.3674993036E-01 3.9083175098E-01 -4.5918179378E-02
1.8367271751E-01 -8.2758168134E-01

H3	Total	8.3651327570E-01	4.3674993036E-01	3.9083175098E-01	-4.5918179378E-02
		1.8367271751E-01	-8.2758168134E-01		

H4 C1 8.3651328405E-01 4.3674993548E-01 3.9083175590E-01 -4.5918179575E-02
1.8367271830E-01 -8.2758169138E-01

H4	Total	8.3651328405E-01	4.3674993548E-01	3.9083175590E-01	-4.5918179575E-02
		1.8367271830E-01	-8.2758169138E-01		

Total	Total	5.0190796995E+00	2.6204996132E+00	2.3449905346E+00	-2.7550907861E-01
		1.1020363144E+00	-4.9654901478E+00		

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

$\text{Area\_ESP+\_IDS}(A)$ = Surface Area of Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Int\_IDS}(A)$ = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

$\text{Area\_ESP-\_IDS}(A)$ = Surface Area of Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Int\_IDS}(A)$ = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Min\_IDS}(A)$ = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Avg\_IDS}(A)$ = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+\_Var\_IDS}(A)$ = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

$\text{ESP+*ESP+\_Int\_IDS}(A)$ = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

$\text{ESP-\_Min\_IDS}(A)$ = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Avg\_IDS}(A)$ = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-\_Var\_IDS}(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$\text{ESP-*ESP-\_Int\_IDS}(A)$ = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	7.0969608469E+01						

H2	4.5063814094E+01						

H3	4.4980846327E+01						

H4	4.5033429167E+01						

Total	2.0604769806E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1 6.2754993800E+01 1.8463217041E+01 3.6764989516E-01 2.5990540768E-01 2.9421112047E-01 2.2728139278E-02 7.6230234740E-04

H2 3.6325839443E+01 9.5988532339E+00 2.9001399074E-01 2.5795545772E-01 2.6424312228E-01 4.6658336329E-03 3.9762180592E-05

H3 3.6262316259E+01 9.5812460860E+00 2.8996230933E-01 2.5794642779E-01 2.6422046561E-01 4.6256905808E-03 3.8497925952E-05

H4 3.6648978720E+01 9.6843415055E+00 2.9006384400E-01 2.5793680150E-01 2.6424587652E-01 4.6639277958E-03 3.9777198075E-05

Total 1.7199212822E+02 4.7327657866E+01 3.6764989516E-01 2.5793680150E-01
2.7517339518E-01 5.1134621556E-04

0.001 IsoDensity Surface:

Atom A |ESP|_Int_IDS(A) ESP*ESP_Int_IDS(A) Area_ESP+_IDS(A) ESP+_Int_IDS(A) Area_ESP-
_IDS(A) ESP-_Int_IDS(A)

C1 1.8463217041E+01 5.4799220520E+00 6.2754993800E+01 1.8463217041E+01
0.0000000000E+00 NULL

H2 9.5988532339E+00 2.5378753435E+00 3.6325839443E+01 9.5988532339E+00
0.0000000000E+00 NULL

H3 9.5812460860E+00 2.5329573259E+00 3.6262316259E+01 9.5812460860E+00
0.0000000000E+00 NULL

H4 9.6843415055E+00 2.5605051033E+00 3.6648978720E+01 9.6843415055E+00
0.0000000000E+00 NULL

Total 4.7327657866E+01 1.3111259825E+01 1.7199212822E+02 4.7327657866E+01
0.0000000000E+00 NULL

0.001 IsoDensity Surface:

Atom A ESP+_Min_IDS(A) ESP+_Avg_IDS(A) ESP+_MAD_IDS(A) ESP+_Var_IDS(A)
ESP*ESP+_Int_IDS(A)

C1 2.5990540768E-01 2.9421112047E-01 2.2728139278E-02 7.6230234740E-04
5.4799220520E+00

H2	2.5795545772E-01	2.6424312228E-01	4.6658336329E-03	3.9762180592E-05
	2.5378753435E+00			
H3	2.5794642779E-01	2.6422046561E-01	4.6256905808E-03	3.8497925952E-05
	2.5329573259E+00			
H4	2.5793680150E-01	2.6424587652E-01	4.6639277958E-03	3.9777198075E-05
	2.5605051033E+00			

Total	2.5793680150E-01	2.7517339518E-01	5.1134621556E-04	1.3111259825E+01

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	NULL	NULL	NULL	NULL	NULL
H2	NULL	NULL	NULL	NULL	NULL
H3	NULL	NULL	NULL	NULL	NULL
H4	NULL	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL	NULL

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	5.6866526928E+01						
H2	2.9936768873E+01						
H3	3.0132648032E+01						
H4	2.9865664009E+01						

Total	1.4680160784E+02						

Atomic Surface Area and Volume Data:

$$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$$

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

N(Vol(A)) = Average Number of Electrons in Vol(A)

$\text{N(Vol(A))}/\text{Vol(A)}$ = Average Electron Density in Vol(A)

$\%N(\text{Vol(A)}) = 100 * \text{N(Vol(A))} / \text{N(A)}$
= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.6446047813E+02	1.1920246270E+02	5.8118124263E+00	4.8755808350E-02	
	9.9783469453E+01				
H2	7.6227437342E+01	4.9760026909E+01	7.1737741450E-01	1.4416740888E-02	
	9.8922357879E+01				
H3	7.6144469513E+01	4.9835827300E+01	7.1740912658E-01	1.4395449327E-02	
	9.8926951927E+01				
H4	7.6197052394E+01	4.9729635920E+01	7.1736487579E-01	1.4425299171E-02	
	9.8920650633E+01				
Total	3.9302943738E+02	2.6852795283E+02	7.9639638432E+00	2.9657857811E-02	
	9.9549554475E+01				

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.3644543503E+02	9.4496162091E+01	5.7957705566E+00	6.1333396281E-02	
	9.9508045318E+01				
H2	6.0889319875E+01	3.5953581639E+01	7.0845109384E-01	1.9704604146E-02	
	9.7691467877E+01				

H3	6.0825796644E+01	3.5966650304E+01	7.0846202855E-01	1.9697748402E-02
9.7693194083E+01				
H4	6.1212459135E+01	3.5952505539E+01	7.0844785762E-01	1.9705103914E-02
9.7691043123E+01				

Total	3.1937301069E+02	2.0236889957E+02	7.9211315366E+00	3.9142039875E-02
9.9014150609E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.1695728480E+02	7.8213610891E+01	5.7724065758E+00	7.3803095267E-02	
9.9106907274E+01					
H2	4.9967021513E+01	2.6696660478E+01	6.9524770804E-01	2.6042497286E-02	
9.5870794367E+01					
H3	5.0162900634E+01	2.6688039829E+01	6.9522780135E-01	2.6050163511E-02	
9.5868263636E+01					
H4	4.9895916635E+01	2.6690120293E+01	6.9523768506E-01	2.6048503245E-02	
9.5869433355E+01					

Total	2.6698312358E+02	1.5828843149E+02	7.8581197703E+00	4.9644308786E-02	
9.8226503478E+01					

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	H2	1.0906826747E-02		
C1	H3	1.0905205747E-02		
C1	H4	1.0906667127E-02		

C1		3.2718699621E-02	1.7557591640E-01
H2	C1	1.3195039003E-01	
H2		1.3195039003E-01	2.7480760681E-01
H3	C1	1.3195201103E-01	
H3		1.3195201103E-01	2.7480922781E-01
H4	C1	1.3195054965E-01	
H4		1.3195054965E-01	2.7480776643E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	-7.1286625380E-07	1.8104067166E-06	1.0975404628E-06
H2	-5.4876710486E-07	-2.9862860937E-11	-5.4879696772E-07
H3	-9.2921253885E-02	7.2165670377E-02	-2.0755583508E-02
H4	9.2921138031E-02	-7.2164871653E-02	2.0756266378E-02

Total	-1.3774873587E-06	2.6091006368E-06	1.2316132782E-06

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	-6.5850422656E-07	-1.2735298747E-06	-1.9320341013E-06
H2	-1.0729530167E-01	8.3328715806E-02	-2.3966585864E-02
H3	5.3647745305E-02	-4.1664869235E-02	1.1982876070E-02
H4	5.3647386737E-02	-4.1664407918E-02	1.1982978819E-02

Total	-8.2813222656E-07	-1.8348760189E-06	-2.6630082455E-06

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	2.2804410733E-06	7.9361492283E-19	2.2804410733E-06
H2	-1.9094679774E-06	9.9442142723E-18	-1.9094679774E-06
H3	1.0382410958E-06	-6.5671583566E-18	1.0382410958E-06
H4	-2.7376245022E-06	6.2231102295E-18	-2.7376245022E-06

Total	-1.3284103105E-06	1.0393781068E-17	-1.3284103105E-06

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	2.4783497737E-06	2.2134703118E-06	3.1839852897E-06
H2	1.0729530169E-01	8.3328715806E-02	2.3966585946E-02
H3	1.0729603907E-01	8.3329738445E-02	2.3966300648E-02
H4	1.0729575949E-01	8.3328816071E-02	2.3966943544E-02

Total	2.0851734606E-06	3.1896984400E-06	3.2207387562E-06

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	H2	-2.4684205203E-12	
C1	H3	-1.3510073310E-02	
C1	H4	1.3511883720E-02	
C1		1.8104067166E-06	
H2	C1	-2.9862860937E-11	

H2		-2.9862860937E-11
H3	C1	7.2165670377E-02
H3		7.2165670377E-02
H4	C1	-7.2164871653E-02
H4		-7.2164871653E-02

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	H2	-1.5602407682E-02	
C1	H3	7.8000444489E-03	
C1	H4	7.8010897035E-03	
C1		-1.2735298747E-06	
H2	C1	8.3328715806E-02	
H2		8.3328715806E-02	
H3	C1	-4.1664869235E-02	
H3		-4.1664869235E-02	
H4	C1	-4.1664407918E-02	
H4		-4.1664407918E-02	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	H2	8.2197424485E-19	
C1	H3	-5.4274438482E-19	
C1	H4	5.1438506280E-19	
C1		7.9361492283E-19	
H2	C1	9.9442142723E-18	
H2		9.9442142723E-18	
H3	C1	-6.5671583566E-18	
H3		-6.5671583566E-18	
H4	C1	6.2231102295E-18	
H4		6.2231102295E-18	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	H2	1.5602407682E-02	
C1	H3	1.5600088918E-02	
C1	H4	1.5602179406E-02	
C1		2.2134703118E-06	
H2	C1	8.3328715806E-02	
H2		8.3328715806E-02	
H3	C1	8.3329738445E-02	
H3		8.3329738445E-02	
H4	C1	8.3328816071E-02	
H4		8.3328816071E-02	

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)

C1	-6.7857675597E-01	2.0165644045E-05	-4.3686863313E-06	-6.7852827683E-01	1.9133289892E-05	1.3571050328E+00
H2	-1.3038214605E-01	-3.6425837631E-06	-4.3570057051E-06	3.1714388077E-01	-5.2920644062E-07	-1.8676173471E-01
H3	2.0525446527E-01	-1.9378778658E-01	8.4854820836E-07	-1.8505883326E-02	-9.5312618823E-07	-1.8674858194E-01

H4 2.0527017556E-01 1.9378491159E-01 8.5751638478E-06 -1.8505158148E-02 -1.0931304909E-05 -1.8676501741E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$

C1	1	-6.7858404755E-01	9.4041203174E-01	-3.4003707228E-01	5.2141523818E-06
C1	2	-6.7852098544E-01	3.4003707232E-01	9.4041203171E-01	-8.1093779323E-06
C1	3	1.3571050330E+00	-2.1459625049E-06	9.3991616880E-06	9.9999999995E-01
H2	1	-1.8676173505E-01	7.7279909220E-05	1.0507680823E-06	9.9999999701E-01
H2	2	-1.3038214575E-01	9.9999999698E-01	8.1392871906E-06	-7.7279917770E-05
H2	3	3.1714388080E-01	-8.1393683695E-06	9.9999999997E-01	-1.0501390757E-06
H3	1	-1.8674858195E-01	1.4769440148E-06	7.3663814825E-06	9.9999999997E-01
H3	2	-1.3039094232E-01	5.0000545736E-01	8.6602225292E-01	-7.1179303552E-06
H3	3	3.1713952426E-01	8.6602225295E-01	-5.0000545736E-01	2.4041645591E-06
H4	1	-1.8676502077E-01	-1.2534416717E-04	2.0932569650E-04	9.9999997024E-01
H4	2	-1.3038397774E-01	-4.9999010336E-01	8.6603108318E-01	-2.4395341004E-04
H4	3	3.1714899851E-01	8.6603110846E-01	4.9999011906E-01	3.8911682367E-06

Atomic Radial Moments:

$R-2(A) = \langle \rho / (r^*r) \rangle (A)$

$R-1(A) = \langle \rho / r \rangle (A)$

$R0(A) = \langle \rho \rangle (A) = N(A)$

$R+1(A) = \langle \rho * r \rangle (A)$

$R+2(A) = \langle \rho * r^*r \rangle (A)$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3792992755E+02	1.4810793991E+01	5.8244240836E+00	5.9254231435E+00	9.1007503069E+00
H2	2.5736072872E+00	1.0271437698E+00	7.2519239319E-01	7.2943200509E-01	9.7309792034E-01
H3	2.5736057082E+00	1.0271422582E+00	7.2519077219E-01	7.2942986664E-01	9.7309309486E-01
H4	2.5736066305E+00	1.0271432677E+00	7.2519223357E-01	7.2943284990E-01	9.7310323146E-01

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3689973613E+02	-2.7830356884E+01	-1.4259346358E+01	-1.7703201771E+01	-3.3742543541E+01
H2	-1.9154311895E+00	-1.4596625011E+00	-1.5841717373E+00	-2.2500249932E+00	-3.9830598124E+00
H3	-1.9154291795E+00	-1.4596600542E+00	-1.5841681834E+00	-2.2500172557E+00	-3.9830268263E+00
H4	-1.9154306971E+00	-1.4596627475E+00	-1.5841737287E+00	-2.2500321477E+00	-3.9830914356E+00

Atomic Electronic Spin Populations:

$$N\_alpha(A) = \text{Average number of Alpha electrons in Atom A}$$

$N_{\text{beta}}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\text{alpha}}(A) + N_{\text{beta}}(A)$

$N_{\text{spin}}(A) = N_{\text{alpha}}(A) - N_{\text{beta}}(A)$

Atom A	$N_{\text{alpha}}(A)$	$N_{\text{beta}}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
C1	2.9122120418E+00	2.9122120418E+00	5.8244240836E+00	0.0000000000E+00
H2	3.6259619660E-01	3.6259619660E-01	7.2519239319E-01	0.0000000000E+00
H3	3.6259538609E-01	3.6259538609E-01	7.2519077219E-01	0.0000000000E+00
H4	3.6259611679E-01	3.6259611679E-01	7.2519223357E-01	0.0000000000E+00
Total	3.9999997413E+00	3.9999997413E+00	7.9999994825E+00	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A)

into interatomic ($V_{ee}X(A,B)$ and $V_{ee}X(A,A')$) and intraatomic ($V_{ee}X(A,A)$) contributions is ambiguous. Currently, interatomic contributions $V_{ee}X(A,B)$ and $V_{ee}X(A,A')$ are calculated using the Hartree-Fock exchange functional while the intratomic contribution $V_{ee}X(A,A)$ is calculated as $V_{ee}X(A) - V_{ee}X(A,A')$. For wavefunctions of non-supported DFT models, $V_{ee}X$ is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E_{IQA}(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CH4

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\ch4\ch4.wfx

Sum File: D:\calc\ellipticity\ch4\ch4.sum

SumViz File: D:\calc\ellipticity\ch4\ch4.sumviz

Wfx Title: nh3_as_pyr_mp2

Total memory allocated for AIMSum = 0.367 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	9.9999999926
Number of Alpha electrons (from MO Occs)	=	4.9999999963
Number of Beta electrons (from MO Occs)	=	4.9999999963
Number of electron pairs ($N*(N-1)/2$)	=	44.9999999295
Number of electron pairs (from Muller 2EDM)	=	44.9999857258
Number of electron pairs (from Muller 2EDM, no SOSI)	=	45.1090414654

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
H2	1.0	1.1898652500E+00	1.1898652500E+00	1.1898652500E+00
H3	1.0	-1.1898652500E+00	-1.1898652500E+00	1.1898652500E+00
H4	1.0	-1.1898652500E+00	1.1898652500E+00	-1.1898652500E+00
H5	1.0	1.1898652500E+00	-1.1898652500E+00	-1.1898652500E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
C1	-1.6202137200E-02	-6.7160175427E-05	3.7868889633E+01	-3.7920219450E+01	3.0117104991E-05
H2	4.0510769600E-03	1.6485159484E-05	6.1402170687E-01	-6.1485398956E-01	1.5367713351E-01

H3 4.0510719600E-03 1.6918326902E-05 6.1402206954E-01 -6.1485435273E-01 1.5367694520E-01

H4 4.0515321600E-03 1.6707646303E-05 6.1402166200E-01 -6.1485394464E-01 1.5367728886E-01

H5 4.0510952300E-03 1.6592989736E-05 6.1402180857E-01 -6.1485409140E-01 1.5367707871E-01

Total 2.6391100003E-06 -4.5605300200E-07 4.0324976880E+01 -4.0379635828E+01

Molecular charge q(Mol) from the wfx file: 7.4225282099E-09

Molecular energy E(Mol) from the wfx file: -4.0379637695E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0013554614E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0013091981E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR
C1	15	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00 13.00
H2	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H3	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00
H4	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00 13.00

H5	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 27

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -9.15708624727454E-24 1.35333141822550E-22 3.41660955509587E-22

Type = (3,-3) NACP C1

Rho = 1.1935915664E+02 Rho at Nucleus = 1.1935915664E+02

GradRho = -9.9283047193E-21 8.1155137187E-19 2.1181739368E-18

HessRho_EigVals = -1.8095596016E+05 -1.8095596016E+05 -1.8095596016E+05

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00

DelSqRho = -5.4286788048E+05

Bond Ellipticity = NA

V = -1.3573241705E+05

G = 7.7234630572E+00

K = 1.3572469358E+05

L = 1.3571697012E+05

Vnuc = 6.0000000194E+08

Ven = -7.1615494216E+10

Vrep = 7.1615358484E+10

DelSqV = 4.5999482305E+09

DelSqVen = 2.1484648195E+27

DelSqVrep = -2.1484648195E+27

DelSqG = 2.0578103975E+08

DelSqK = -4.8057292703E+09

Stress_EigVals = -4.5244139016E+04 -4.5244139016E+04 -4.5244139016E+04
Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec2 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 1.0000000000E+00 0.0000000000E+00
-DivStress = 1.4638174560E-14 -1.8025385109E-13 -4.8082853750E-13

CP# 2 Coords = 1.17389648512364E+00 1.17389648511150E+00 1.17389648509859E+00

Type = (3,-3) NACP H2

Rho = 4.2583650272E-01 Rho at Nucleus = 4.2274345394E-01

GradRho = -3.6647427143E-14 -3.5568213571E-14 -3.5482539438E-14

HessRho_EigVals = -8.4956717610E+00 -8.4956717610E+00 -7.8563986794E+00

HessRho_EigVec1 = 7.1139924203E-01 -8.6645518485E-03 -7.0273468961E-01

HessRho_EigVec2 = -4.0072158063E-01 8.1645060634E-01 -4.1572902499E-01

HessRho_EigVec3 = -5.7735026912E-01 -5.7735026886E-01 -5.7735026959E-01

DelSqRho = -2.4847742201E+01

Bond Ellipticity = NA

V = -6.2322754143E+00

G = 1.0169931961E-02

K = 6.2221054823E+00

L = 6.2119355504E+00

Vnuc = 4.0003340206E+01

Ven = -1.7034882490E+01

Vrep = 1.0802607076E+01

DelSqV = 1.6077671312E+03

DelSqVen = 9.9399268462E+02

DelSqVrep = 6.1377444656E+02

DelSqG = 1.2203358320E+02

DelSqK = -1.7298007144E+03

Stress_EigVals = -2.1310995969E+00 -2.1310995969E+00 -1.9700762205E+00

Stress_EigVec1 = 7.1514671821E-01 -1.6363923617E-02 -6.9878279418E-01

Stress_EigVec2 = -3.9399471838E-01 8.1633258482E-01 -4.2233786574E-01

Stress_EigVec3 = 5.7735026918E-01 5.7735026886E-01 5.7735026953E-01

-DivStress = 8.3147177972E+00 8.3147178032E+00 8.3147178100E+00

CP# 3 Coords = -1.17389648512364E+00 -1.17389648511150E+00 1.17389648509859E+00

Type = (3,-3) NACP H3

Rho = 4.2583650272E-01 Rho at Nucleus = 4.2274345394E-01

GradRho = 3.6661304925E-14 3.5557805250E-14 -3.5472131104E-14

HessRho_EigVals = -8.4956717610E+00 -8.4956717610E+00 -7.8563986794E+00

HessRho_EigVec1 = 7.1142728010E-01 -8.7216815785E-03 7.0270559795E-01

HessRho_EigVec2 = 4.0067180069E-01 -8.1644999805E-01 -4.1577819665E-01

HessRho_EigVec3 = -5.7735026912E-01 -5.7735026886E-01 5.7735026959E-01

DelSqRho = -2.4847742201E+01

Bond Ellipticity = NA

V = -6.2322754143E+00

G = 1.0169931961E-02

K = 6.2221054823E+00

L = 6.2119355504E+00

Vnuc = 4.0003340206E+01

Ven = -1.7034882490E+01

Vrep = 1.0802607076E+01

DelSqV = 1.6077671312E+03

DelSqVen = 9.9399268462E+02

DelSqVrep = 6.1377444656E+02

DelSqG = 1.2203358320E+02

DelSqK = -1.7298007144E+03

Stress_EigVals = -2.1310995969E+00 -2.1310995969E+00 -1.9700762205E+00

Stress_EigVec1 = -7.1516987331E-01 1.6411902074E-02 -6.9875797082E-01

Stress_EigVec2 = -3.9395268624E-01 8.1633162165E-01 4.2237893472E-01

Stress_EigVec3 = 5.7735026918E-01 5.7735026886E-01 -5.7735026953E-01

-DivStress = -8.3147177972E+00 -8.3147178032E+00 8.3147178100E+00

CP# 4 Coords = -1.17389648512364E+00 1.17389648511150E+00 -1.17389648509859E+00

Type = (3,-3) NACP H4

Rho = 4.2583650272E-01 Rho at Nucleus = 4.2274345394E-01
GradRho = 3.6664774363E-14 -3.5575152518E-14 3.5503356090E-14
HessRho_EigVals = -8.4956717610E+00 -8.4956717610E+00 -7.8563986794E+00
HessRho_EigVec1 = 7.1139924203E-01 8.6645518485E-03 -7.0273468961E-01
HessRho_EigVec2 = -4.0072158063E-01 -8.1645060634E-01 -4.1572902499E-01
HessRho_EigVec3 = 5.7735026912E-01 -5.7735026886E-01 5.7735026959E-01
DelSqRho = -2.4847742201E+01
Bond Ellipticity = NA
V = -6.2322754143E+00
G = 1.0169931961E-02
K = 6.2221054823E+00
L = 6.2119355504E+00
Vnuc = 4.0003340206E+01
Ven = -1.7034882490E+01
Vrep = 1.0802607076E+01
DelSqV = 1.6077671312E+03
DelSqVen = 9.9399268462E+02
DelSqVrep = 6.1377444656E+02
DelSqG = 1.2203358320E+02
DelSqK = -1.7298007144E+03
Stress_EigVals = -2.1310995969E+00 -2.1310995969E+00 -1.9700762205E+00
Stress_EigVec1 = 7.1514671821E-01 1.6363923617E-02 -6.9878279418E-01
Stress_EigVec2 = -3.9399471838E-01 -8.1633258482E-01 -4.2233786574E-01
Stress_EigVec3 = -5.7735026918E-01 5.7735026886E-01 -5.7735026953E-01
-DivStress = -8.3147177972E+00 8.3147178032E+00 -8.3147178100E+00

CP# 5 Coords = 1.17389648512364E+00 -1.17389648511150E+00 -1.17389648509859E+00

Type = (3,-3) NACP H5

Rho = 4.2583650272E-01 Rho at Nucleus = 4.2274345394E-01
GradRho = -3.6664774362E-14 3.5564744158E-14 3.5489478329E-14
HessRho_EigVals = -8.4956717610E+00 -8.4956717610E+00 -7.8563986794E+00
HessRho_EigVec1 = 7.1137832131E-01 8.6219288754E-03 7.0275639187E-01

HessRho_EigVec2 = 4.0075871882E-01 8.1645105756E-01 -4.1569233802E-01
HessRho_EigVec3 = 5.7735026912E-01 -5.7735026886E-01 -5.7735026959E-01
DelSqRho = -2.4847742201E+01
Bond Ellipticity = NA
V = -6.2322754143E+00
G = 1.0169931961E-02
K = 6.2221054823E+00
L = 6.2119355504E+00
Vnuc = 4.0003340206E+01
Ven = -1.7034882490E+01
Vrep = 1.0802607076E+01
DelSqV = 1.6077671312E+03
DelSqVen = 9.9399268462E+02
DelSqVrep = 6.1377444656E+02
DelSqG = 1.2203358320E+02
DelSqK = -1.7298007144E+03
Stress_EigVals = -2.1310995969E+00 -2.1310995969E+00 -1.9700762205E+00
Stress_EigVec1 = -7.1519557375E-01 -1.6465160539E-02 -6.9873041280E-01
Stress_EigVec2 = -3.9390602682E-01 -8.1633054918E-01 4.2242452167E-01
Stress_EigVec3 = -5.7735026918E-01 5.7735026886E-01 5.7735026953E-01
-DivStress = 8.3147177972E+00 -8.3147178032E+00 -8.3147178100E+00

CP# 6 Coords = 7.56904285163685E-01 7.56904285557802E-01 7.56904284987262E-01

Type = (3,-1) BCP H2 C1

Rho = 2.7188214671E-01

GradRho = 2.5163909150E-14 2.5222953581E-14 2.5148320543E-14

HessRho_EigVals = -6.8455732839E-01 -6.8455732800E-01 4.5854367437E-01

HessRho_EigVec1 = -7.0386636498E-01 -6.4368848699E-03 7.1030324986E-01

HessRho_EigVec2 = 4.1381010936E-01 -8.1647120817E-01 4.0266109772E-01

HessRho_EigVec3 = 5.7735026946E-01 5.7735026867E-01 5.7735026944E-01

DelSqRho = -9.1057098201E-01

Bond Ellipticity = 5.6713411745E-10

V = -3.2536622984E-01
G = 4.8861742169E-02
K = 2.7650448767E-01
L = 2.2764274550E-01
Vnuc = 6.9865958353E+00
Ven = -1.8995306739E+00
Vrep = 1.5741644440E+00
DelSqV = -2.3079565577E+00
DelSqVen = 6.3617914306E+00
DelSqVrep = -8.6697479884E+00
DelSqG = 1.5632267781E+00
DelSqK = 7.4472977961E-01
Stress_EigVals = -2.1173586210E-01 -2.1173586202E-01 9.8105494279E-02
Stress_EigVec1 = -7.1245069763E-01 1.0811824929E-02 7.0163887284E-01
Stress_EigVec2 = -3.9884918186E-01 8.1642499439E-01 -4.1757581188E-01
Stress_EigVec3 = -5.7735026940E-01 -5.7735026888E-01 -5.7735026929E-01
-DivStress = -8.3325150342E-02 -8.3325150222E-02 -8.3325150391E-02
BPL = 2.0332483550E+00 = 7.2225167655E-01 + 1.3109966785E+00
GBL_I = 2.0332483550E+00
GBL_II = 2.0609070672E+00
GBL_III = 2.0332483550E+00 = 7.2225167655E-01 + 1.3109966785E+00
GBL_IV = 2.0609070672E+00 = 7.4991038866E-01 + 1.3109966785E+00

CP# 7 Coords = -7.56904285163685E-01 -7.56904285557802E-01 7.56904284987262E-01

Type = (3,-1) BCP C1 H3
Rho = 2.7188214671E-01
GradRho = -2.5170847996E-14 -2.5202136890E-14 2.5134442704E-14
HessRho_EigVals = -6.8455732839E-01 -6.8455732800E-01 4.5854367437E-01
HessRho_EigVec1 = 7.0386660116E-01 6.4364188659E-03 7.1030302004E-01
HessRho_EigVec2 = 4.1380970763E-01 -8.1647121185E-01 -4.0266150312E-01
HessRho_EigVec3 = 5.7735026946E-01 5.7735026867E-01 -5.7735026944E-01
DelSqRho = -9.1057098201E-01

Bond Ellipticity = 5.6713611585E-10

V = -3.2536622984E-01

G = 4.8861742169E-02

K = 2.7650448767E-01

L = 2.2764274550E-01

Vnuc = 6.9865958353E+00

Ven = -1.8995306739E+00

Vrep = 1.5741644440E+00

DelSqV = -2.3079565577E+00

DelSqVen = 6.3617914306E+00

DelSqVrep = -8.6697479884E+00

DelSqG = 1.5632267781E+00

DelSqK = 7.4472977961E-01

Stress_EigVals = -2.1173586210E-01 -2.1173586202E-01 9.8105494279E-02

Stress_EigVec1 = 7.1245148884E-01 -1.0813444506E-02 7.0163804448E-01

Stress_EigVec2 = -3.9884776854E-01 8.1642497294E-01 4.1757720375E-01

Stress_EigVec3 = -5.7735026940E-01 -5.7735026888E-01 5.7735026929E-01

-DivStress = 8.3325150342E-02 8.3325150222E-02 -8.3325150391E-02

BPL = 2.0332483550E+00 = 1.3109966785E+00 + 7.2225167655E-01

GBL_I = 2.0332483550E+00

GBL_II = 2.0609070672E+00

GBL_III = 2.0332483550E+00 = 1.3109966785E+00 + 7.2225167655E-01

GBL_IV = 2.0609070672E+00 = 1.3109966785E+00 + 7.4991038866E-01

CP# 8 Coords = -7.56904285163685E-01 7.56904285557802E-01 -7.56904284987262E-01

Type = (3,-1) BCP H4 C1

Rho = 2.7188214671E-01

GradRho = -2.5108398019E-14 2.5195198007E-14 -2.5280159545E-14

HessRho_EigVals = -6.8455732839E-01 -6.8455732800E-01 4.5854367437E-01

HessRho_EigVec1 = -7.0386673001E-01 6.4361646496E-03 7.1030289467E-01

HessRho_EigVec2 = 4.1380948847E-01 8.1647121385E-01 4.0266172428E-01

HessRho_EigVec3 = -5.7735026946E-01 5.7735026867E-01 -5.7735026944E-01

DelSqRho = -9.1057098201E-01

Bond Ellipticity = 5.6713522767E-10

V = -3.2536622984E-01

G = 4.8861742169E-02

K = 2.7650448767E-01

L = 2.2764274550E-01

Vnuc = 6.9865958353E+00

Ven = -1.8995306739E+00

Vrep = 1.5741644440E+00

DelSqV = -2.3079565577E+00

DelSqVen = 6.3617914306E+00

DelSqVrep = -8.6697479884E+00

DelSqG = 1.5632267781E+00

DelSqK = 7.4472977961E-01

Stress_EigVals = -2.1173586210E-01 -2.1173586202E-01 9.8105494279E-02

Stress_EigVec1 = -7.1245093822E-01 -1.0812317403E-02 7.0163862096E-01

Stress_EigVec2 = -3.9884875210E-01 -8.1642498787E-01 -4.1757623511E-01

Stress_EigVec3 = 5.7735026940E-01 -5.7735026888E-01 5.7735026929E-01

-DivStress = 8.3325150342E-02 -8.3325150222E-02 8.3325150391E-02

BPL = 2.0332483550E+00 = 7.2225167655E-01 + 1.3109966785E+00

GBL_I = 2.0332483550E+00

GBL_II = 2.0609070672E+00

GBL_III = 2.0332483550E+00 = 7.2225167655E-01 + 1.3109966785E+00

GBL_IV = 2.0609070672E+00 = 7.4991038866E-01 + 1.3109966785E+00

CP# 9 Coords = 7.56904285163685E-01 -7.56904285557802E-01 -7.56904284987262E-01

Type = (3,-1) BCP C1 H5

Rho = 2.7188214671E-01

GradRho = 2.5129214618E-14 -2.5313159182E-14 -2.5155259370E-14

HessRho_EigVals = -6.8455732839E-01 -6.8455732800E-01 4.5854367437E-01

HessRho_EigVec1 = 7.0386654208E-01 -6.4365354316E-03 7.1030307753E-01

HessRho_EigVec2 = 4.1380980811E-01 8.1647121093E-01 -4.0266140172E-01

HessRho_EigVec3 = -5.7735026946E-01 5.7735026867E-01 5.7735026944E-01

DelSqRho = -9.1057098201E-01

Bond Ellipticity = 5.6713522767E-10

V = -3.2536622984E-01

G = 4.8861742169E-02

K = 2.7650448767E-01

L = 2.2764274550E-01

Vnuc = 6.9865958353E+00

Ven = -1.8995306739E+00

Vrep = 1.5741644440E+00

DelSqV = -2.3079565577E+00

DelSqVen = 6.3617914306E+00

DelSqVrep = -8.6697479884E+00

DelSqG = 1.5632267781E+00

DelSqK = 7.4472977961E-01

Stress_EigVals = -2.1173586210E-01 -2.1173586202E-01 9.8105494279E-02

Stress_EigVec1 = 7.1245076595E-01 1.0811964779E-02 7.0163880131E-01

Stress_EigVec2 = -3.9884905982E-01 -8.1642499254E-01 4.1757593207E-01

Stress_EigVec3 = 5.7735026940E-01 -5.7735026888E-01 -5.7735026929E-01

-DivStress = -8.3325150342E-02 8.3325150222E-02 8.3325150391E-02

BPL = 2.0332483550E+00 = 1.3109966785E+00 + 7.2225167655E-01

GBL_I = 2.0332483550E+00

GBL_II = 2.0609070672E+00

GBL_III = 2.0332483550E+00 = 1.3109966785E+00 + 7.2225167655E-01

GBL_IV = 2.0609070672E+00 = 1.3109966785E+00 + 7.4991038866E-01

Number of NACPs = 5

Number of NNACPs = 0

Number of BCPs = 4

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H3	C1	H2	109.47122070	109.47122064	109.47122063	109.47122066	109.47122066
H4	C1	H2	109.47122052	109.47122063	109.47122063	109.47122060	109.47122060
H4	C1	H3	109.47122068	109.47122063	109.47122063	109.47122064	109.47122064
H5	C1	H2	109.47122068	109.47122063	109.47122063	109.47122064	109.47122064
H5	C1	H3	109.47122052	109.47122063	109.47122063	109.47122060	109.47122060
H5	C1	H4	109.47122070	109.47122064	109.47122063	109.47122066	109.47122066

Total time for electron density critical point search, analysis and connectivity = 1 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$E_e(A) = E(A) - W(A) = -T(A)$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A) = V_{ee}(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7868889633E+01	3.7868889633E+01	-1.0109396796E+02	-8.9866531424E+01		
H2	-6.1402170687E-01	6.1402170687E-01	-4.7188831948E+00	-1.2644321537E+00		
H3	-6.1402206954E-01	6.1402206954E-01	-4.7188842535E+00	-1.2644323823E+00		
H4	-6.1402166200E-01	6.1402166200E-01	-4.7188812035E+00	-1.2644318340E+00		
H5	-6.1402180857E-01	6.1402180857E-01	-4.7188833604E+00	-1.2644321867E+00		
Total	-4.0324976880E+01	4.0324976880E+01	-1.1996949997E+02	-9.4924259981E+01		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

C1	-3.7870076367E+01	-3.7868889633E+01	-1.1867341037E-03			
H2	-6.1419141444E-01	-6.1402170687E-01	-1.6970756821E-04			
H3	-6.1419177711E-01	-6.1402206954E-01	-1.6970756821E-04			
H4	-6.1419136957E-01	-6.1402166200E-01	-1.6970756821E-04			
H5	-6.1419151614E-01	-6.1402180857E-01	-1.6970756821E-04			

Total	-4.0326842444E+01	-4.0324976880E+01	-1.8655643766E-03			

IQA Atomic Energy Components:

E_IQA(A) = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

Vne(A,Mol)/2 = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

Ven(A,Mol)/2 = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

Vnn(A,Mol)/2 = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

VeeC(A) = Coulomb Part of Vee(A)

VeeX(A) = Exchange-Correlation Part of Vee(A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2

C1			3.7868889633E+01	-5.0148783542E+01	-5.0546983979E+01	
	5.8226788540E+00					
H2			6.1402170687E-01	-2.4589933552E+00	-2.3594415974E+00	
	1.9013757175E+00					

H3	6.1402206954E-01	-2.4589933552E+00	-2.3594421268E+00
1.9013757175E+00			
H4	6.1402166200E-01	-2.4589933552E+00	-2.3594406017E+00
1.9013757175E+00			
H5	6.1402180857E-01	-2.4589933552E+00	-2.3594416802E+00
1.9013757175E+00			

Total	4.0324976880E+01	-5.9984756963E+01	-5.9984749985E+01
1.3428181724E+01			

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to E_IQA(A)

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

Vee(A,A) = Two-electron Interaction Energy of Atom A With Itself

VeeC(A,A) = Coulomb Part of Vee(A,A)

VeeX(A,A) = Exchange-Correlation Part of Vee(A,A)

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Intra(A)	T(A)	Vne(A,A)	Vee(A,A)	VeeC(A,A)	VeeX(A,A)

C1	3.7868889633E+01	-8.9866531424E+01				
H2	6.1402170687E-01	-1.2644321537E+00				
H3	6.1402206954E-01	-1.2644323823E+00				
H4	6.1402166200E-01	-1.2644318340E+00				
H5	6.1402180857E-01	-1.2644321867E+00				

Total	4.0324976880E+01	-9.4924259981E+01				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$	$VeeX(A,A')$

C1	-5.2155178299E+00	-5.6137182675E+00		5.8226788540E+00			
H2	-1.8267772783E+00	-1.7272255205E+00		1.9013757175E+00			
H3	-1.8267771640E+00	-1.7272259356E+00		1.9013757175E+00			
H4	-1.8267774381E+00	-1.7272246847E+00		1.9013757175E+00			
H5	-1.8267772618E+00	-1.7272255869E+00		1.9013757175E+00			

Total	-1.2522626972E+01	-1.2522619995E+01		1.3428181724E+01			

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$$\%Loc(A) = 100 * LI(A) / N(A)$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A)$$

$$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1	6.0162021372E+00	4.2806188976E+00	7.1151513863E+01	1.7355832395E+00	2.8848486137E+01
H2	9.9594892319E-01	5.0865582434E-01	5.1072480977E+01	4.8729309885E-01	4.8927519023E+01
H3	9.9594892806E-01	5.0865589252E-01	5.1072487573E+01	4.8729303555E-01	4.8927512427E+01
H4	9.9594846782E-01	5.0865547484E-01	5.1072469237E+01	4.8729299298E-01	4.8927530763E+01
H5	9.9594890474E-01	5.0865582928E-01	5.1072482419E+01	4.8729307546E-01	4.8927517581E+01
Total	9.9999973610E+00	6.3152419186E+00	6.3152435852E+01	3.6847554424E+00	3.6847564148E+01

More Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that
are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2	
C1	6.0162021372E+00	4.2806188976E+00	1.7355832395E+00	1.7355875221E+00	-	4.2825642070E-06
H2	9.9594892319E-01	5.0865582434E-01	4.8729309885E-01	4.3389892189E-01	5.3394176961E-02	
H3	9.9594892806E-01	5.0865589252E-01	4.8729303555E-01	4.3389707653E-01	5.3395959018E-02	
H4	9.9594846782E-01	5.0865547484E-01	4.8729299298E-01	4.3389522121E-01	5.3397771763E-02	
H5	9.9594890474E-01	5.0865582928E-01	4.8729307546E-01	4.3389630247E-01	5.3396772993E-02	
Total	9.9999973610E+00	6.3152419186E+00	3.6847554424E+00	3.4711750442E+00	2.1358039817E-01	

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A')$ = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.5957034629E+01	1.1115872085E+01	2.7072906714E+01
H2	2.4162921663E-01	4.2401381035E+00	4.4817673201E+00
H3	2.4162918740E-01	4.2401381546E+00	4.4817673420E+00
H4	2.4162893785E-01	4.2401363328E+00	4.4817652707E+00
H5	2.4162919579E-01	4.2401380410E+00	4.4817672368E+00
Total	1.6923551166E+01	2.8076422717E+01	4.4999973883E+01

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized
 (Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
C1	H2	5.5579311183E+00	8.6779784378E-01	7.2121732615E+00	4.3566382953E+01 (Bonded)
C1	H3	5.5579329930E+00	8.6779415306E-01	7.2121425883E+00	4.3566197453E+01 (Bonded)
H2	H3	9.7411375093E-01	3.5601023051E-02	1.7872916081E+00	1.7872915994E+00
C1	H4	5.5579320794E+00	8.6779044243E-01	7.2121117496E+00	4.3566031299E+01 (Bonded)
H2	H4	9.7411328437E-01	3.5601039411E-02	1.7872924295E+00	1.7872932467E+00

H3	H4	9.7411331824E-01	3.5600981374E-02	1.7872895071E+00	1.7872903330E+00
C1	H5	5.5579336267E+00	8.6779260493E-01	7.2121297219E+00	4.3566120752E+01 (Bonded)
H2	H5	9.7411369490E-01	3.5601088654E-02	1.7872949016E+00	1.7872949347E+00
H3	H5	9.7411372538E-01	3.5601037405E-02	1.7872923200E+00	1.7872923619E+00
H4	H5	9.7411328296E-01	3.5601005486E-02	1.7872915435E+00	1.7872907594E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	H2	4.0904550675E+01	3.1765623304E+01	2.5496777221E+01
C1	H3	4.0904561665E+01	3.1765461793E+01	2.5496778720E+01
C1	H4	4.0908343764E+01	3.1768883340E+01	2.5496731931E+01
C1	H5	4.0908547626E+01	3.1768882924E+01	2.5496737495E+01

C1	Total	1.6362600373E+02	1.2706885136E+02	1.0198702537E+02
H2	C1	4.0904550675E+01	3.1765623304E+01	2.5496777221E+01

H2	Total	4.0904550675E+01	3.1765623304E+01	2.5496777221E+01
H3	C1	4.0904561665E+01	3.1765461793E+01	2.5496778720E+01

H3	Total	4.0904561665E+01	3.1765461793E+01	2.5496778720E+01

H4	C1	4.0908343765E+01	3.1768883339E+01	2.5496731931E+01

H4	Total	4.0908343765E+01	3.1768883339E+01	2.5496731931E+01
H5	C1	4.0908547627E+01	3.1768882923E+01	2.5496737496E+01

H5	Total	4.0908547627E+01	3.1768882923E+01	2.5496737496E+01

Total	Total	3.2725200746E+02	2.5413770272E+02	2.0397405074E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta \rho\_IAS(A B)$ $V\_IAS(A B)$

C1	H2	9.5412688452E-01	5.2831296846E-01	3.9906348685E-01	-1.2924948162E-01	5.1699792647E-01 -9.2737645531E-01
C1	H3	9.5412688550E-01	5.2831296786E-01	3.9906348714E-01	-1.2924948073E-01	5.1699792291E-01 -9.2737645500E-01
C1	H4	9.5412742556E-01	5.2831321592E-01	3.9906371989E-01	-1.2924949603E-01	5.1699798411E-01 -9.2737693581E-01

C1 H5 9.5412742652E-01 5.2831321534E-01 3.9906372017E-01 -1.2924949516E-01
5.1699798065E-01 -9.2737693551E-01

C1 Total 3.8165086221E+00 2.1132523676E+00 1.5962544141E+00 -5.1699795354E-01
2.0679918141E+00 -3.7095067816E+00

H2 C1 9.5412688452E-01 5.2831296846E-01 3.9906348685E-01 -1.2924948162E-01
5.1699792647E-01 -9.2737645531E-01

H2 Total 9.5412688452E-01 5.2831296846E-01 3.9906348685E-01 -1.2924948162E-01
5.1699792647E-01 -9.2737645531E-01

H3 C1 9.5412688550E-01 5.2831296786E-01 3.9906348714E-01 -1.2924948073E-01
5.1699792291E-01 -9.2737645500E-01

H3 Total 9.5412688550E-01 5.2831296786E-01 3.9906348714E-01 -1.2924948073E-01
5.1699792291E-01 -9.2737645500E-01

H4 C1 9.5412742555E-01 5.2831321592E-01 3.9906371989E-01 -1.2924949603E-01
5.1699798411E-01 -9.2737693581E-01

H4 Total 9.5412742555E-01 5.2831321592E-01 3.9906371989E-01 -1.2924949603E-01
5.1699798411E-01 -9.2737693581E-01

H5 C1 9.5412742652E-01 5.2831321534E-01 3.9906372017E-01 -1.2924949516E-01
5.1699798065E-01 -9.2737693551E-01

H5 Total 9.5412742652E-01 5.2831321534E-01 3.9906372017E-01 -1.2924949516E-01
5.1699798065E-01 -9.2737693551E-01

Total Total 7.6330172442E+00 4.2265047352E+00 3.1925088281E+00 -1.0339959071E+00
4.1359836283E+00 -7.4190135633E+00

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 4.2361761662E+01
H2 5.4752085396E+01
H3 5.5089479305E+01
H4 5.4910770319E+01
H5 5.4913056471E+01

Total 2.6202715315E+02

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	3.7993315356E+01	-1.1749173708E-01	-2.2769151701E-03	-3.6363281382E-03	-3.0924318128E-03
	3.0877948348E-04	1.3044082690E-07			

H2	4.4446883460E+01	1.6472956786E-01	1.3163665085E-02	-2.9339280502E-03	3.7062118879E-03
	4.1260870486E-03	2.2527153486E-05			

H3	4.4579529153E+01	1.6440932202E-01	1.3161520323E-02	-2.9164904272E-03	3.6880004150E-03
	4.1295805130E-03	2.2571271463E-05			

H4	4.4578508345E+01	1.6436300914E-01	1.3179828231E-02	-2.9332298585E-03	3.6870459609E-03
	4.1310466229E-03	2.2584879324E-05			

H5	4.4306083145E+01	1.6512996782E-01	1.3166126844E-02	-2.9159356930E-03	3.7270269926E-03
	4.1192543334E-03	2.2462097808E-05			

Total	2.1590431946E+02	5.4114012976E-01	1.3179828231E-02	-3.6363281382E-03	2.5063886221E-03
		2.5288016403E-05			

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
	ESP-_Int_IDS(A)				

C1	1.1749173708E-01	3.6829106495E-04	0.0000000000E+00	NULL	3.7993315356E+01
	1.1749173708E-01				

H2	2.0636283977E-01	1.6117844484E-03	3.0973687700E+01	1.8554620381E-01	
	1.3473195760E+01	-2.0816635953E-02			

H3	2.0669738288E-01	1.6125583020E-03	3.1086890801E+01	1.8555335245E-01
	1.3492638352E+01	-2.1144030430E-02		
H4	2.0674450412E-01	1.6128142004E-03	3.1028340997E+01	1.8555375663E-01
	1.3550167348E+01	-2.1190747489E-02		
H5	2.0597861565E-01	1.6106514205E-03	3.1081524655E+01	1.8555429173E-01
	1.3224558490E+01	-2.0424323917E-02		

Total	9.4327507950E-01	6.8160994363E-03	1.2417044415E+02	7.4220760462E-01
	9.1733875306E+01	-2.0106747487E-01		

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				
C1	NULL	NULL	NULL	NULL
H2	1.1858422529E-05	5.9904460073E-03	3.3441375809E-03	1.4835404319E-05
	1.5710116961E-03			
H3	2.6495568448E-06	5.9688617184E-03	3.3508246485E-03	1.4908816426E-05
	1.5710110504E-03			
H4	1.5886025281E-06	5.9801378567E-03	3.3456790927E-03	1.4869446267E-05
	1.5710112937E-03			
H5	1.5512540959E-05	5.9699224473E-03	3.3501526660E-03	1.4904896066E-05
	1.5710116260E-03			
Total	1.5886025281E-06	5.9773290632E-03	1.4879761386E-05	6.2840456662E-03

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
C1	-2.2769151701E-03	-3.0924318128E-03	3.0877948348E-04	1.3044082690E-07	3.6829106495E-04
H2	-9.7981900974E-06	-1.5450407108E-03	6.8512489516E-04	6.3906161599E-07	4.0772752264E-05

H3	-2.8552067304E-05	-1.5670790158E-03	6.7903512927E-04	6.2351669533E-07
4.1547251673E-05				
H4	-1.3963934707E-05	-1.5638734892E-03	6.8620807656E-04	6.3934697617E-07
4.1802906735E-05				
H5	-7.4706759820E-05	-1.5444238787E-03	6.7185887713E-04	6.1219290895E-07
3.9639794495E-05				

Total	-9.7981900974E-06	-2.1918563257E-03	9.9573634201E-07	5.3205377012E-04

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	3.5746351529E+01
H2	3.7128500064E+01
H3	3.7072297598E+01
H4	3.7017565018E+01
H5	3.6906870271E+01

Total	1.8387158448E+02

Atomic Surface Area and Volume Data:

$$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$$
$$\text{Vol(A)} = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$$
$$\text{Isosurface of the Electron Density Distribution (IsoDensity Surface)}$$
$$\text{N(Vol(A))} = \text{Average Number of Electrons in Vol(A)}$$
$$\text{N(Vol(A))}/\text{Vol(A)} = \text{Average Electron Density in Vol(A)}$$
$$\% \text{N(Vol(A))} = 100 * \text{N(Vol(A))} / \text{N(A)}$$
$$= \text{Percentage of Atom A's Electron Population in Vol(A)}$$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.0598776539E+02	1.0242592711E+02	6.0071857368E+00	5.8649073591E-02	9.9850131359E+01
H2	9.5656636071E+01	7.1115891525E+01	9.8359214459E-01	1.3830834761E-02	9.8759295967E+01
H3	9.5994040970E+01	7.1138670543E+01	9.8360093644E-01	1.3826529635E-02	9.8760178233E+01
H4	9.5819114084E+01	7.1150133314E+01	9.8360566023E-01	1.3824368479E-02	9.8760698168E+01
H5	9.5821604098E+01	7.1117064368E+01	9.8359298757E-01	1.3830618520E-02	9.8759382420E+01
Total	5.8927916062E+02	3.8694768686E+02	9.9415774656E+00	2.5692303645E-02	9.9415800892E+01

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.6506216672E+02	8.4299642978E+01	5.9954368016E+00	7.1120547961E-02	9.9654843120E+01
H2	7.6212506764E+01	5.1133398505E+01	9.7066011619E-01	1.8982898547E-02	9.7460832954E+01
H3	7.6344990946E+01	5.1190033837E+01	9.7071582267E-01	1.8962984587E-02	9.7466425771E+01
H4	7.6347391684E+01	5.1169854634E+01	9.7069527489E-01	1.8970061217E-02	9.7464407671E+01
H5	7.6074966068E+01	5.1108571204E+01	9.7063372279E-01	1.8991603559E-02	9.7458184666E+01
Total	4.7004202218E+02	2.8890150116E+02	9.8781417381E+00	3.4192074802E-02	9.8781443450E+01

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.3773337690E+02	7.1387251136E+01	5.9768964556E+00	8.3724983950E-02	9.9346669532E+01
H2	6.2625277285E+01	3.7807460036E+01	9.5148968825E-01	2.5166718085E-02	9.5535992483E+01
H3	6.2569076318E+01	3.7837464586E+01	9.5155111353E-01	2.5148384648E-02	9.5542159516E+01
H4	6.2514296949E+01	3.7810701393E+01	9.5149593071E-01	2.5164725743E-02	9.5536662933E+01
H5	6.2403607767E+01	3.7792632365E+01	9.5146036515E-01	2.5175816174E-02	9.5533049998E+01
Total	3.8784563522E+02	2.2263550952E+02	9.7828935532E+00	4.3941299277E-02	9.7828961350E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
C1	H2	-4.0504904911E-03		
C1	H3	-4.0504854911E-03		
C1	H4	-4.0509456911E-03		
C1	H5	-4.0505087611E-03		
C1		-1.6202430434E-02	-1.6202137200E-02	
H2	C1	4.0507837256E-03		
H2		4.0507837256E-03	4.0510769600E-03	
H3	C1	4.0507787256E-03		

H3		4.0507787256E-03	4.0510719600E-03
H4	C1	4.0512389256E-03	
H4		4.0512389256E-03	4.0515321600E-03
H5	C1	4.0508019956E-03	
H5		4.0508019956E-03	4.0510952300E-03

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	2.4521621075E-05	-3.2692966788E-07	2.4194691407E-05
H2	-8.8725798631E-02	1.7538312302E-03	-8.6971967401E-02
H3	8.8725690382E-02	-1.7538290654E-03	8.6971861317E-02
H4	8.8725340026E-02	-1.7540283140E-03	8.6971311712E-02
H5	-8.8725144626E-02	1.7538391404E-03	-8.6971305486E-02

Total	2.4608772075E-05	-5.1393849742E-07	2.4094833578E-05

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	-1.0822466946E-05	3.3449871086E-07	-1.0487968235E-05
H2	-8.8725580703E-02	1.7538312286E-03	-8.6971749474E-02
H3	8.8725279909E-02	-1.7538290638E-03	8.6971450845E-02
H4	-8.8725469644E-02	1.7540283124E-03	-8.6971441332E-02
H5	8.8725892363E-02	-1.7538391388E-03	8.6972053224E-02

Total	-1.0700541946E-05	5.2583714985E-07	-1.0174704796E-05

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	1.3733328879E-05	-3.6215599329E-07	1.3371172886E-05
H2	-8.8725223862E-02	1.7538312309E-03	-8.6971392631E-02
H3	-8.8725306747E-02	1.7538290661E-03	-8.6971477681E-02
H4	8.8726062609E-02	-1.7540283147E-03	8.6972034294E-02
H5	8.8725471301E-02	-1.7538391411E-03	8.6971632160E-02

Total	1.4736629879E-05	-5.6931482625E-07	1.4167315053E-05

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	3.0117104991E-05	5.9154827258E-07	2.9566346313E-05
H2	1.5367713351E-01	3.0377247980E-03	1.5063940871E-01
H3	1.5367694520E-01	3.0377210485E-03	1.5063922415E-01
H4	1.5367728886E-01	3.0380661572E-03	1.5063922271E-01
H5	1.5367707871E-01	3.0377384989E-03	1.5063934022E-01

Total	3.0614727194E-05	9.2992303912E-07	2.9745561663E-05

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	H2	3.0658336097E-03	
C1	H3	-3.0658298252E-03	
C1	H4	-3.0661781526E-03	

C1	H5	3.0658474384E-03
C1		-3.2692966788E-07
H2	C1	1.7538312302E-03
H2		1.7538312302E-03
H3	C1	-1.7538290654E-03
H3		-1.7538290654E-03
H4	C1	-1.7540283140E-03
H4		-1.7540283140E-03
H5	C1	1.7538391404E-03
H5		1.7538391404E-03

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	H2	3.0658336113E-03	
C1	H3	-3.0658298268E-03	
C1	H4	3.0661781542E-03	
C1	H5	-3.0658474400E-03	
C1		3.3449871086E-07	
H2	C1	1.7538312286E-03	
H2		1.7538312286E-03	
H3	C1	-1.7538290638E-03	
H3		-1.7538290638E-03	
H4	C1	1.7540283124E-03	
H4		1.7540283124E-03	
H5	C1	-1.7538391388E-03	
H5		-1.7538391388E-03	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	H2	3.0658336090E-03	
C1	H3	3.0658298245E-03	
C1	H4	-3.0661781519E-03	

C1	H5	-3.0658474377E-03
C1		-3.6215599329E-07
H2	C1	1.7538312309E-03
H2		1.7538312309E-03
H3	C1	1.7538290661E-03
H3		1.7538290661E-03
H4	C1	-1.7540283147E-03
H4		-1.7540283147E-03
H5	C1	-1.7538391411E-03
H5		-1.7538391411E-03

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	H2	5.3101795801E-03	
C1	H3	5.3101730251E-03	
C1	H4	5.3107763458E-03	
C1	H5	5.3102035320E-03	
C1		5.9154827258E-07	
H2	C1	3.0377247980E-03	
H2		3.0377247980E-03	
H3	C1	3.0377210485E-03	
H3		3.0377210485E-03	
H4	C1	3.0380661572E-03	
H4		3.0380661572E-03	
H5	C1	3.0377384989E-03	
H5		3.0377384989E-03	

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$Q_{XX}(A) = -[3\langle Rho * x * x \rangle(A) - \langle Rho * r * r \rangle(A)]$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	3.4661749338E-05	-1.6316458870E-04	-1.2452256492E-05	4.8487721352E-04	-1.4409786473E-04	-5.1953896287E-04
H2	2.0043208081E-07	2.3364597242E-01	2.3364549526E-01	-5.0117292517E-07	2.3364593936E-01	3.0074084414E-07
H3	4.6714928411E-07	2.3364493444E-01	-2.3364406199E-01	-5.2505145772E-07	-2.3364536888E-01	5.7902177204E-08
H4	-5.0490338492E-07	-2.3364498455E-01	2.3364519767E-01	1.9117563356E-08	-2.3364517599E-01	4.8578582121E-07
H5	-1.4844649650E-06	-2.3364692221E-01	-2.3364579855E-01	6.3991017715E-07	2.3364399452E-01	8.4455479509E-07

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$$Q\_EigVal\_n(A) = \text{nth Eigenvalue of } Q(A)$$

$$Q\_EigVal\_n\_X(A) = \text{X Component of the nth Eigenvector of } Q(A)$$

$$Q\_EigVal\_n\_Y(A) = \text{Y Component of the nth Eigenvector of } Q(A)$$

$$Q\_EigVal\_n\_Z(A) = \text{Z Component of the nth Eigenvector of } Q(A)$$

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
C1	1	-5.4202775502E-04	6.3337413278E-02	1.4854446635E-01	9.8687532829E-01
C1	2	-1.2377040510E-05	9.5354433196E-01	2.8281697429E-01	-1.0376784688E-01
C1	3	5.5440479552E-04	-2.9451923378E-01	9.4760176265E-01	-1.2373083835E-01
H2	1	-2.3364636209E-01	4.3824653496E-01	-8.1574300211E-01	3.7749613125E-01
H2	2	-2.3364524261E-01	-6.8891696230E-01	-3.5074289385E-02	7.2399116934E-01
H2	3	4.6729160469E-01	-5.7735032143E-01	-5.7735010932E-01	-5.7735037682E-01

H3	1	-2.3364584400E-01	2.7618020706E-01	-8.0351717668E-01	-5.2733731141E-01
H3	2	-2.3364373288E-01	-7.6836922612E-01	1.4500559263E-01	-6.2336354598E-01
H3	3	4.6728957687E-01	5.7735017587E-01	5.7735043508E-01	-5.7735019662E-01
H4	1	-2.3364531562E-01	-8.1613541896E-01	-4.2910589117E-01	3.8702856753E-01
H4	2	-2.3364492319E-01	2.4293592351E-02	-6.9464728970E-01	-7.1894016739E-01
H4	3	4.6729023881E-01	-5.7734980670E-01	5.7735022047E-01	-5.7735078040E-01
H5	1	-2.3364799683E-01	8.0755927704E-01	5.0811565104E-01	2.9944364953E-01
H5	2	-2.3364314669E-01	-1.2047652262E-01	6.3912812402E-01	-7.5960558751E-01
H5	3	4.6729114352E-01	-5.7735034560E-01	5.7735060947E-01	5.7734985249E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3755376780E+02	1.4977755237E+01	6.0162021372E+00	6.1947408202E+00	9.7085846754E+00
H2	2.8848356088E+00	1.2644321537E+00	9.9594892304E-01	1.1256823136E+00	1.7019718867E+00
H3	2.8848359120E+00	1.2644323823E+00	9.9594892804E-01	1.1256818299E+00	1.7019704356E+00
H4	2.8848353164E+00	1.2644318340E+00	9.9594846784E-01	1.1256815278E+00	1.7019701997E+00
H5	2.8848356366E+00	1.2644321867E+00	9.9594890477E-01	1.1256821873E+00	1.7019715623E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\text{Rho}/dx) + y^*(d\text{Rho}/dy) + z^*(d\text{Rho}/dz)$$

$$GR-2(A) = \langle \text{Dot}/(r*r) \rangle (A)$$

$$GR-1(A) = \langle \text{Dot}/r \rangle (A)$$

$$GR0(A) = \langle \text{Dot} \rangle (A)$$

$$GR+1(A) = \langle \text{Dot}*r \rangle (A)$$

$$GR+2(A) = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3602488380E+02	-2.7446922241E+01	-1.3760951610E+01	-1.7055788123E+01	-3.3667839891E+01
H2	-2.2250258103E+00	-1.8280850768E+00	-2.1685475789E+00	-3.4135660380E+00	-6.8084036966E+00
H3	-2.2250259316E+00	-1.8280847260E+00	-2.1685463117E+00	-3.4135632183E+00	-6.8083976652E+00
H4	-2.2250255450E+00	-1.8280844862E+00	-2.1685463384E+00	-3.4135631595E+00	-6.8083916333E+00
H5	-2.2250259084E+00	-1.8280850303E+00	-2.1685473404E+00	-3.4135657432E+00	-6.8084014498E+00

Atomic Electronic Spin Populations:

$N\_alpha(A)$ = Average number of Alpha electrons in Atom A

$N\_beta(A)$ = Average number of Beta electrons in Atom A

$N\_total(A) = N\_alpha(A) + N\_beta(A)$

$N\_spin(A) = N\_alpha(A) - N\_beta(A)$

Atom A	$N\_alpha(A)$	$N\_beta(A)$	$N\_total(A)$	$N\_spin(A)$
C1	3.0081010686E+00	3.0081010686E+00	6.0162021372E+00	0.0000000000E+00
H2	4.9797446152E-01	4.9797446152E-01	9.9594892304E-01	0.0000000000E+00
H3	4.9797446402E-01	4.9797446402E-01	9.9594892804E-01	0.0000000000E+00
H4	4.9797423392E-01	4.9797423392E-01	9.9594846784E-01	0.0000000000E+00
H5	4.9797445238E-01	4.9797445238E-01	9.9594890477E-01	0.0000000000E+00

Total 4.9999986804E+00 4.9999986804E+00 9.999973609E+00 0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

CMe3plus

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\cme3\Cme3_plane_mp2.wfx

Sum File: D:\calc\ellipticity\cme3\Cme3_plane_mp2.sum

Wfx Title: Cme3_plane_mp2

Total memory allocated for AIMSum = 1.019 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	31.9999999912
Number of Alpha electrons (from MO Occs)	=	15.9999999956
Number of Beta electrons (from MO Occs)	=	15.9999999956
Number of electron pairs ($N*(N-1)/2$)	=	495.9999997228
Number of electron pairs (from Muller 2EDM)	=	495.9999647912
Number of electron pairs (from Muller 2EDM, no SOSI)	=	496.3631717587

Nuclear Charges and Cartesian Coordinates:

Atom Charge X Y Z

C1	6.0	0.0000000000E+00	0.0000000000E+00	1.3023286200E-01
C2	6.0	0.0000000000E+00	2.7670837100E+00	2.7521380400E-02
H3	1.0	1.7164990400E+00	3.6056692600E+00	8.0021432900E-01
H4	1.0	0.0000000000E+00	3.1865760700E+00	-2.0260226700E+00
H5	1.0	-1.7164990400E+00	3.6056692600E+00	8.0021432900E-01
C6	6.0	-2.3963647900E+00	-1.3835418500E+00	2.7521380400E-02
H7	1.0	-2.7596558300E+00	-1.5932880400E+00	-2.0260226700E+00
H8	1.0	-2.2643516500E+00	-3.2893664000E+00	8.0021432900E-01
H9	1.0	-3.9808506900E+00	-3.1630285600E-01	8.0021432900E-01
C10	6.0	2.3963647900E+00	-1.3835418500E+00	2.7521380400E-02
H11	1.0	2.2643516500E+00	-3.2893664000E+00	8.0021432900E-01
H12	1.0	2.7596558300E+00	-1.5932880400E+00	-2.0260226700E+00
H13	1.0	3.9808506900E+00	-3.1630285600E-01	8.0021432900E-01

Some Atomic Properties:

 $q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

C1	5.1745338400E-02	-1.7156338871E-04	3.7941475329E+01	-3.7984154002E+01	4.2741973219E-02
C2	-4.3447536700E-02	-2.5320645235E-04	3.7953578517E+01	-3.7996270804E+01	2.4082655575E-01
H3	1.0884627666E-01	4.1040628132E-05	5.7343189399E-01	-5.7407692194E-01	1.3124829771E-01
H4	1.4166375268E-01	4.1469067487E-05	5.4556727713E-01	-5.4618096142E-01	1.2872159354E-01
H5	1.0884766939E-01	4.2313572352E-05	5.7343215478E-01	-5.7407718302E-01	1.3124815629E-01

C6 -4.3420662800E-02 -2.4416888653E-04 3.7953583273E+01 -3.7996275565E+01 2.4086562736E-01

H7 1.4166246947E-01 4.1401048476E-05 5.4556776184E-01 -5.4618144667E-01 1.2872102303E-01

H8 1.0884706036E-01 4.2301696366E-05 5.7343238847E-01 -5.7407741698E-01 1.3124859650E-01

H9 1.0885411559E-01 4.7734262209E-05 5.7343250981E-01 -5.7407753845E-01 1.3125058094E-01

C10 -4.3489808400E-02 -3.1012073295E-04 3.7953566811E+01 -3.7996259085E+01 2.4085017460E-01

H11 1.0884920179E-01 4.3882811587E-05 5.7343229489E-01 -5.7407732329E-01 1.3124948611E-01

H12 1.4166315944E-01 4.0910573844E-05 5.4556706813E-01 -5.4618075218E-01 1.2872130520E-01

H13 1.0885314011E-01 4.6975992234E-05 5.7343241019E-01 -5.7407743872E-01 1.3125099170E-01

Total 9.9947417599E-01 -5.9102980785E-04 1.5687949969E+02 -1.5705596644E+02

Molecular charge q(Mol) from the wfx file: 1.0000000088E+00

Molecular energy E(Mol) from the wfx file: -1.5705611371E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 2.0011248554E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 2.0011248524E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	127	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
C2	91	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H3	22	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	20	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H5	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C6	67	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H7	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H9	18	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C10	68	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H11	17	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H12	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H13	16	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 511

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 1.05723090986645E-18 1.45901005931620E-13 1.30232296138826E-01

Type = (3,-3) NACP C1

Rho = 1.1990152420E+02 Rho at Nucleus = 1.1990152417E+02

GradRho = 1.6116543583E-16 1.1993986533E-17 -8.4544815593E-11

HessRho_EigVals = -1.8181026477E+05 -1.8180109589E+05 -1.8180109589E+05

HessRho_EigVec1 = 6.2787481161E-14 -1.7643815209E-09 1.0000000000E+00

HessRho_EigVec2 = 5.6998143970E-06 9.9999999998E-01 1.7643815205E-09

HessRho_EigVec3 = 9.9999999998E-01 -5.6998143970E-06 -7.2844128354E-14

DelSqRho = -5.4541245654E+05

Bond Ellipticity = NA

V = -1.3636657887E+05

G = 6.7323664239E+00

K = 1.3635984650E+05

L = 1.3635311414E+05

Vnuc = 1.0603316207E+07

Ven = -1.2713537747E+09

Vrep = 1.2712174082E+09

DelSqV = 4.6214093552E+09

DelSqVen = 5.7831818527E+12

DelSqVrep = -5.7785604433E+12

DelSqG = 2.0677259749E+08

DelSqK = -4.8281819527E+09

Stress_EigVals = -4.5456362951E+04 -4.5456362951E+04 -4.5453852967E+04

Stress_EigVec1 = 9.9999999997E-01 -7.4156622149E-06 -7.4368869846E-14

Stress_EigVec2 = 7.4156622149E-06 9.9999999997E-01 7.6786039910E-10

Stress_EigVec3 = 6.8674676496E-14 -7.6786039963E-10 1.0000000000E+00

-DivStress = -1.4453080946E-09 -2.0146029712E-04 8.5004281320E+02

CP# 2 Coords = -6.12090573376850E-18 2.76708116764996E+00 2.75203427920283E-02

Type = (3,-3) NACP C2

Rho = 1.1941246302E+02 Rho at Nucleus = 1.1941246234E+02

GradRho = 1.6545941592E-17 -8.7208895660E-09 -3.5523749498E-09

HessRho_EigVals = -1.8103599508E+05 -1.8103535156E+05 -1.8103454142E+05

HessRho_EigVec1 = 3.2674744476E-14 9.8018340785E-01 -1.9809211741E-01

HessRho_EigVec2 = -2.1937698095E-13 1.9809211741E-01 9.8018340785E-01

HessRho_EigVec3 = 1.0000000000E+00 1.1429608275E-14 2.2150228611E-13

DelSqRho = -5.4310588806E+05

Bond Ellipticity = NA

V = -1.3579188205E+05
G = 7.7050150646E+00
K = 1.3578417703E+05
L = 1.3577647202E+05
Vnuc = 2.1850530866E+06
Ven = -2.6092257090E+08
Vrep = 2.6078677902E+08
DelSqV = 4.6019515859E+09
DelSqVen = 1.1867152384E+12
DelSqVrep = -1.1821132868E+12
DelSqG = 2.0586953424E+08
DelSqK = -4.8078211201E+09
Stress_EigVals = -4.5264164242E+04 -4.5263934803E+04 -4.5263783000E+04
Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 8.7175378597E-14
Stress_EigVec2 = -8.3429223268E-14 2.8999761023E-01 9.5702736955E-01
Stress_EigVec3 = 2.5280651464E-14 9.5702736955E-01 -2.8999761023E-01
-DivStress = 9.3674881602E-09 3.8067103892E+03 1.5533843434E+03

CP# 3 Coords = 1.69212006185635E+00 3.59269776992133E+00 7.89050471448927E-01

Type = (3,-3) NACP H3

Rho = 4.1492029467E-01 Rho at Nucleus = 4.1144268376E-01

GradRho = -7.4940054162E-16 8.6085652495E-16 -4.1459891076E-16

HessRho_EigVals = -8.2718940226E+00 -8.2668397414E+00 -7.5801136975E+00

HessRho_EigVec1 = -5.2308765821E-01 8.2837517229E-01 2.0043421803E-01

HessRho_EigVec2 = -2.2461040429E-01 -3.6084924320E-01 9.0517290611E-01

HessRho_EigVec3 = 8.2214929794E-01 4.2846516499E-01 3.7481746795E-01

DelSqRho = -2.4118847462E+01

Bond Ellipticity = NA

V = -6.0484925686E+00

G = 9.3903516127E-03

K = 6.0391022170E+00

L = 6.0297118654E+00

Vnuc = 4.1656992063E+01
Ven = -1.7284331422E+01
Vrep = 1.1235838853E+01
DelSqV = 1.5544182726E+03
DelSqVen = 1.0047186373E+03
DelSqVrep = 5.4969963532E+02
DelSqG = 1.1798736995E+02
DelSqK = -1.6724056426E+03
Stress_EigVals = -2.0740276427E+00 -2.0735956446E+00 -1.9008692814E+00
Stress_EigVec1 = -5.6889642233E-01 6.5200160650E-01 5.0124920526E-01
Stress_EigVec2 = -2.9623941877E-02 -6.2533937709E-01 7.7979041128E-01
Stress_EigVec3 = 8.2187546668E-01 4.2877099782E-01 3.7506819207E-01
-DivStress = 1.2322469718E+01 6.5525028748E+00 5.6428054055E+00

CP# 4 Coords = -2.24297774648436E-15 3.17929682707528E+00 -1.99805083021781E+00

Type = (3,-3) NACP H4

Rho = 3.9098441885E-01 Rho at Nucleus = 3.8788522660E-01

GradRho = 2.2086384100E-19 -4.1910919180E-15 1.8724605200E-14

HessRho_EigVals = -7.8046929490E+00 -7.8030127143E+00 -7.1889760340E+00

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 9.7164514592E-01 2.3644388427E-01

HessRho_EigVec3 = 0.0000000000E+00 -2.3644388427E-01 9.7164514592E-01

DelSqRho = -2.2796681697E+01

Bond Ellipticity = NA

V = -5.7189489660E+00

G = 9.8892708136E-03

K = 5.7090596952E+00

L = 5.6991704243E+00

Vnuc = 4.2806721840E+01

Ven = -1.6736761261E+01

Vrep = 1.1017812295E+01

DelSqV = 1.4723017017E+03

DelSqVen = 9.7585121230E+02

DelSqVrep = 4.9645048937E+02

DelSqG = 1.1188206944E+02

DelSqK = -1.5841837711E+03

Stress_EigVals = -1.9582820293E+00 -1.9576130184E+00 -1.8030539182E+00

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 9.7196575312E-01 2.3512246760E-01

Stress_EigVec3 = 0.0000000000E+00 -2.3512246760E-01 9.7196575312E-01

-DivStress = 1.1966118929E-12 3.4698953367E+00 -1.3367594124E+01

CP# 5 Coords = -1.69212006185634E+00 3.59269776992133E+00 7.89050471448923E-01

Type = (3,-3) NACP H5

Rho = 4.1492029467E-01 Rho at Nucleus = 4.1144268376E-01

GradRho = 1.5196177650E-15 9.5019478397E-16 -3.5388358910E-16

HessRho_EigVals = -8.2718940226E+00 -8.2668397414E+00 -7.5801136975E+00

HessRho_EigVec1 = 5.2308765821E-01 8.2837517229E-01 2.0043421803E-01

HessRho_EigVec2 = 2.2461040429E-01 -3.6084924321E-01 9.0517290611E-01

HessRho_EigVec3 = 8.2214929794E-01 -4.2846516499E-01 -3.7481746795E-01

DelSqRho = -2.4118847462E+01

Bond Ellipticity = NA

V = -6.0484925686E+00

G = 9.3903516127E-03

K = 6.0391022170E+00

L = 6.0297118654E+00

Vnuc = 4.1656992063E+01

Ven = -1.7284331422E+01

Vrep = 1.1235838853E+01

DelSqV = 1.5544182726E+03

DelSqVen = 1.0047186373E+03

DelSqVrep = 5.4969963532E+02

DelSqG = 1.1798736995E+02

DelSqK = -1.6724056426E+03

Stress_EigVals = -2.0740276427E+00 -2.0735956446E+00 -1.9008692814E+00
Stress_EigVec1 = 5.6889642233E-01 6.5200160651E-01 5.0124920526E-01
Stress_EigVec2 = 2.9623941881E-02 -6.2533937709E-01 7.7979041128E-01
Stress_EigVec3 = 8.2187546668E-01 -4.2877099782E-01 -3.7506819207E-01
-DivStress = -1.2322469718E+01 6.5525028748E+00 5.6428054055E+00

CP# 6 Coords = -2.39636258826202E+00 -1.38354057882234E+00 2.75203427938538E-02

Type = (3,-3) NACP C6

Rho = 1.1941246267E+02 Rho at Nucleus = 1.1941246198E+02

GradRho = 7.5667455079E-09 4.3417404116E-09 -3.5519400199E-09

HessRho_EigVals = -1.8103599439E+05 -1.8103535087E+05 -1.8103454072E+05

HessRho_EigVec1 = 8.4886380306E-01 4.9009168308E-01 1.9809186258E-01

HessRho_EigVec2 = -1.7155257396E-01 -9.9045950907E-02 9.8018345935E-01

HessRho_EigVec3 = -4.9999995822E-01 8.6602542791E-01 3.2857630950E-08

DelSqRho = -5.4310588599E+05

Bond Ellipticity = NA

V = -1.3579188153E+05

G = 7.7050148191E+00

K = 1.3578417651E+05

L = 1.3577647150E+05

Vnuc = 2.1850537736E+06

Ven = -2.6092265217E+08

Vrep = 2.6078686029E+08

DelSqV = 4.6019515680E+09

DelSqVen = 1.1867155988E+12

DelSqVrep = -1.1821136473E+12

DelSqG = 2.0586953328E+08

DelSqK = -4.8078211013E+09

Stress_EigVals = -4.5264164069E+04 -4.5263934630E+04 -4.5263782827E+04

Stress_EigVec1 = -5.0000018881E-01 8.6602529478E-01 3.5949222068E-07

Stress_EigVec2 = -2.5114495847E-01 -1.4499907965E-01 9.5702741692E-01

Stress_EigVec3 = 8.2881000297E-01 4.7851379887E-01 2.8999745390E-01

-DivStress = -3.2967052965E+03 -1.9033591407E+03 1.5533815961E+03

CP# 7 Coords = -2.75335182220163E+00 -1.58964841587023E+00 -1.99805083363676E+00

Type = (3,-3) NACP H7

Rho = 3.9098441165E-01 Rho at Nucleus = 3.8788522013E-01

GradRho = 2.5951463201E-15 2.5689086275E-15 1.8565010640E-14

HessRho_EigVals = -7.8046928700E+00 -7.8030126390E+00 -7.1889760205E+00

HessRho_EigVec1 = -4.9999972485E-01 8.6602556264E-01 -1.3271424718E-07

HessRho_EigVec2 = 8.4146954573E-01 4.8582227605E-01 -2.3644390394E-01

HessRho_EigVec3 = 2.0476640046E-01 1.1822199859E-01 9.7164514114E-01

DelSqRho = -2.2796681530E+01

Bond Ellipticity = NA

V = -5.7189489204E+00

G = 9.8892689869E-03

K = 5.7090596514E+00

L = 5.6991703824E+00

Vnuc = 4.2806725777E+01

Ven = -1.6736762492E+01

Vrep = 1.1017813572E+01

DelSqV = 1.4723017019E+03

DelSqVen = 9.7585129485E+02

DelSqVrep = 4.9645040710E+02

DelSqG = 1.1188206981E+02

DelSqK = -1.5841837718E+03

Stress_EigVals = -1.9582820093E+00 -1.9576129986E+00 -1.8030539124E+00

Stress_EigVec1 = -5.0000002237E-01 8.6602539087E-01 -5.4846435927E-08

Stress_EigVec2 = 8.4174702430E-01 4.8598288516E-01 -2.3512248386E-01

Stress_EigVec3 = 2.0362201434E-01 1.1756129336E-01 9.7196574918E-01

-DivStress = -3.0050167914E+00 -1.7349489139E+00 -1.3367592458E+01

CP# 8 Coords = -2.26530749981002E+00 -3.26176784031314E+00 7.89050471551676E-01

Type = (3,-3) NACP H8

Rho = 4.1492029448E-01 Rho at Nucleus = 4.1144268366E-01
GradRho = -1.7694179455E-15 2.2729214344E-14 -9.3328123008E-15
HessRho_EigVals = -8.2718937253E+00 -8.2668394508E+00 -7.5801133942E+00
HessRho_EigVec1 = 9.7893766559E-01 -3.8819821422E-02 -2.0043469847E-01
HessRho_EigVec2 = 2.0019993275E-01 3.7494290067E-01 9.0517280569E-01
HessRho_EigVec3 = -4.0012920565E-02 9.2623476652E-01 -3.7481745355E-01
DelSqRho = -2.4118846570E+01
Bond Ellipticity = NA
V = -6.0484923439E+00
G = 9.3903506791E-03
K = 6.0391019933E+00
L = 6.0297116426E+00
Vnuc = 4.1656991817E+01
Ven = -1.7284331312E+01
Vrep = 1.1235838968E+01
DelSqV = 1.5544182075E+03
DelSqVen = 1.0047185942E+03
DelSqVrep = 5.4969961332E+02
DelSqG = 1.1798736143E+02
DelSqK = -1.6724055690E+03
Stress_EigVals = -2.0740275689E+00 -2.0735955709E+00 -1.9008692042E+00
Stress_EigVec1 = 8.4909655450E-01 -1.6667897931E-01 -5.0125159251E-01
Stress_EigVec2 = 5.2675041277E-01 3.3832425617E-01 7.7978888190E-01
Stress_EigVec3 = -3.9611157279E-02 9.2615053611E-01 -3.7506818137E-01
-DivStress = 4.8660121714E-01 -1.3947822816E+01 5.6428051225E+00

CP# 9 Coords = -3.95742756190818E+00 -3.30929924650125E-01 7.89050470996460E-01

Type = (3,-3) NACP H9

Rho = 4.1492027843E-01 Rho at Nucleus = 4.1144266802E-01
GradRho = -1.4311468677E-16 -2.1684043450E-16 1.6046192153E-17
HessRho_EigVals = -8.2718933623E+00 -8.2668390813E+00 -7.5801131017E+00
HessRho_EigVec1 = 4.5585014102E-01 8.6719478952E-01 -2.0043414370E-01

HessRho_EigVec2 = 4.2480978408E-01 -1.4093766743E-02 9.0517291889E-01

HessRho_EigVec3 = 7.8213636681E-01 -4.9776958803E-01 -3.7481747685E-01

DelSqRho = -2.4118845545E+01

Bond Ellipticity = NA

V = -6.0484920921E+00

G = 9.3903528789E-03

K = 6.0391017392E+00

L = 6.0297113863E+00

Vnuc = 4.1656993086E+01

Ven = -1.7284331170E+01

Vrep = 1.1235839078E+01

DelSqV = 1.5544181459E+03

DelSqVen = 1.0047185821E+03

DelSqVrep = 5.4969956377E+02

DelSqG = 1.1798735606E+02

DelSqK = -1.6724055020E+03

Stress_EigVals = -2.0740274771E+00 -2.0735954803E+00 -1.9008691347E+00

Stress_EigVec1 = -2.8020160078E-01 -8.1867948854E-01 5.0124939697E-01

Stress_EigVec2 = 5.5637183340E-01 2.8701480177E-01 7.7979028370E-01

Stress_EigVec3 = 7.8226430694E-01 -4.9737953175E-01 -3.7506820111E-01

-DivStress = -1.1835867386E+01 7.3953194360E+00 5.6428051621E+00

CP# 10 Coords = 2.39636258826202E+00 -1.38354057882234E+00 2.75203427938538E-02

Type = (3,-3) NACP C10

Rho = 1.1941246267E+02 Rho at Nucleus = 1.1941246198E+02

GradRho = -7.5675572475E-09 4.3412743400E-09 -3.5520035802E-09

HessRho_EigVals = -1.8103599439E+05 -1.8103535087E+05 -1.8103454072E+05

HessRho_EigVec1 = 8.4886380308E-01 -4.9009168307E-01 -1.9809186255E-01

HessRho_EigVec2 = 1.7155257392E-01 -9.9045950887E-02 9.8018345935E-01

HessRho_EigVec3 = 4.9999995820E-01 8.6602542792E-01 3.2861299236E-08

DelSqRho = -5.4310588599E+05

Bond Ellipticity = NA

V = -1.3579188153E+05
G = 7.7050148191E+00
K = 1.3578417651E+05
L = 1.3577647150E+05
Vnuc = 2.1850537736E+06
Ven = -2.6092265217E+08
Vrep = 2.6078686029E+08
DelSqV = 4.6019515680E+09
DelSqVen = 1.1867155988E+12
DelSqVrep = -1.1821136473E+12
DelSqG = 2.0586953328E+08
DelSqK = -4.8078211013E+09
Stress_EigVals = -4.5264164069E+04 -4.5263934630E+04 -4.5263782827E+04
Stress_EigVec1 = 5.0000018883E-01 8.6602529476E-01 3.5949723511E-07
Stress_EigVec2 = 2.5114495848E-01 -1.4499907967E-01 9.5702741691E-01
Stress_EigVec3 = 8.2881000296E-01 -4.7851379889E-01 -2.8999745391E-01
-DivStress = 3.2967052965E+03 -1.9033591407E+03 1.5533815961E+03

CP# 11 Coords = 2.26530749981002E+00 -3.26176784031314E+00 7.89050471551675E-01

Type = (3,-3) NACP H11

Rho = 4.1492029448E-01 Rho at Nucleus = 4.1144268366E-01

GradRho = 2.1701390684E-15 2.3532824994E-14 -9.6068986100E-15

HessRho_EigVals = -8.2718937253E+00 -8.2668394508E+00 -7.5801133942E+00

HessRho_EigVec1 = 9.7893766559E-01 3.8819821420E-02 2.0043469846E-01

HessRho_EigVec2 = -2.0019993274E-01 3.7494290067E-01 9.0517280569E-01

HessRho_EigVec3 = 4.0012920565E-02 9.2623476652E-01 -3.7481745355E-01

DelSqRho = -2.4118846570E+01

Bond Ellipticity = NA

V = -6.0484923439E+00

G = 9.3903506791E-03

K = 6.0391019932E+00

L = 6.0297116426E+00

Vnuc = 4.1656991817E+01
Ven = -1.7284331312E+01
Vrep = 1.1235838968E+01
DelSqV = 1.5544182075E+03
DelSqVen = 1.0047185942E+03
DelSqVrep = 5.4969961332E+02
DelSqG = 1.1798736143E+02
DelSqK = -1.6724055690E+03
Stress_EigVals = -2.0740275689E+00 -2.0735955709E+00 -1.9008692042E+00
Stress_EigVec1 = 8.4909655449E-01 1.6667897931E-01 5.0125159252E-01
Stress_EigVec2 = -5.2675041278E-01 3.3832425617E-01 7.7978888189E-01
Stress_EigVec3 = 3.9611157279E-02 9.2615053611E-01 -3.7506818137E-01
-DivStress = -4.8660121715E-01 -1.3947822816E+01 5.6428051225E+00

CP# 12 Coords = 2.75335182220163E+00 -1.58964841587023E+00 -1.99805083363677E+00

Type = (3,-3) NACP H12

Rho = 3.9098441165E-01 Rho at Nucleus = 3.8788522013E-01

GradRho = -4.3316045195E-15 3.0762339290E-15 1.8087961684E-14

HessRho_EigVals = -7.8046928700E+00 -7.8030126390E+00 -7.1889760205E+00

HessRho_EigVec1 = 4.9999972485E-01 8.6602556264E-01 -1.3271452784E-07

HessRho_EigVec2 = 8.4146954573E-01 -4.8582227604E-01 2.3644390394E-01

HessRho_EigVec3 = -2.0476640046E-01 1.1822199859E-01 9.7164514114E-01

DelSqRho = -2.2796681530E+01

Bond Ellipticity = NA

V = -5.7189489204E+00

G = 9.8892689869E-03

K = 5.7090596514E+00

L = 5.6991703824E+00

Vnuc = 4.2806725777E+01

Ven = -1.6736762492E+01

Vrep = 1.1017813572E+01

DelSqV = 1.4723017019E+03

DelSqVen = 9.7585129485E+02
DelSqVrep = 4.9645040710E+02
DelSqG = 1.1188206981E+02
DelSqK = -1.5841837718E+03
Stress_EigVals = -1.9582820093E+00 -1.9576129986E+00 -1.8030539124E+00
Stress_EigVec1 = 5.0000002237E-01 8.6602539087E-01 -5.4845342739E-08
Stress_EigVec2 = 8.4174702429E-01 -4.8598288516E-01 2.3512248386E-01
Stress_EigVec3 = -2.0362201434E-01 1.1756129336E-01 9.7196574918E-01
-DivStress = 3.0050167914E+00 -1.7349489139E+00 -1.3367592458E+01

CP# 13 Coords = 3.95742756190819E+00 -3.30929924650124E-01 7.89050470996462E-01

Type = (3,-3) NACP H13

Rho = 4.1492027843E-01 Rho at Nucleus = 4.1144266802E-01

GradRho = 1.4224732503E-16 -2.7321894747E-16 3.0444397003E-16

HessRho_EigVals = -8.2718933623E+00 -8.2668390813E+00 -7.5801131017E+00

HessRho_EigVec1 = -4.5585014102E-01 8.6719478952E-01 -2.0043414370E-01

HessRho_EigVec2 = -4.2480978408E-01 -1.4093766744E-02 9.0517291889E-01

HessRho_EigVec3 = 7.8213636681E-01 4.9776958803E-01 3.7481747685E-01

DelSqRho = -2.4118845545E+01

Bond Ellipticity = NA

V = -6.0484920921E+00

G = 9.3903528789E-03

K = 6.0391017392E+00

L = 6.0297113863E+00

Vnuc = 4.1656993086E+01

Ven = -1.7284331170E+01

Vrep = 1.1235839078E+01

DelSqV = 1.5544181459E+03

DelSqVen = 1.0047185821E+03

DelSqVrep = 5.4969956377E+02

DelSqG = 1.1798735606E+02

DelSqK = -1.6724055020E+03

Stress_EigVals = -2.0740274771E+00 -2.0735954803E+00 -1.9008691347E+00
Stress_EigVec1 = 2.8020160078E-01 -8.1867948854E-01 5.0124939696E-01
Stress_EigVec2 = -5.5637183340E-01 2.8701480177E-01 7.7979028370E-01
Stress_EigVec3 = 7.8226430694E-01 4.9737953175E-01 3.7506820111E-01
-DivStress = 1.1835867386E+01 7.3953194360E+00 5.6428051621E+00

CP# 14 Coords = 1.51877410226325E-15 1.51862042799155E+00 9.22611452462579E-02

Type = (3,-1) BCP C2 C1

Rho = 2.7570817785E-01

GradRho = -3.5557384335E-18 -7.5894152074E-17 4.1633363423E-17

HessRho_EigVals = -5.3289554075E-01 -5.0489887006E-01 2.9348271623E-01

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 3.8725722795E-02 9.9924987786E-01

HessRho_EigVec3 = 0.0000000000E+00 9.9924987786E-01 -3.8725722795E-02

DelSqRho = -7.4431169458E-01

Bond Ellipticity = 5.5450056147E-02

V = -3.6369013927E-01

G = 8.8806107813E-02

K = 2.7488403146E-01

L = 1.8607792365E-01

Vnuc = 1.4275904649E+01

Ven = -3.9359836579E+00

Vrep = 3.5722935186E+00

DelSqV = -1.3322712980E+00

DelSqVen = 1.0625722781E+01

DelSqVrep = -1.1957994079E+01

DelSqG = 1.2804249503E+00

DelSqK = 5.1846347716E-02

Stress_EigVals = -2.0615288418E-01 -2.0501277397E-01 4.7475518879E-02

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 2.9923870111E-02 9.9955218073E-01

Stress_EigVec3 = 0.0000000000E+00 9.9955218073E-01 -2.9923870111E-02

-DivStress = 4.0677739239E-17 2.2739914333E-01 -1.9219413936E-02
BPL = 2.7694364457E+00 = 1.2501895851E+00 + 1.5192468606E+00
GBL_I = 2.7689868063E+00
GBL_II = 2.7689893294E+00
GBL_III = 2.7692332921E+00 = 1.2501382283E+00 + 1.5190950637E+00
GBL_IV = 2.7692357914E+00 = 1.2501407136E+00 + 1.5190950779E+00

CP# 15 Coords = 1.12844655380292E+00 3.30400213709645E+00 5.32700519739014E-01

Type = (3,-1) BCP H3 C2

Rho = 2.7579682329E-01

GradRho = 2.7755575616E-17 1.0408340856E-16 -4.1633363423E-17

HessRho_EigVals = -7.3335338301E-01 -7.1829540633E-01 5.0622786834E-01

HessRho_EigVec1 = -5.1569425499E-01 8.2990767275E-01 2.1286777606E-01

HessRho_EigVec2 = 2.2307322627E-01 3.6994235484E-01 -9.0187637169E-01

HessRho_EigVec3 = 8.2722292708E-01 4.1760736202E-01 3.7590732914E-01

DelSqRho = -9.4542092099E-01

Bond Ellipticity = 2.0963487374E-02

V = -3.2040777616E-01

G = 4.2026272959E-02

K = 2.7838150321E-01

L = 2.3635523025E-01

Vnuc = 1.1496404046E+01

Ven = -3.1706717151E+00

Vrep = 2.8502639389E+00

DelSqV = -2.9299686211E+00

DelSqVen = 1.0868940901E+01

DelSqVrep = -1.3798909522E+01

DelSqG = 1.6013820158E+00

DelSqK = 1.3285866053E+00

Stress_EigVals = -2.1616047997E-01 -2.1469444547E-01 1.1044714928E-01

Stress_EigVec1 = -4.9988360861E-01 2.4824045660E-01 8.2975481532E-01

Stress_EigVec2 = 2.5195068963E-01 -8.7493039273E-01 4.1354281261E-01

Stress_EigVec3 = 8.2863576307E-01 4.1578057143E-01 3.7481900776E-01

-DivStress = -3.1074915529E-02 -1.2575334383E-02 -1.4317997061E-02

BPL = 2.0313726131E+00 = 6.8322383249E-01 + 1.3481487806E+00

GBL_I = 2.0309705105E+00

GBL_II = 2.0607399331E+00

GBL_III = 2.0311370008E+00 = 6.8321906431E-01 + 1.3479179364E+00

GBL_IV = 2.0609189316E+00 = 7.1300239671E-01 + 1.3479165349E+00

CP# 16 Coords = 1.55389193071111E-15 3.02256981899377E+00 -1.31495189608928E+00

Type = (3,-1) BCP C2 H4

Rho = 2.5464758727E-01

GradRho = 2.1279585217E-18 -1.5265566589E-16 -8.3266726847E-17

HessRho_EigVals = -6.3924165727E-01 -6.3862637546E-01 4.6381584915E-01

HessRho_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 9.7734812774E-01 2.1163798622E-01

HessRho_EigVec3 = 0.0000000000E+00 -2.1163798622E-01 9.7734812774E-01

DelSqRho = -8.1405218358E-01

Bond Ellipticity = 9.6344565545E-04

V = -2.9357825269E-01

G = 4.5032603398E-02

K = 2.4854564929E-01

L = 2.0351304590E-01

Vnuc = 1.1590557963E+01

Ven = -2.9515076205E+00

Vrep = 2.6579293678E+00

DelSqV = -2.4942311959E+00

DelSqVen = 9.4353190190E+00

DelSqVrep = -1.1929550215E+01

DelSqG = 1.4209175787E+00

DelSqK = 1.0733136172E+00

Stress_EigVals = -1.9775889747E-01 -1.9526741021E-01 9.9448054982E-02

Stress_EigVec1 = 1.0000000000E+00 0.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 9.7876932465E-01 2.0496489732E-01

Stress_EigVec3 = 0.0000000000E+00 -2.0496489732E-01 9.7876932465E-01

-DivStress = -1.2016635665E-15 -1.1291570389E-02 5.0288299757E-02

BPL = 2.0675574365E+00 = 1.3666887846E+00 + 7.0086865187E-01

GBL_I = 2.0670898207E+00

GBL_II = 2.0959525298E+00

GBL_III = 2.0674149992E+00 = 1.3665672918E+00 + 7.0084770733E-01

GBL_IV = 2.0963073071E+00 = 1.3665678358E+00 + 7.2973947124E-01

CP# 17 Coords = -1.12844655380293E+00 3.30400213709646E+00 5.32700519739016E-01

Type = (3,-1) BCP C2 H5

Rho = 2.7579682329E-01

GradRho = 2.4286128664E-17 -2.0643209364E-16 5.5511151231E-17

HessRho_EigVals = -7.3335338301E-01 -7.1829540633E-01 5.0622786834E-01

HessRho_EigVec1 = 5.1569425499E-01 8.2990767275E-01 2.1286777606E-01

HessRho_EigVec2 = -2.2307322627E-01 3.6994235484E-01 -9.0187637169E-01

HessRho_EigVec3 = 8.2722292708E-01 -4.1760736202E-01 -3.7590732914E-01

DelSqRho = -9.4542092099E-01

Bond Ellipticity = 2.0963487374E-02

V = -3.2040777616E-01

G = 4.2026272959E-02

K = 2.7838150321E-01

L = 2.3635523025E-01

Vnuc = 1.1496404046E+01

Ven = -3.1706717151E+00

Vrep = 2.8502639389E+00

DelSqV = -2.9299686211E+00

DelSqVen = 1.0868940901E+01

DelSqVrep = -1.3798909522E+01

DelSqG = 1.6013820158E+00

DelSqK = 1.3285866053E+00

Stress_EigVals = -2.1616047997E-01 -2.1469444547E-01 1.1044714928E-01

Stress_EigVec1 = 4.9988360861E-01 2.4824045660E-01 8.2975481532E-01

Stress_EigVec2 = -2.5195068963E-01 -8.7493039273E-01 4.1354281261E-01

Stress_EigVec3 = 8.2863576307E-01 -4.1578057143E-01 -3.7481900776E-01

-DivStress = 3.1074915529E-02 -1.2575334383E-02 -1.4317997061E-02

BPL = 2.0313726131E+00 = 1.3481487806E+00 + 6.8322383249E-01

GBL_I = 2.0309705105E+00

GBL_II = 2.0607399331E+00

GBL_III = 2.0311370008E+00 = 1.3479179364E+00 + 6.8321906431E-01

GBL_IV = 2.0609189316E+00 = 1.3479165349E+00 + 7.1300239671E-01

CP# 18 Coords = -1.31516381686619E+00 -7.59310183841452E-01 9.22611550110862E-02

Type = (3,-1) BCP C1 C6

Rho = 2.7570817794E-01

GradRho = -9.0639301620E-17 -2.0816681712E-16 4.1633363423E-17

HessRho_EigVals = -5.3289554098E-01 -5.0489887170E-01 2.9348273996E-01

HessRho_EigVec1 = -5.0000000259E-01 8.6602540229E-01 7.8858534815E-08

HessRho_EigVec2 = -3.3537429103E-02 -1.9362934844E-02 9.9924987746E-01

HessRho_EigVec3 = 8.6537577864E-01 4.9962493868E-01 3.8725733003E-02

DelSqRho = -7.4431167272E-01

Bond Ellipticity = 5.5450053154E-02

V = -3.6369012006E-01

G = 8.8806100939E-02

K = 2.7488401912E-01

L = 1.8607791818E-01

Vnuc = 1.4275904604E+01

Ven = -3.9359836467E+00

Vrep = 3.5722935267E+00

DelSqV = -1.3322713611E+00

DelSqVen = 1.0625722435E+01

DelSqVrep = -1.1957993796E+01

DelSqG = 1.2804247909E+00

DelSqK = 5.1846570180E-02

Stress_EigVals = -2.0615287779E-01 -2.0501276387E-01 4.7475521609E-02
Stress_EigVec1 = -5.0000002581E-01 8.6602538888E-01 6.8620133833E-07
Stress_EigVec2 = -2.5914497867E-02 -1.4962535351E-02 9.9955218040E-01
Stress_EigVec3 = 8.6563757601E-01 4.9977609821E-01 2.9923881155E-02
-DivStress = -1.9693337886E-01 -1.1369953905E-01 -1.9219408335E-02
BPL = 2.7694364458E+00 = 1.5192468000E+00 + 1.2501896458E+00
GBL_I = 2.7689868062E+00
GBL_II = 2.7689893293E+00
GBL_III = 2.7692332921E+00 = 1.5190950030E+00 + 1.2501382892E+00
GBL_IV = 2.7692357915E+00 = 1.5190950171E+00 + 1.2501407744E+00

CP# 19 Coords = -2.61762225330878E+00 -1.51128489283146E+00 -1.31495192669616E+00

Type = (3,-1) BCP C6 H7
Rho = 2.5464757830E-01
GradRho = 2.2443852332E-13 1.2964602265E-13 -6.4699547803E-13
HessRho_EigVals = -6.3924164960E-01 -6.3862637520E-01 4.6381592074E-01
HessRho_EigVec1 = -4.9999672196E-01 8.6602729635E-01 -8.2252040759E-07
HessRho_EigVec2 = 8.4641024004E-01 4.8867070721E-01 -2.1163800571E-01
HessRho_EigVec3 = 1.8328388795E-01 1.0581900529E-01 9.7734812351E-01
DelSqRho = -8.1405210406E-01
Bond Ellipticity = 9.6343407116E-04
V = -2.9357822797E-01
G = 4.5032600978E-02
K = 2.4854562699E-01
L = 2.0351302601E-01
Vnuc = 1.1590557906E+01
Ven = -2.9515075020E+00
Vrep = 2.6579292741E+00
DelSqV = -2.4942318143E+00
DelSqVen = 9.4353180509E+00
DelSqVrep = -1.1929549865E+01
DelSqG = 1.4209175836E+00

DelSqK = 1.0733142307E+00

Stress_EigVals = -1.9775889089E-01 -1.9526740530E-01 9.9448068222E-02

Stress_EigVec1 = -5.0000000705E-01 8.6602539971E-01 9.7400551691E-09

Stress_EigVec2 = 8.4763909272E-01 4.8938466986E-01 -2.0496490770E-01

Stress_EigVec3 = 1.7750482089E-01 1.0248244704E-01 9.7876932247E-01

-DivStress = 9.7787709187E-03 5.6457913436E-03 5.0288253244E-02

BPL = 2.0675574416E+00 = 1.3666888144E+00 + 7.0086862719E-01

GBL_I = 2.0670898250E+00

GBL_II = 2.0959525307E+00

GBL_III = 2.0674150039E+00 = 1.3665673212E+00 + 7.0084768265E-01

GBL_IV = 2.0963073085E+00 = 1.3665678652E+00 + 7.2973944325E-01

CP# 20 Coords = -2.29712648669961E+00 -2.62926444336550E+00 5.32700528975053E-01

Type = (3,-1) BCP C6 H8

Rho = 2.7579682885E-01

GradRho = 1.5612511284E-16 3.1225022568E-17 -1.2836953722E-16

HessRho_EigVals = -7.3335338853E-01 -7.1829542143E-01 5.0622784788E-01

HessRho_EigVec1 = 9.7656822325E-01 -3.1650572062E-02 -2.1286790886E-01

HessRho_EigVec2 = 2.0884301907E-01 3.7815823734E-01 9.0187634458E-01

HessRho_EigVec3 = -5.1952850968E-02 9.2519975617E-01 -3.7590731898E-01

DelSqRho = -9.4542096208E-01

Bond Ellipticity = 2.0963473596E-02

V = -3.2040778575E-01

G = 4.2026272616E-02

K = 2.7838151314E-01

L = 2.3635524052E-01

Vnuc = 1.1496404054E+01

Ven = -3.1706717814E+00

Vrep = 2.8502639957E+00

DelSqV = -2.9299684657E+00

DelSqVen = 1.0868941382E+01

DelSqVrep = -1.3798909847E+01

DelSqG = 1.6013819846E+00

DelSqK = 1.3285864811E+00

Stress_EigVals = -2.1616048356E-01 -2.1469444584E-01 1.1044714365E-01

Stress_EigVec1 = 4.6492392410E-01 -3.0879178679E-01 -8.2975501035E-01

Stress_EigVec2 = 8.8368751515E-01 2.1926932478E-01 4.1354242681E-01

Stress_EigVec3 = -5.4241315968E-02 9.2550991114E-01 -3.7481900168E-01

-DivStress = -4.6469110446E-03 3.3199343374E-02 -1.4317997985E-02

BPL = 2.0313726154E+00 = 1.3481487842E+00 + 6.8322383123E-01

GBL_I = 2.0309705116E+00

GBL_II = 2.0607399344E+00

GBL_III = 2.0311370024E+00 = 1.3479179393E+00 + 6.8321906307E-01

GBL_IV = 2.0609189334E+00 = 1.3479165377E+00 + 7.1300239570E-01

CP# 21 Coords = -3.42557307165949E+00 -6.74737668118747E-01 5.32700525209041E-01

Type = (3,-1) BCP C6 H9

Rho = 2.7579681851E-01

GradRho = 1.7694179455E-16 -2.4286128664E-17 -2.7755575616E-17

HessRho_EigVals = -7.3335336592E-01 -7.1829538576E-01 5.0622790139E-01

HessRho_EigVec1 = -4.6087406692E-01 -8.6155816540E-01 2.1286761631E-01

HessRho_EigVec2 = 4.3191600931E-01 -8.2160516160E-03 9.0187640916E-01

HessRho_EigVec3 = 7.7527005317E-01 -5.0759237989E-01 -3.7590732971E-01

DelSqRho = -9.4542085029E-01

Bond Ellipticity = 2.0963492827E-02

V = -3.2040775411E-01

G = 4.2026270770E-02

K = 2.7838148334E-01

L = 2.3635521257E-01

Vnuc = 1.1496404036E+01

Ven = -3.1706716573E+00

Vrep = 2.8502639032E+00

DelSqV = -2.9299690753E+00

DelSqVen = 1.0868940079E+01

DelSqVrep = -1.3798909154E+01

DelSqG = 1.6013819735E+00

DelSqK = 1.3285871018E+00

Stress_EigVals = -2.1616047200E-01 -2.1469443951E-01 1.1044715740E-01

Stress_EigVec1 = 3.4959450152E-02 -5.5703193430E-01 8.2975494034E-01

Stress_EigVec2 = 6.3173658347E-01 6.5566106637E-01 4.1354256753E-01

Stress_EigVec3 = 7.7439442531E-01 -5.0972933035E-01 -3.7481900143E-01

-DivStress = 2.6427957399E-02 -2.0623964631E-02 -1.4317973983E-02

BPL = 2.0313726045E+00 = 1.3481487954E+00 + 6.8322380917E-01

GBL_I = 2.0309705014E+00

GBL_II = 2.0607399230E+00

GBL_III = 2.0311369918E+00 = 1.3479179508E+00 + 6.8321904100E-01

GBL_IV = 2.0609189217E+00 = 1.3479165492E+00 + 7.1300237250E-01

CP# 22 Coords = 1.31516381686625E+00 -7.59310183841476E-01 9.22611550110820E-02

Type = (3,-1) BCP C10 C1

Rho = 2.7570817794E-01

GradRho = -1.8214596498E-17 6.2450045135E-17 6.2450045135E-17

HessRho_EigVals = -5.3289554098E-01 -5.0489887170E-01 2.9348273996E-01

HessRho_EigVec1 = 5.0000000259E-01 8.6602540229E-01 7.8858509729E-08

HessRho_EigVec2 = 3.3537429103E-02 -1.9362934844E-02 9.9924987746E-01

HessRho_EigVec3 = 8.6537577864E-01 -4.9962493868E-01 -3.8725733003E-02

DelSqRho = -7.4431167272E-01

Bond Ellipticity = 5.5450053154E-02

V = -3.6369012006E-01

G = 8.8806100939E-02

K = 2.7488401912E-01

L = 1.8607791818E-01

Vnuc = 1.4275904604E+01

Ven = -3.9359836467E+00

Vrep = 3.5722935267E+00

DelSqV = -1.3322713611E+00

DelSqVen = 1.0625722435E+01

DelSqVrep = -1.1957993796E+01

DelSqG = 1.2804247909E+00

DelSqK = 5.1846570180E-02

Stress_EigVals = -2.0615287779E-01 -2.0501276387E-01 4.7475521609E-02

Stress_EigVec1 = 5.0000002581E-01 8.6602538888E-01 6.8620195896E-07

Stress_EigVec2 = 2.5914497867E-02 -1.4962535352E-02 9.9955218040E-01

Stress_EigVec3 = 8.6563757601E-01 -4.9977609821E-01 -2.9923881155E-02

-DivStress = 1.9693337886E-01 -1.1369953905E-01 -1.9219408335E-02

BPL = 2.7694364458E+00 = 1.2501896458E+00 + 1.5192468000E+00

GBL_I = 2.7689868062E+00

GBL_II = 2.7689893293E+00

GBL_III = 2.7692332921E+00 = 1.2501382892E+00 + 1.5190950030E+00

GBL_IV = 2.7692357915E+00 = 1.2501407744E+00 + 1.5190950171E+00

CP# 23 Coords = 2.29712648669962E+00 -2.62926444336552E+00 5.32700528975066E-01

Type = (3,-1) BCP C10 H11

Rho = 2.7579682885E-01

GradRho = -9.0205620751E-17 7.8062556419E-18 -5.1174342541E-17

HessRho_EigVals = -7.3335338853E-01 -7.1829542143E-01 5.0622784788E-01

HessRho_EigVec1 = 9.7656822325E-01 3.1650572062E-02 2.1286790886E-01

HessRho_EigVec2 = -2.0884301906E-01 3.7815823734E-01 9.0187634458E-01

HessRho_EigVec3 = 5.1952850968E-02 9.2519975617E-01 -3.7590731898E-01

DelSqRho = -9.4542096208E-01

Bond Ellipticity = 2.0963473596E-02

V = -3.2040778575E-01

G = 4.2026272616E-02

K = 2.7838151314E-01

L = 2.3635524052E-01

Vnuc = 1.1496404054E+01

Ven = -3.1706717814E+00

Vrep = 2.8502639957E+00

DelSqV = -2.9299684657E+00

DelSqVen = 1.0868941382E+01

DelSqVrep = -1.3798909847E+01

DelSqG = 1.6013819846E+00

DelSqK = 1.3285864811E+00

Stress_EigVals = -2.1616048356E-01 -2.1469444584E-01 1.1044714365E-01

Stress_EigVec1 = 4.6492392410E-01 3.0879178679E-01 8.2975501035E-01

Stress_EigVec2 = -8.8368751515E-01 2.1926932478E-01 4.1354242681E-01

Stress_EigVec3 = 5.4241315968E-02 9.2550991114E-01 -3.7481900168E-01

-DivStress = 4.6469110446E-03 3.3199343374E-02 -1.4317997985E-02

BPL = 2.0313726154E+00 = 1.3481487842E+00 + 6.8322383123E-01

GBL_I = 2.0309705116E+00

GBL_II = 2.0607399344E+00

GBL_III = 2.0311370024E+00 = 1.3479179393E+00 + 6.8321906307E-01

GBL_IV = 2.0609189334E+00 = 1.3479165377E+00 + 7.1300239570E-01

CP# 24 Coords = 2.61762225330877E+00 -1.51128489283147E+00 -1.31495192669614E+00

Type = (3,-1) BCP C10 H12

Rho = 2.5464757830E-01

GradRho = -2.2446627890E-13 1.2961100292E-13 -6.4726869697E-13

HessRho_EigVals = -6.3924164960E-01 -6.3862637520E-01 4.6381592074E-01

HessRho_EigVec1 = 4.9999672195E-01 8.6602729636E-01 -8.2252137025E-07

HessRho_EigVec2 = 8.4641024005E-01 -4.8867070721E-01 2.1163800571E-01

HessRho_EigVec3 = -1.8328388795E-01 1.0581900529E-01 9.7734812351E-01

DelSqRho = -8.1405210406E-01

Bond Ellipticity = 9.6343407114E-04

V = -2.9357822797E-01

G = 4.5032600978E-02

K = 2.4854562699E-01

L = 2.0351302601E-01

Vnuc = 1.1590557906E+01

Ven = -2.9515075020E+00

Vrep = 2.6579292741E+00
DelSqV = -2.4942318143E+00
DelSqVen = 9.4353180509E+00
DelSqVrep = -1.1929549865E+01
DelSqG = 1.4209175836E+00
DelSqK = 1.0733142307E+00
Stress_EigVals = -1.9775889089E-01 -1.9526740530E-01 9.9448068222E-02
Stress_EigVec1 = 5.0000000705E-01 8.6602539971E-01 9.7401805155E-09
Stress_EigVec2 = 8.4763909272E-01 -4.8938466986E-01 2.0496490770E-01
Stress_EigVec3 = -1.7750482089E-01 1.0248244704E-01 9.7876932247E-01
-DivStress = -9.7787709187E-03 5.6457913436E-03 5.0288253244E-02
BPL = 2.0675574416E+00 = 1.3666888144E+00 + 7.0086862719E-01
GBL_I = 2.0670898250E+00
GBL_II = 2.0959525307E+00
GBL_III = 2.0674150039E+00 = 1.3665673212E+00 + 7.0084768265E-01
GBL_IV = 2.0963073085E+00 = 1.3665678652E+00 + 7.2973944325E-01

CP# 25 Coords = 3.42557307165950E+00 -6.74737668118750E-01 5.32700525209038E-01

Type = (3,-1) BCP H13 C10
Rho = 2.7579681851E-01
GradRho = 2.0816681712E-16 5.7245874707E-17 6.7654215563E-17
HessRho_EigVals = -7.3335336592E-01 -7.1829538576E-01 5.0622790139E-01
HessRho_EigVec1 = 4.6087406692E-01 -8.6155816540E-01 2.1286761631E-01
HessRho_EigVec2 = -4.3191600931E-01 -8.2160516160E-03 9.0187640916E-01
HessRho_EigVec3 = 7.7527005317E-01 5.0759237989E-01 3.7590732971E-01
DelSqRho = -9.4542085029E-01
Bond Ellipticity = 2.0963492827E-02
V = -3.2040775411E-01
G = 4.2026270770E-02
K = 2.7838148334E-01
L = 2.3635521257E-01
Vnuc = 1.1496404036E+01

$$\text{Ven} = -3.1706716573\text{E}+00$$

$$\text{Vrep} = 2.8502639032\text{E}+00$$

$$\text{DelSqV} = -2.9299690753\text{E}+00$$

$$\text{DelSqVen} = 1.0868940079\text{E}+01$$

$$\text{DelSqVrep} = -1.3798909154\text{E}+01$$

$$\text{DelSqG} = 1.6013819735\text{E}+00$$

$$\text{DelSqK} = 1.3285871018\text{E}+00$$

$$\text{Stress\_EigVals} = -2.1616047200\text{E}-01 \ -2.1469443951\text{E}-01 \ 1.1044715740\text{E}-01$$

$$\text{Stress\_EigVec1} = -3.4959450153\text{E}-02 \ -5.5703193430\text{E}-01 \ 8.2975494034\text{E}-01$$

$$\text{Stress\_EigVec2} = -6.3173658347\text{E}-01 \ 6.5566106637\text{E}-01 \ 4.1354256753\text{E}-01$$

$$\text{Stress\_EigVec3} = 7.7439442531\text{E}-01 \ 5.0972933035\text{E}-01 \ 3.7481900143\text{E}-01$$

$$-\text{DivStress} = -2.6427957399\text{E}-02 \ -2.0623964631\text{E}-02 \ -1.4317973983\text{E}-02$$

$$\text{BPL} = 2.0313726045\text{E}+00 = 6.8322380917\text{E}-01 + 1.3481487954\text{E}+00$$

$$\text{GBL\_I} = 2.0309705014\text{E}+00$$

$$\text{GBL\_II} = 2.0607399230\text{E}+00$$

$$\text{GBL\_III} = 2.0311369918\text{E}+00 = 6.8321904100\text{E}-01 + 1.3479179508\text{E}+00$$

$$\text{GBL\_IV} = 2.0609189217\text{E}+00 = 7.1300237250\text{E}-01 + 1.3479165492\text{E}+00$$

$$\text{Number of NACPs} = 13$$

$$\text{Number of NNACPs} = 0$$

$$\text{Number of BCPs} = 12$$

$$\text{Number of RCPs} = 0$$

$$\text{Number of CCPs} = 0$$

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H3	C2	C1	110.84506586	113.09924324	113.12544732	112.23399644	112.23392950
H4	C2	C1	103.25095227	103.62874819	103.67116909	103.74372216	103.74355578
H4	C2	H3	107.39699395	106.64023455	106.61425587	107.07998106	107.08002965
H5	C2	C1	110.84506586	113.09924324	113.12544732	112.23399644	112.23392950
H5	C2	H3	116.17061556	112.84911668	112.80652954	113.68651749	113.68669988
H5	C2	H4	107.39699395	106.64023455	106.61425587	107.07998106	107.08002965
C6	C1	C2	119.99272942	119.86354616	119.86354766	119.93801520	119.93801335
H7	C6	C1	103.25095124	103.62874829	103.67116921	103.74372207	103.74355570
H8	C6	C1	110.84506307	113.09924289	113.12544696	112.23399498	112.23392805
H8	C6	H7	107.39699679	106.64023440	106.61425563	107.07998222	107.08003080
H9	C6	C1	110.84506453	113.09924330	113.12544738	112.23399627	112.23392934
H9	C6	H7	107.39699329	106.64023474	106.61425614	107.07998089	107.08002947
H9	C6	H8	116.17061834	112.84911685	112.80652972	113.68651829	113.68670067
C10	C1	C2	119.99272942	119.86354616	119.86354766	119.93801520	119.93801335
C10	C1	C6	119.99272978	119.86354651	119.86354801	119.93801520	119.93801335
H11	C10	C1	110.84506307	113.09924289	113.12544696	112.23399498	112.23392805
H12	C10	C1	103.25095124	103.62874829	103.67116921	103.74372207	103.74355570
H12	C10	H11	107.39699679	106.64023440	106.61425563	107.07998222	107.08003080
H13	C10	C1	110.84506453	113.09924330	113.12544738	112.23399627	112.23392934
H13	C10	H11	116.17061834	112.84911685	112.80652972	113.68651829	113.68670067
H13	C10	H12	107.39699329	106.64023474	106.61425614	107.07998089	107.08002947

Total time for electron density critical point search, analysis and connectivity = 19 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular Ee unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Ven(A) = Ven(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$VenO(A) = Ven(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A) = Vee(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus
the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $Vnn(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
C1	-3.7941475329E+01	3.7941475329E+01	-1.4141847717E+02	-8.9628589459E+01		
C2	-3.7953578517E+01	3.7953578517E+01	-1.3259848037E+02	-9.0120279680E+01		
H3	-5.7343189399E-01	5.7343189399E-01	-7.9682476646E+00	-1.1754956965E+00		
H4	-5.4556727713E-01	5.4556727713E-01	-7.7885142912E+00	-1.1237446735E+00		
H5	-5.7343215478E-01	5.7343215478E-01	-7.9682372200E+00	-1.1754950124E+00		
C6	-3.7953583273E+01	3.7953583273E+01	-1.3259824722E+02	-9.0120244985E+01		
H7	-5.4556776184E-01	5.4556776184E-01	-7.7885264519E+00	-1.1237457666E+00		
H8	-5.7343238847E-01	5.7343238847E-01	-7.9682420654E+00	-1.1754955007E+00		
H9	-5.7343250981E-01	5.7343250981E-01	-7.9681804779E+00	-1.1754912656E+00		
C10	-3.7953566811E+01	3.7953566811E+01	-1.3259870459E+02	-9.0120350372E+01		
H11	-5.7343229489E-01	5.7343229489E-01	-7.9682240825E+00	-1.1754940876E+00		
H12	-5.4556706813E-01	5.4556706813E-01	-7.7885187396E+00	-1.1237449794E+00		
H13	-5.7343241019E-01	5.7343241019E-01	-7.9681873345E+00	-1.1754916503E+00		
Total	-1.5687949969E+02	1.5687949969E+02	-6.1038878768E+02	-3.7041366313E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) = \text{Contribution of Atom A to Total Energy E of Molecule}$$

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$$W(A) = \text{Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule}$$

$$V_{nn}(A) = \text{Contribution of Atom A to Nuclear Repulsion Energy of Molecule}$$

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$$V_{eeC}(A) = \text{Coulomb Part of } V_{ee}(A)$$

$$V_{eeX}(A) = \text{Exchange-Correlation Part of } V_{ee}(A)$$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

C1	-3.7941475019E+01	-3.7941475329E+01	3.1032240684E-07			

C2	-3.7953578658E+01	-3.7953578517E+01	-1.4052759974E-07			

H3	-5.7343192562E-01	-5.7343189399E-01	-3.1626455274E-08			

H4	-5.4556733074E-01	-5.4556727713E-01	-5.3608868487E-08			

H5	-5.7343218641E-01	-5.7343215478E-01	-3.1626454167E-08			

C6	-3.7953583414E+01	-3.7953583273E+01	-1.4052582973E-07			

H7	-5.4556781545E-01	-5.4556776184E-01	-5.3608897846E-08			

H8	-5.7343242010E-01	-5.7343238847E-01	-3.1626420040E-08			

H9	-5.7343254144E-01	-5.7343250981E-01	-3.1626416678E-08			

C10	-3.7953566952E+01	-3.7953566811E+01	-1.4052582165E-07			

H11	-5.7343232652E-01	-5.7343229489E-01	-3.1626424166E-08			

H12	-5.4556712174E-01	-5.4556706813E-01	-5.3608895252E-08			

H13	-5.7343244182E-01	-5.7343241019E-01	-3.1626423471E-08			

Total	-1.5687950015E+02	-1.5687949969E+02	-4.6184209966E-07			

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
$VeeC(A)$	$VeeX(A)$					

C1			3.7941475329E+01	-6.9548295553E+01	-7.0709238585E+01	
2.6286158587E+01						

C2			3.7953578517E+01	-6.5150905779E+01	-6.6299240185E+01	
2.1534360464E+01						

H3			5.7343189399E-01	-4.4515800571E+00	-3.9841238323E+00	
4.0103045664E+00						

H4			5.4556727713E-01	-4.4938961808E+00	-3.8942571456E+00	
4.0737729262E+00						

H5			5.7343215478E-01	-4.4515800571E+00	-3.9841186100E+00	
4.0103045664E+00						

C6			3.7953583273E+01	-6.5150905752E+01	-6.6299123608E+01	
2.1534360464E+01						

H7			5.4556776184E-01	-4.4938961677E+00	-3.8942632260E+00	
4.0737729233E+00						

H8 4.0103045678E+00	5.7343238847E-01 -4.4515800700E+00 -3.9841210327E+00
H9 4.0103045755E+00	5.7343250981E-01 -4.4515800655E+00 -3.9840902390E+00
C10 2.1534360464E+01	3.7953566811E+01 -6.5150905752E+01 -6.6299352295E+01
H11 4.0103045678E+00	5.7343229489E-01 -4.4515800700E+00 -3.9841120412E+00
H12 4.0737729233E+00	5.4556706813E-01 -4.4938961677E+00 -3.8942593698E+00
H13 4.0103045755E+00	5.7343241019E-01 -4.4515800655E+00 -3.9840936673E+00

Total 1.2717238617E+02	1.5687949969E+02 -3.0519218174E+02 -3.0519439384E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

$$= \text{Intraatomic ("Self") Contribution to } E\_IQA(A)$$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$
C1	3.7941475329E+01	-8.9628589459E+01				
C2	3.7953578517E+01	-9.0120279680E+01				
H3	5.7343189399E-01	-1.1754956965E+00				
H4	5.4556727713E-01	-1.1237446735E+00				

H5	5.7343215478E-01 -1.1754950124E+00
C6	3.7953583273E+01 -9.0120244985E+01
H7	5.4556776184E-01 -1.1237457666E+00
H8	5.7343238847E-01 -1.1754955007E+00
H9	5.7343250981E-01 -1.1754912656E+00
C10	3.7953566811E+01 -9.0120350372E+01
H11	5.7343229489E-01 -1.1754940876E+00
H12	5.4556706813E-01 -1.1237449794E+00
H13	5.7343241019E-01 -1.1754916503E+00

Total	1.5687949969E+02 -3.7041366313E+02

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$Vnn(A) = Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A,A')$ = Coulomb Part of $Vee(A,A')$

$VeeX(A,A')$ = Exchange-Correlation Part of $Vee(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$Vne(A,A')/2$	$Ven(A,A')/2$	$Vee(A,A')$	$Vnn(A)$	$VeeC(A,A')$
	$VeeX(A,A')$					

C1	-2.4734000824E+01 -2.5894943855E+01	2.6286158587E+01
C2	-2.0090765939E+01 -2.1239100345E+01	2.1534360464E+01
H3	-3.8638322088E+00 -3.3963759840E+00	4.0103045664E+00
H4	-3.9320238440E+00 -3.3323848089E+00	4.0737729262E+00
H5	-3.8638325509E+00 -3.3963711038E+00	4.0103045664E+00
C6	-2.0090783259E+01 -2.1239001115E+01	2.1534360464E+01
H7	-3.9320232844E+00 -3.3323903427E+00	4.0737729233E+00
H8	-3.8638323196E+00 -3.3963732823E+00	4.0103045678E+00
H9	-3.8638344327E+00 -3.3963446061E+00	4.0103045755E+00
C10	-2.0090730566E+01 -2.1239177109E+01	2.1534360464E+01
H11	-3.8638330262E+00 -3.3963649975E+00	4.0103045678E+00
H12	-3.9320236780E+00 -3.3323868801E+00	4.0737729233E+00
H13	-3.8638342404E+00 -3.3963478421E+00	4.0103045755E+00
Total	-1.1998535017E+02 -1.1998756227E+02	1.2717238617E+02

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A
that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')

C1	5.9482546619E+00	4.2739801965E+00	7.1852676784E+01	1.6742744654E+00	
2.8147323216E+01					
C2	6.0434475363E+00	4.3020064546E+00	7.1184641362E+01	1.7414410817E+00	
2.8815358638E+01					
H3	8.9115372315E-01	4.2247244906E-01	4.7407359481E+01	4.6868127409E-01	
5.2592640519E+01					
H4	8.5833624761E-01	3.9530772800E-01	4.6055112911E+01	4.6302851962E-01	
5.3944887089E+01					
H5	8.9115233079E-01	4.2247141633E-01	4.7407317664E+01	4.6868091447E-01	
5.2592682336E+01					
C6	6.0434206630E+00	4.3019869380E+00	7.1184634959E+01	1.7414337250E+00	
2.8815365041E+01					
H7	8.5833753058E-01	3.9530870041E-01	4.6055157363E+01	4.6302883017E-01	
5.3944842637E+01					
H8	8.9115293950E-01	4.2247180385E-01	4.7407328767E+01	4.6868113566E-01	
5.2592671233E+01					
H9	8.9114588380E-01	4.2246671147E-01	4.7407132676E+01	4.6867917233E-01	
5.2592867324E+01					
C10	6.0434898082E+00	4.3020423811E+00	7.1184737919E+01	1.7414474271E+00	
2.8815262081E+01					
H11	8.9115079858E-01	4.2247023119E-01	4.7407266184E+01	4.6868056739E-01	
5.2592733816E+01					
H12	8.5833684090E-01	3.9530817999E-01	4.6055133737E+01	4.6302866091E-01	
5.3944866263E+01					
H13	8.9114685981E-01	4.2246720849E-01	4.7407136528E+01	4.6867965132E-01	
5.2592863472E+01					

Total	3.2000525824E+01	2.0900760399E+01	6.5313803010E+01	1.1099765425E+01	
3.4686196990E+01					

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

= LI(A) + DI(A,A')/2 = LI(A) + DI_Bond(A,A')/2 + DI_NonBond(A,A')/2

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	5.9482546619E+00	4.2739801965E+00	1.6742744654E+00	1.4302647875E+00	2.4400967794E-01
C2	6.0434475363E+00	4.3020064546E+00	1.7414410817E+00	1.6817494577E+00	5.9691624036E-02
H3	8.9115372315E-01	4.2247244906E-01	4.6868127409E-01	4.0941377302E-01	5.9267501071E-02
H4	8.5833624761E-01	3.9530772800E-01	4.6302851962E-01	3.8616208785E-01	7.6866431770E-02
H5	8.9115233079E-01	4.2247141633E-01	4.6868091447E-01	4.0940534498E-01	5.9275569492E-02
C6	6.0434206630E+00	4.3019869380E+00	1.7414337250E+00	1.6817326155E+00	5.9701109471E-02
H7	8.5833753058E-01	3.9530870041E-01	4.6302883017E-01	3.8614059884E-01	7.6888231332E-02
H8	8.9115293950E-01	4.2247180385E-01	4.6868113566E-01	4.0943508747E-01	5.9246048185E-02
H9	8.9114588380E-01	4.2246671147E-01	4.6867917233E-01	4.0939077452E-01	5.9288397813E-02
C10	6.0434898082E+00	4.3020423811E+00	1.7414474271E+00	1.6817229315E+00	5.9724495559E-02
H11	8.9115079858E-01	4.2247023119E-01	4.6868056739E-01	4.0944578083E-01	5.9234786568E-02

H12	8.5833684090E-01	3.9530817999E-01	4.6302866091E-01	3.8615150379E-01
7.6877157116E-02				
H13	8.9114685981E-01	4.2246720849E-01	4.6867965132E-01	4.0939526599E-01
5.9284385332E-02				

Total	3.2000525824E+01	2.0900760399E+01	1.1099765425E+01	1.0090410009E+01
1.0093554157E+00				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.5553876663E+01	7.6644065295E+01	9.2197941958E+01
C2	1.6110625835E+01	7.7562807843E+01	9.3673433677E+01
H3	1.8584125462E-01	1.3627039115E+01	1.3812880369E+01
H4	1.7071669299E-01	1.3133493030E+01	1.3304209723E+01
H5	1.8584053018E-01	1.3627018264E+01	1.3812858794E+01
C6	1.6110473186E+01	7.7562543942E+01	9.3673017128E+01
H7	1.7071730800E-01	1.3133512301E+01	1.3304229609E+01
H8	1.8584087887E-01	1.3627027347E+01	1.3812868226E+01
H9	1.8583713737E-01	1.3626921726E+01	1.3812758864E+01
C10	1.6110863341E+01	7.7563225541E+01	9.3674088881E+01
H11	1.8583975731E-01	1.3626995284E+01	1.3812835041E+01
H12	1.7071697623E-01	1.3133501943E+01	1.3304218919E+01

H13 1.8583775863E-01 1.3626936232E+01 1.3812773991E+01

Total 6.5513027319E+01 4.3049508786E+02 4.9600811518E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) = \text{Average Number of Electron Pairs Formed Between Atoms A and B}$
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) = \text{Electron Delocalization Index. Average Number of Electrons Delocalized}$
 (Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
C1	C2	3.5471196730E+01	9.5353650365E-01	8.0152629455E+00	7.8890111804E+00 (Bonded)
C1	H3	5.2803512044E+00	4.0916167766E-02	3.4393423021E-01	2.2956851721E+00
C2	H3	4.9762269996E+00	8.1882754605E-01	6.7745069443E+00	4.5941992093E+01 (Bonded)
C1	H4	5.0651699374E+00	8.0865298021E-02	6.7973971036E-01	4.7105838909E+00
C2	H4	4.8011479931E+00	7.7232417570E-01	6.3897648739E+00	4.4989605055E+01 (Bonded)
H3	H4	7.5304225650E-01	2.3734572567E-02	1.3316766766E+00	1.3825917659E+00
C1	H5	5.2803196167E+00	4.0962778933E-02	3.4432603563E-01	2.2983039778E+00
C2	H5	4.9762270130E+00	8.1881068996E-01	6.7743674867E+00	4.5941118127E+01 (Bonded)
H3	H5	7.8205691558E-01	2.4193603816E-02	1.3574315624E+00	1.3574336833E+00
H4	H5	7.5304113838E-01	2.3734418566E-02	1.3825827950E+00	1.3316701166E+00
C1	C6	3.5471038978E+01	9.5353230942E-01	8.0152276895E+00	7.8890115598E+00 (Bonded)
C2	C6	3.6504457201E+01	3.7277030068E-02	3.0840865122E-01	3.0841002262E-01
H3	C6	5.3822482759E+00	6.7370969025E-03	3.7799858360E-01	5.5739102722E-02

H4	C6	5.1842362553E+00	6.1015186832E-03	3.5542706603E-01	5.0480671655E-02	
H5	C6	5.3807902928E+00	9.6362340064E-03	5.4066143763E-01	7.9724998008E-02	
C1	H7	5.0651701332E+00	8.0880169175E-02	6.7986471471E-01	4.7114431266E+00	
C2	H7	5.1842661419E+00	6.1033852167E-03	5.0495889805E-02	3.5553526435E-01	
H3	H7	7.6448646360E-01	8.4844499288E-04	4.7603739447E-02	4.9423738486E-02	
H4	H7	7.3442501206E-01	4.6344062484E-03	2.6996449592E-01	2.6996409240E-01	
H5	H7	7.6433844400E-01	1.1420939745E-03	6.4079615515E-02	6.6529420756E-02	
C6	H7	4.8011541693E+00	7.7228119767E-01	6.3894377104E+00	4.4987034247E+01	(Bonded)
C1	H8	5.2803392257E+00	4.0930802382E-02	3.4405724627E-01	2.2965082966E+00	
C2	H8	5.3822671880E+00	6.7376974364E-03	5.5743823339E-02	3.7803261021E-01	
H3	H8	7.9302481443E-01	2.2588910098E-03	1.2673969435E-01	1.2673980580E-01	
H4	H8	7.6448464571E-01	8.4844887733E-04	4.9424038638E-02	4.7603999253E-02	
H5	H8	7.9386630228E-01	5.7343371392E-04	3.2173720143E-02	3.2173698167E-02	
C6	H8	4.9761770010E+00	8.1887017494E-01	6.7748897570E+00	4.5944424276E+01	(Bonded)
H7	H8	7.5304277008E-01	2.3734486770E-02	1.3825847015E+00	1.3316730338E+00	
C1	H9	5.2802827133E+00	4.0959888979E-02	3.4430174318E-01	2.2981584567E+00	
C2	H9	5.3807716931E+00	9.6434056705E-03	7.9783977710E-02	5.4106773346E-01	
H3	H9	7.9386127882E-01	5.7338679995E-04	3.2171037670E-02	3.2171320677E-02	
H4	H9	7.6433176324E-01	1.1421014864E-03	6.6529957787E-02	6.4080500576E-02	
H5	H9	7.9017309749E-01	7.9472678787E-03	4.4589839492E-01	4.4590162077E-01	
C6	H9	4.9761786734E+00	8.1878154904E-01	6.7741565142E+00	4.5939815462E+01	(Bonded)
H7	H9	7.5303686336E-01	2.3734187860E-02	1.3825672894E+00	1.3316668063E+00	
H8	H9	7.8205072861E-01	2.4193090532E-02	1.3574039573E+00	1.3574147046E+00	
C1	C10	3.5471486045E+01	9.5346076186E-01	8.0146262732E+00	7.8883293604E+00	(Bonded)
C2	C10	3.6504873498E+01	3.7280188164E-02	3.0843477948E-01	3.0843262210E-01	
H3	C10	5.3808599096E+00	9.6370676853E-03	5.4070736815E-01	7.9730983182E-02	
H4	C10	5.1842945735E+00	6.1035819346E-03	3.5554725503E-01	5.0497164124E-02	
H5	C10	5.3823008729E+00	6.7383115786E-03	3.7806732619E-01	5.5748514455E-02	
C6	C10	3.6504679514E+01	3.7343339532E-02	3.0895863133E-01	3.0895509645E-01	
H7	C10	5.1843017017E+00	6.1048327469E-03	3.5561958608E-01	5.0507512552E-02	
H8	C10	5.3808401064E+00	9.6672020870E-03	5.4239859728E-01	7.9980296102E-02	

H9	C10	5.3822608272E+00	6.7404783236E-03	3.7819163204E-01	5.5766440728E-02
C1	H11	5.2803313452E+00	4.0921093957E-02	3.4397563893E-01	2.2959691010E+00
C2	H11	5.3822543836E+00	6.7374290275E-03	5.5741602679E-02	3.7801845873E-01
H3	H11	7.9386563674E-01	5.7343060718E-04	3.2173495564E-02	3.2173601151E-02
H4	H11	7.6448280360E-01	8.4845782601E-04	4.9424559919E-02	4.7604615704E-02
H5	H11	7.9302167271E-01	2.2588770662E-03	1.2673911004E-01	1.2673932795E-01
C6	H11	5.3807668271E+00	9.6646456979E-03	7.9960061006E-02	5.4225646845E-01
H7	H11	7.6433711744E-01	1.1421167766E-03	6.6530749027E-02	6.4081005054E-02
H8	H11	7.9017796175E-01	7.9473838958E-03	4.4590459973E-01	4.4590567099E-01
H9	H11	7.9385866596E-01	5.7340008297E-04	3.2172065954E-02	3.2171888522E-02
C10	H11	4.9762149880E+00	8.1889156165E-01	6.7749891837E+00	4.5945734603E+01
(Bonded)					
C1	H12	5.0651726990E+00	8.0866832789E-02	6.7975261135E-01	4.7106700386E+00
C2	H12	5.1842627887E+00	6.1017555299E-03	5.0482406716E-02	3.5544061720E-01
H3	H12	7.6433901607E-01	1.1421108394E-03	6.4080461639E-02	6.6530456634E-02
H4	H12	7.3442439113E-01	4.6344641620E-03	2.6996786952E-01	2.6996768292E-01
H5	H12	7.6448465451E-01	8.4844373425E-04	4.7603743206E-02	4.9423704880E-02
C6	H12	5.1842395201E+00	6.1021600296E-03	5.0485977809E-02	3.5546418019E-01
H7	H12	7.3442554872E-01	4.6343514227E-03	2.6996089869E-01	2.6996111560E-01
H8	H12	7.6433834353E-01	1.1421106469E-03	6.4080507188E-02	6.6530445420E-02
H9	H12	7.6447912924E-01	8.4842689293E-04	4.7603142670E-02	4.9422723836E-02
C10	H12	4.8011984462E+00	7.7230300759E-01	6.3895450484E+00	4.4988340870E+01
(Bonded)					
H11	H12	7.5304037295E-01	2.3734376551E-02	1.3316700489E+00	1.3825793919E+00
C1	H13	5.2803114196E+00	4.0914087467E-02	3.4391674359E-01	2.2955861325E+00
C2	H13	5.3807761365E+00	9.6463158412E-03	7.9808054783E-02	5.4123042319E-01
H3	H13	7.9017511480E-01	7.9474543878E-03	4.4590816271E-01	4.4591159696E-01
H4	H13	7.6433258571E-01	1.1421320236E-03	6.6531736649E-02	6.4082143761E-02
H5	H13	7.9386089469E-01	5.7341301857E-04	3.2172558986E-02	3.2172756502E-02
C6	H13	5.3822059160E+00	6.7388606512E-03	5.5753695027E-02	3.7810045432E-01
H7	H13	7.6448057934E-01	8.4843139320E-04	4.9422946275E-02	4.7603343032E-02
H8	H13	7.9386142425E-01	5.7343879672E-04	3.2173983348E-02	3.2174202849E-02
H9	H13	7.9301241891E-01	2.2588741452E-03	1.2673986304E-01	1.2673972423E-01

C10	H13	4.9762416989E+00	8.1879053198E-01	6.7741533283E+00	4.5940269158E+01
(Bonded)					
H11	H13	7.8204974980E-01	2.4192971946E-02	1.3574005648E+00	1.3574065644E+00
H12	H13	7.5303708843E-01	2.3734183993E-02	1.3825681750E+00	1.3316651308E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	C2	6.6523580633E+01	5.2023052648E+01	4.1159555665E+01
C1	C6	6.6523580744E+01	5.2023052814E+01	4.1159555823E+01
C1	C10	6.6523580744E+01	5.2023052814E+01	4.1159555823E+01

C1	Total	1.9957074212E+02	1.5606915828E+02	1.2347866731E+02

C2	C1	6.6523580633E+01	5.2023052648E+01	4.1159555665E+01
C2	H3	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01
C2	H4	4.0726328815E+01	3.1581672571E+01	2.5160774829E+01
C2	H5	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01

C2	Total	1.9184228393E+02	1.4989533354E+02	1.1942748327E+02

H3	C2	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01

H3	Total	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01
H4	C2	4.0726328815E+01	3.1581672571E+01	2.5160774829E+01

H4	Total	4.0726328815E+01	3.1581672571E+01	2.5160774829E+01
H5	C2	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01

H5	Total	4.2296187240E+01	3.3145304160E+01	2.6553576387E+01
C6	C1	6.6523580744E+01	5.2023052814E+01	4.1159555823E+01
C6	H7	4.0724302756E+01	3.1585854798E+01	2.5169310903E+01
C6	H8	4.2285569793E+01	3.3133256670E+01	2.6554820271E+01
C6	H9	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01

C6	Total	1.9182469439E+02	1.4987943630E+02	1.1943233519E+02
H7	C6	4.0724302756E+01	3.1585854798E+01	2.5169310903E+01

H7	Total	4.0724302756E+01	3.1585854798E+01	2.5169310903E+01
H8	C6	4.2285569793E+01	3.3133256670E+01	2.6554820271E+01

H8	Total	4.2285569793E+01	3.3133256670E+01	2.6554820271E+01
H9	C6	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01

H9	Total	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01
C10	C1	6.6523580744E+01	5.2023052814E+01	4.1159555823E+01
C10	H11	4.2291241444E+01	3.3137272280E+01	2.6548648386E+01
C10	H12	4.0726328713E+01	3.1581672424E+01	2.5160774711E+01

C10	H13	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01

C10	Total	1.9183239200E+02	1.4987926954E+02	1.1941762711E+02
H11	C10	4.2291241444E+01	3.3137272280E+01	2.6548648386E+01

H11	Total	4.2291241444E+01	3.3137272280E+01	2.6548648386E+01
H12	C10	4.0726328713E+01	3.1581672424E+01	2.5160774711E+01

H12	Total	4.0726328713E+01	3.1581672424E+01	2.5160774711E+01
H13	C10	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01

H13	Total	4.2291241095E+01	3.3137272022E+01	2.6548648192E+01

Total	Total	1.1509987406E+03	8.9930807877E+02	7.1655489114E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	N_IAS(A B)	G_IAS(A B)	K_IAS(A B)	L_IAS(A B)	DelSqRho_IAS(A B)
V_IAS(A B)						

C1	C2	1.3044978227E+00	9.1446962611E-01	4.5571008378E-01	-4.5875954233E-01	1.8350381693E+00 -1.3701797099E+00
C1	C6	1.3044978201E+00	9.1446961581E-01	4.5571007404E-01	-4.5875954176E-01	1.8350381671E+00 -1.3701796899E+00
C1	C10	1.3044978201E+00	9.1446961581E-01	4.5571007404E-01	-4.5875954176E-01	1.8350381671E+00 -1.3701796898E+00

C1	Total	3.9134934629E+00	2.7434088577E+00	1.3671302319E+00	-1.3762786258E+00	5.5051145035E+00 -4.1105390896E+00
C2	C1	1.3044978227E+00	9.1446962611E-01	4.5571008378E-01	-4.5875954233E-01	1.8350381693E+00 -1.3701797099E+00
C2	H3	9.3668918058E-01	5.1946492281E-01	3.8693251159E-01	-1.3253241122E-01	5.3012964488E-01 -9.0639743440E-01
C2	H4	8.9602157570E-01	4.9526191091E-01	3.5505458587E-01	-1.4020732504E-01	5.6082930016E-01 -8.5031649677E-01
C2	H5	9.3668918058E-01	5.1946492281E-01	3.8693251159E-01	-1.3253241122E-01	5.3012964488E-01 -9.0639743440E-01

C2	Total	4.0738977596E+00	2.4486613826E+00	1.5846296928E+00	-8.6403168981E-01	3.4561267592E+00 -4.0332910755E+00
H3	C2	9.3668918058E-01	5.1946492281E-01	3.8693251159E-01	-1.3253241122E-01	5.3012964488E-01 -9.0639743440E-01

H3	Total	9.3668918058E-01	5.1946492281E-01	3.8693251159E-01	-1.3253241122E-01	5.3012964488E-01 -9.0639743440E-01
H4	C2	8.9602157570E-01	4.9526191091E-01	3.5505458587E-01	-1.4020732504E-01	5.6082930016E-01 -8.5031649677E-01

H4	Total	8.9602157570E-01	4.9526191091E-01	3.5505458587E-01	-1.4020732504E-01	5.6082930016E-01 -8.5031649677E-01

H5 C2 9.3668918058E-01 5.1946492281E-01 3.8693251159E-01 -1.3253241122E-01
5.3012964488E-01 -9.0639743440E-01

H5 Total 9.3668918058E-01 5.1946492281E-01 3.8693251159E-01 -1.3253241122E-01
5.3012964488E-01 -9.0639743440E-01

C6 C1 1.3044978201E+00 9.1446961581E-01 4.5571007404E-01 -4.5875954176E-01
1.8350381671E+00 -1.3701796899E+00

C6 H7 8.9602154783E-01 4.9526186232E-01 3.5505454723E-01 -1.4020731508E-01
5.6082926034E-01 -8.5031640955E-01

C6 H8 9.3668517165E-01 5.1946404796E-01 3.8692931331E-01 -1.3253473465E-01
5.3013893859E-01 -9.0639336127E-01

C6 H9 9.3668870485E-01 5.1946471720E-01 3.8693251098E-01 -1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01

C6 Total 4.0738932444E+00 2.4486602433E+00 1.5846264456E+00 -8.6403379771E-01
3.4561351909E+00 -4.0332866889E+00

H7 C6 8.9602154783E-01 4.9526186232E-01 3.5505454723E-01 -1.4020731508E-01
5.6082926034E-01 -8.5031640955E-01

H7 Total 8.9602154783E-01 4.9526186232E-01 3.5505454723E-01 -1.4020731508E-01
5.6082926034E-01 -8.5031640955E-01

H8 C6 9.3668517165E-01 5.1946404796E-01 3.8692931331E-01 -1.3253473465E-01
5.3013893859E-01 -9.0639336127E-01

H8 Total 9.3668517165E-01 5.1946404796E-01 3.8692931331E-01 -1.3253473465E-01
5.3013893859E-01 -9.0639336127E-01

H9 C6 9.3668870485E-01 5.1946471720E-01 3.8693251098E-01 -1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01

H9 Total 9.3668870485E-01 5.1946471720E-01 3.8693251098E-01 -1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01

C10	C1	1.3044978201E+00	9.1446961581E-01	4.5571007404E-01	-4.5875954176E-01
1.8350381671E+00 -1.3701796898E+00					
C10	H11	9.3668871573E-01	5.1946474922E-01	3.8693253830E-01	-1.3253221092E-01
5.3012884368E-01 -9.0639728753E-01					
C10	H12	8.9602152921E-01	4.9526188100E-01	3.5505453552E-01	-1.4020734549E-01
5.6082938195E-01 -8.5031641652E-01					
C10	H13	9.3668870485E-01	5.1946471720E-01	3.8693251098E-01	-1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01					

C10	Total	4.0738967699E+00	2.4486609632E+00	1.5846296588E+00	-8.6403130439E-01
3.4561252176E+00 -4.0332906220E+00					
H11	C10	9.3668871573E-01	5.1946474922E-01	3.8693253830E-01	-1.3253221092E-01
5.3012884368E-01 -9.0639728753E-01					

H11	Total	9.3668871573E-01	5.1946474922E-01	3.8693253830E-01	-1.3253221092E-01
5.3012884368E-01 -9.0639728753E-01					
H12	C10	8.9602152921E-01	4.9526188100E-01	3.5505453552E-01	-1.4020734549E-01
5.6082938195E-01 -8.5031641652E-01					

H12	Total	8.9602152921E-01	4.9526188100E-01	3.5505453552E-01	-1.4020734549E-01
5.6082938195E-01 -8.5031641652E-01					
H13	C10	9.3668870485E-01	5.1946471720E-01	3.8693251098E-01	-1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01					

H13	Total	9.3668870485E-01	5.1946471720E-01	3.8693251098E-01	-1.3253220622E-01
5.3012882490E-01 -9.0639722818E-01					

Total	Total	2.4443375548E+01	1.4691965178E+01	9.5077715945E+00	-5.1841935838E+00
2.0736774336E+01 -2.4199736773E+01					

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1 9.9868831184E+00
C2 2.6212368622E+01
H3 4.1835713863E+01
H4 4.3143491809E+01
H5 4.1732093911E+01
C6 2.6066649413E+01
H7 4.3649132443E+01
H8 4.1981264196E+01
H9 4.2044770106E+01
C10 2.6290259043E+01
H11 4.1867161081E+01
H12 4.3401366459E+01
H13 4.1776660307E+01

Total 4.6998781437E+02

0.001 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 1.0983044340E+01 2.4096520668E+00 2.3210531688E-01 2.0166214248E-01 2.1939746322E-
01 6.3322931366E-03 5.4675768430E-05
C2 2.5474894981E+01 4.6020245898E+00 2.2421124829E-01 1.6398309307E-01 1.8064940378E-
01 1.2892174215E-02 2.1566866397E-04
H3 3.5720481603E+01 6.3275653545E+00 1.9964900809E-01 1.6404916642E-01 1.7714109862E-
01 8.2295083570E-03 9.2894978549E-05
H4 3.7313421526E+01 7.1150564585E+00 2.2479532421E-01 1.7009889747E-01 1.9068357088E-
01 1.1770326468E-02 1.9681822178E-04
H5 3.5762449273E+01 6.3379732850E+00 1.9945481814E-01 1.6402718858E-01 1.7722425096E-
01 8.2800039509E-03 9.4048705874E-05
C6 2.5938953187E+01 4.7085948306E+00 2.2826411659E-01 1.6398113068E-01 1.8152601597E-
01 1.3451733864E-02 2.3616843898E-04
H7 3.7105401792E+01 7.0748010576E+00 2.2648296128E-01 1.7014146094E-01 1.9066768492E-
01 1.1752601399E-02 1.9680931789E-04

H8	3.5602392241E+01	6.3043974860E+00	1.9996358157E-01	1.6407477523E-01	1.7707791778E-01	8.1727714816E-03	9.1501240177E-05
H9	3.5644764009E+01	6.3115816590E+00	1.9778536381E-01	1.6400910858E-01	1.7706897028E-01	8.1961775363E-03	9.1917417845E-05
C10	2.5936346000E+01	4.7055472971E+00	2.2901674027E-01	1.6398183289E-01	1.8142676294E-01	1.3374464737E-02	2.3413186698E-04
H11	3.5995179513E+01	6.3785067617E+00	1.9901665783E-01	1.6402310670E-01	1.7720447149E-01	8.2751793430E-03	9.3541857699E-05
H12	3.7275712207E+01	7.1054506220E+00	2.2733473633E-01	1.7012141038E-01	1.9061877564E-01	1.1753282059E-02	1.9694143165E-04
H13	3.5906997624E+01	6.3640140550E+00	1.9972976585E-01	1.6402924508E-01	1.7723603966E-01	8.3127917334E-03	9.4821717929E-05

Total	4.1466003830E+02	7.5745165524E+01	2.3210531688E-01	1.6398113068E-01	1.8266811009E-01	2.1440670246E-04	

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)	ESP-_Int_IDS(A)
C1	2.4096520668E+00	5.2927205709E-01	1.0983044340E+01	2.4096520668E+00	0.0000000000E+00	NULL
C2	4.6020245898E+00	8.3684713490E-01	2.5474894981E+01	4.6020245898E+00	0.0000000000E+00	NULL
H3	6.3275653545E+00	1.1241901319E+00	3.5720481603E+01	6.3275653545E+00	0.0000000000E+00	NULL
H4	7.1150564585E+00	1.3640683338E+00	3.7313421526E+01	7.1150564585E+00	0.0000000000E+00	NULL
H5	6.3379732850E+00	1.1266059801E+00	3.5762449273E+01	6.3379732850E+00	0.0000000000E+00	NULL
C6	4.7085948306E+00	8.6085842253E-01	2.5938953187E+01	4.7085948306E+00	0.0000000000E+00	NULL
H7	7.0748010576E+00	1.3562386277E+00	3.7105401792E+01	7.0748010576E+00	0.0000000000E+00	NULL
H8	6.3043974860E+00	1.1196272427E+00	3.5602392241E+01	6.3043974860E+00	0.0000000000E+00	NULL

H9	6.3115816590E+00	1.1208616399E+00	3.5644764009E+01	6.3115816590E+00
0.0000000000E+00	NULL			
C10	4.7055472971E+00	8.5978473906E-01	2.5936346000E+01	4.7055472971E+00
0.0000000000E+00	NULL			
H11	6.3785067617E+00	1.1336669755E+00	3.5995179513E+01	6.3785067617E+00
0.0000000000E+00	NULL			
H12	7.1054506220E+00	1.3617734300E+00	3.7275712207E+01	7.1054506220E+00
0.0000000000E+00	NULL			
H13	6.3640140550E+00	1.1313374106E+00	3.5906997624E+01	6.3640140550E+00
0.0000000000E+00	NULL			

Total	7.5745165524E+01	1.3925132126E+01	4.1466003830E+02	7.5745165524E+01
0.0000000000E+00	NULL			

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
ESP+*ESP+_Int_IDS(A)				

C1	2.0166214248E-01	2.1939746322E-01	6.3322931366E-03	5.4675768430E-05
5.2927205709E-01				
C2	1.6398309307E-01	1.8064940378E-01	1.2892174215E-02	2.1566866397E-04
8.3684713490E-01				
H3	1.6404916642E-01	1.7714109862E-01	8.2295083570E-03	9.2894978549E-05
1.1241901319E+00				
H4	1.7009889747E-01	1.9068357088E-01	1.1770326468E-02	1.9681822178E-04
1.3640683338E+00				
H5	1.6402718858E-01	1.7722425096E-01	8.2800039509E-03	9.4048705874E-05
1.1266059801E+00				
C6	1.6398113068E-01	1.8152601597E-01	1.3451733864E-02	2.3616843898E-04
8.6085842253E-01				
H7	1.7014146094E-01	1.9066768492E-01	1.1752601399E-02	1.9680931789E-04
1.3562386277E+00				
H8	1.6407477523E-01	1.7707791778E-01	8.1727714816E-03	9.1501240177E-05
1.1196272427E+00				
H9	1.6400910858E-01	1.7706897028E-01	8.1961775363E-03	9.1917417845E-05
1.1208616399E+00				

C10	1.6398183289E-01	1.8142676294E-01	1.3374464737E-02	2.3413186698E-04
	8.5978473906E-01			
H11	1.6402310670E-01	1.7720447149E-01	8.2751793430E-03	9.3541857699E-05
	1.1336669755E+00			
H12	1.7012141038E-01	1.9061877564E-01	1.1753282059E-02	1.9694143165E-04
	1.3617734300E+00			
H13	1.6402924508E-01	1.7723603966E-01	8.3127917334E-03	9.4821717929E-05
	1.1313374106E+00			

Total	1.6398113068E-01	1.8266811009E-01	2.1440670246E-04	1.3925132126E+01

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	NULL	NULL	NULL	NULL	NULL
C2	NULL	NULL	NULL	NULL	NULL
H3	NULL	NULL	NULL	NULL	NULL
H4	NULL	NULL	NULL	NULL	NULL
H5	NULL	NULL	NULL	NULL	NULL
C6	NULL	NULL	NULL	NULL	NULL
H7	NULL	NULL	NULL	NULL	NULL
H8	NULL	NULL	NULL	NULL	NULL
H9	NULL	NULL	NULL	NULL	NULL
C10	NULL	NULL	NULL	NULL	NULL
H11	NULL	NULL	NULL	NULL	NULL
H12	NULL	NULL	NULL	NULL	NULL
H13	NULL	NULL	NULL	NULL	NULL

Total	NULL	NULL	NULL	NULL	NULL

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1 1.2659789085E+01

C2 2.5687568444E+01

H3 3.1229206367E+01

H4 3.1634645914E+01

H5 3.1056447421E+01

C6 2.5796989652E+01

H7 3.1985712250E+01

H8 3.1010835663E+01

H9 3.1126335495E+01

C10 2.5621705311E+01

H11 3.0978053025E+01

H12 3.1985417400E+01

H13 3.1031082120E+01

Total 3.7180378815E+02

Atomic Surface Area and Volume Data:

Area(A) = Area_IAS(A|Total) + Area_IDS(A)

Vol(A) = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an

IsoSurface of the Electron Density Distribution (IsoDensity Surface)

N(Vol(A)) = Average Number of Electrons in Vol(A)

N(Vol(A))/Vol(A) = Average Electron Density in Vol(A)

%N(Vol(A)) = 100 * N(Vol(A)) / N(A)

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1 9.9972205570E+01	2.0955762524E+02		6.6726749853E+01	5.9466013781E+00	8.9118702638E-02
C2 9.9917440857E+01	2.1805465255E+02		8.5886938503E+01	6.0384581182E+00	7.0307059764E-02
H3 9.9094701071E+01	8.4131901103E+01		5.9307394150E+01	8.8308611823E-01	1.4889983465E-02
H4 9.9018165903E+01	8.3869820624E+01		5.9713892254E+01	8.4990880938E-01	1.4233016427E-02
H5 9.9091708249E+01	8.4028281151E+01		5.9239760736E+01	8.8305806750E-01	1.4906509691E-02
C6 9.9917408774E+01	2.1789134380E+02		8.5850309784E+01	6.0384293276E+00	7.0336721473E-02
H7 9.9018052612E+01	8.4373435199E+01		5.9715151679E+01	8.4990910757E-01	1.4232721239E-02
H8 9.9095957774E+01	8.4266833989E+01		5.9335983635E+01	8.8309654077E-01	1.4882984770E-02
H9 9.9094266673E+01	8.4336011201E+01		5.9297378398E+01	8.8307447914E-01	1.4892302206E-02
C10 9.9917254913E+01	2.1812265104E+02		8.5934323785E+01	6.0384891175E+00	7.0268652287E-02
H11 9.9092664308E+01	8.4158402525E+01		5.9264036209E+01	8.8306506895E-01	1.4900521892E-02
H12 9.9016346474E+01	8.4127695172E+01		5.9676391626E+01	8.4989377996E-01	1.4241708602E-02
H13 9.9093785935E+01	8.4067901402E+01		5.9287132802E+01	8.8307116171E-01	1.4894819836E-02

Total 9.9717552299E+01	1.6209865550E+03		8.5923544341E+02	3.1910141075E+01	3.7137831451E-02

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.6705220262E+02	6.1779572245E+01	5.9433166508E+00	9.6201971539E-02
9.9916983870E+01				
C2	1.7537022852E+02	7.4570135930E+01	6.0310764177E+00	8.0877905644E-02
9.9795296990E+01				
H3	6.8865785763E+01	4.4060726597E+01	8.7322845198E-01	1.9818748337E-02
9.7988532069E+01				
H4	6.8895094097E+01	4.3919073544E+01	8.3974098279E-01	1.9120188907E-02
9.7833568769E+01				
H5	6.8907753433E+01	4.4089266489E+01	8.7325490354E-01	1.9806519207E-02
9.7991653452E+01				
C6	1.7581838949E+02	7.4566528815E+01	6.0310305577E+00	8.0881203048E-02
9.9794981918E+01				
H7	6.8691256590E+01	4.3944113614E+01	8.3976774941E-01	1.9109903019E-02
9.7836540934E+01				
H8	6.8735648911E+01	4.4068278502E+01	8.7323438103E-01	1.9815486574E-02
9.7989283566E+01				
H9	6.8782036031E+01	4.4068582193E+01	8.7322900278E-01	1.9815227977E-02
9.7989455829E+01				
C10	1.7581561554E+02	7.4559777192E+01	6.0310249632E+00	8.0888452064E-02
9.9793747560E+01				
H11	6.9132451793E+01	4.4132772640E+01	8.7329665722E-01	1.9787940004E-02
9.7996507322E+01				
H12	6.8857384631E+01	4.3913288231E+01	8.3973591725E-01	1.9122592524E-02
9.7832910994E+01				
H13	6.9044269646E+01	4.4089232573E+01	8.7324924820E-01	1.9806406173E-02
9.7991620406E+01				

Total	1.3139681171E+03	6.8176134856E+02	3.1795185884E+01	4.6636826729E-02
9.9358323230E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.3613845639E+02	5.7399909465E+01	5.9369420403E+00	1.0343120914E-01	
9.9809816123E+01					
C2	1.4511505171E+02	6.5776815207E+01	6.0184314136E+00	9.1497762465E-02	
9.9586062046E+01					

H3	5.7782782754E+01	3.3624345258E+01	8.5825295828E-01	2.5524748562E-02
9.6308070740E+01				
H4	5.6795420743E+01	3.2911746031E+01	8.2396577381E-01	2.5035614125E-02
9.5995686584E+01				
H5	5.7610023808E+01	3.3695542280E+01	8.5839553450E-01	2.5475047334E-02
9.6324220340E+01				
C6	1.4522932484E+02	6.5718233422E+01	6.0182757899E+00	9.1576956296E-02
9.9583929792E+01				
H7	5.7155023153E+01	3.2884391317E+01	8.2390908231E-01	2.5054715910E-02
9.5988938268E+01				
H8	5.7565655934E+01	3.3682222868E+01	8.5836919512E-01	2.5484339276E-02
9.6321198858E+01				
H9	5.7674983687E+01	3.3668501494E+01	8.5833386663E-01	2.5493675945E-02
9.6317997047E+01				
C10	1.4503933242E+02	6.5702528039E+01	6.0182488766E+00	9.1598437021E-02
9.9582345092E+01				
H11	5.7526701411E+01	3.3632716635E+01	8.5826948426E-01	2.5518886671E-02
9.6310241318E+01				
H12	5.7146192111E+01	3.2885045298E+01	8.2391111935E-01	2.5054279594E-02
9.5989252752E+01				
H13	5.7579730312E+01	3.3648025035E+01	8.5829458884E-01	2.5508022772E-02
9.6313484059E+01				

Total	1.0883586793E+03	5.5523002235E+02	3.1613599724E+01	5.6937842788E-02
9.8790875804E+01				

Bond Contributions to Atomic Net Charges:

 $q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	C2	3.9215742868E-03		
C1	C6	3.8887536968E-03		

C1	C10	3.9560433768E-03
C1		1.1766371360E-02 5.1745338400E-02
C2	C1	3.6057392753E-02
C2	H3	-2.8888342581E-02
C2	H4	-6.1705818601E-02
C2	H5	-2.8889735311E-02
C2		-8.3426503740E-02 -4.3447536700E-02
H3	C2	6.8867309620E-02
H3		6.8867309620E-02 1.0884627666E-01
H4	C2	1.0168478564E-01
H4		1.0168478564E-01 1.4166375268E-01
H5	C2	6.8868702350E-02
H5		6.8868702350E-02 1.0884766939E-01
C6	C1	3.6090213343E-02
C6	H7	-6.1704535391E-02
C6	H8	-2.8889126281E-02
C6	H9	-2.8896181511E-02
C6		-8.3399629840E-02 -4.3420662800E-02
H7	C6	1.0168350243E-01
H7		1.0168350243E-01 1.4166246947E-01
H8	C6	6.8868093320E-02
H8		6.8868093320E-02 1.0884706036E-01
H9	C6	6.8875148550E-02
H9		6.8875148550E-02 1.0885411559E-01
C10	C1	3.6022923663E-02
C10	H11	-2.8891267711E-02
C10	H12	-6.1705225361E-02
C10	H13	-2.8895206031E-02
C10		-8.3468775440E-02 -4.3489808400E-02
H11	C10	6.8870234750E-02
H11		6.8870234750E-02 1.0884920179E-01
H12	C10	1.0168419240E-01

H12 1.0168419240E-01 1.4166315944E-01
H13 C10 6.8874173070E-02
H13 6.8874173070E-02 1.0885314011E-01

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A Mu_Intra_X(A) Mu_Bond_X(A) Mu_X(A)

C1 4.8143898349E-04 -8.8496952385E-05 3.9294203111E-04
C2 -3.3948576256E-05 -1.5716213692E-06 -3.5520197625E-05
H3 -1.0903860590E-01 4.0497592640E-02 -6.8541013260E-02
H4 -1.6523744182E-06 -1.5800716788E-16 -1.6523744184E-06
H5 1.0903857820E-01 -4.0498411638E-02 6.8540166562E-02
C6 2.0747805317E-01 -7.9546644205E-02 1.2793140896E-01
H7 1.3547777427E-02 -1.4442471541E-02 -8.9469411368E-04
H8 -9.8072794809E-03 2.2571405124E-03 -7.5501389685E-03
H9 9.9235167711E-02 -3.8244828450E-02 6.0990339261E-02
C10 -2.0743002573E-01 7.9472826715E-02 -1.2795719902E-01
H11 9.8085750500E-03 -2.2572106974E-03 7.5513643526E-03
H12 -1.3547579975E-02 1.4442569540E-02 8.9498956459E-04
H13 -9.9234169219E-02 3.8244286788E-02 -6.0989882431E-02

Total 4.9632928592E-04 -1.6521891088E-04 3.3111037504E-04

Atom A Mu_Intra_Y(A) Mu_Bond_Y(A) Mu_Y(A)

C1 -1.4558265611E-04 1.2514863341E-06 -1.4433116978E-04

C2	-2.3970555304E-01	9.1803425096E-02	-1.4790212794E-01
H3	-5.1627336049E-02	2.0775003155E-02	-3.0852332894E-02
H4	-1.5642879803E-02	1.6676940477E-02	1.0340606743E-03
H5	-5.1627711916E-02	2.0775423296E-02	-3.0852288620E-02
C6	1.2021249159E-01	-4.5917082130E-02	7.4295409460E-02
H7	7.8194760517E-03	-8.3383672144E-03	-5.1889116271E-04
H8	1.2024245184E-01	-4.5459963150E-02	7.4782488690E-02
H9	-6.8613546652E-02	2.4687250930E-02	-4.3926295722E-02
C10	1.2024491327E-01	-4.5878524971E-02	7.4366388299E-02
H11	1.2024245049E-01	-4.5461376713E-02	7.4781073777E-02
H12	7.8221017401E-03	-8.3384237941E-03	-5.1632205402E-04
H13	-6.8614679082E-02	2.4686901284E-02	-4.3927777798E-02

Total	6.0659578369E-04	1.2457752539E-05	6.1905353623E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	-4.2739013757E-02	4.4678924391E-04	-4.2292224513E-02
C2	2.3209408455E-02	-5.5984479941E-02	-3.2775071486E-02
H3	-5.1684777718E-02	1.8422956330E-02	-3.3261821388E-02
H4	1.2776755829E-01	-7.2305079220E-02	5.5462479070E-02
H5	-5.1684101579E-02	1.8423328905E-02	-3.3260772674E-02
C6	2.2761036063E-02	-5.5981231485E-02	-3.3220195422E-02
H7	1.2776703522E-01	-7.2304163655E-02	5.5462871565E-02
H8	-5.1689110335E-02	1.8423165345E-02	-3.3265944990E-02
H9	-5.1684404818E-02	1.8425052975E-02	-3.3259351843E-02
C10	2.2863767504E-02	-5.5977212419E-02	-3.3113444915E-02
H11	-5.1691126509E-02	1.8423738207E-02	-3.3267388302E-02
H12	1.2776717972E-01	-7.2304654272E-02	5.5462525448E-02
H13	-5.1685861669E-02	1.8424792021E-02	-3.3261069648E-02

Total	9.9277588867E-02	-2.7386699797E-01	-1.7458940910E-01

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	4.2741973219E-02	4.5547108061E-04	4.2294296178E-02
C2	2.4082655575E-01	1.0752734934E-01	1.5149008556E-01
H3	1.3124829771E-01	4.9102556814E-02	8.2195411707E-02
H4	1.2872159354E-01	7.4203401706E-02	5.5472117940E-02
H5	1.3124815629E-01	4.9103549834E-02	8.2194264668E-02
C6	2.4086562736E-01	1.0756368027E-01	1.5162399101E-01
H7	1.2872102303E-01	7.4202462451E-02	5.5472514346E-02
H8	1.3124859650E-01	4.9103115525E-02	8.2195184221E-02
H9	1.3125058094E-01	4.9108144323E-02	8.2192003407E-02
C10	2.4085017460E-01	1.0749054633E-01	1.5165719476E-01
H11	1.3124948611E-01	4.9104642370E-02	8.2194593638E-02
H12	1.2872130520E-01	7.4202965950E-02	5.5472149082E-02
H13	1.3125099170E-01	4.9107448803E-02	8.2193151633E-02

Total	9.9280682675E-02	2.7386704809E-01	1.7459082058E-01

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	C2	-5.9559854669E-18	
C1	C6	5.1143481547E-03	
C1	C10	-5.2028451071E-03	
C1		-8.8496952385E-05	
C2	C1	-5.4763034308E-17	

C2	H3	3.2598950630E-02
C2	H4	9.5884173602E-17
C2	H5	-3.2600522252E-02
C2		-1.5716213692E-06
H3	C2	4.0497592640E-02
H3		4.0497592640E-02
H4	C2	-1.5800716788E-16
H4		-1.5800716788E-16
H5	C2	-4.0498411638E-02
H5		-4.0498411638E-02
C6	C1	-3.9020773787E-02
C6	H7	-1.3652588975E-02
C6	H8	2.8669078759E-03
C6	H9	-2.9740189319E-02
C6		-7.9546644205E-02
H7	C6	-1.4442471541E-02
H7		-1.4442471541E-02
H8	C6	2.2571405124E-03
H8		2.2571405124E-03
H9	C6	-3.8244828450E-02
H9		-3.8244828450E-02
C10	C1	3.8948020119E-02
C10	H11	-2.8671203878E-03
C10	H12	1.3652741636E-02
C10	H13	2.9739185347E-02
C10		7.9472826715E-02
H11	C10	-2.2572106974E-03
H11		-2.2572106974E-03
H12	C10	1.4442569540E-02
H12		1.4442569540E-02
H13	C10	3.8244286788E-02
H13		3.8244286788E-02

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	C2	-5.9553828218E-03	
C1	C6	2.9527702844E-03	
C1	C10	3.0038640237E-03	
C1		1.2514863341E-06	
C2	C1	4.5016330897E-02	
C2	H3	1.5510683460E-02	
C2	H4	1.5764979497E-02	
C2	H5	1.5511431242E-02	
C2		9.1803425096E-02	
H3	C2	2.0775003155E-02	
H3		2.0775003155E-02	
H4	C2	1.6676940477E-02	
H4		1.6676940477E-02	
H5	C2	2.0775423296E-02	
H5		2.0775423296E-02	
C6	C1	-2.2528654007E-02	
C6	H7	-7.8823251073E-03	
C6	H8	-3.5987837311E-02	
C6	H9	2.0481734295E-02	
C6		-4.5917082130E-02	
H7	C6	-8.3383672144E-03	
H7		-8.3383672144E-03	
H8	C6	-4.5459963150E-02	
H8		-4.5459963150E-02	
H9	C6	2.4687250930E-02	
H9		2.4687250930E-02	
C10	C1	-2.2486649658E-02	
C10	H11	-3.5990504938E-02	
C10	H12	-7.8824132462E-03	

C1	C2	-5.9553828218E-03	
C1	C6	2.9527702844E-03	
C1	C10	3.0038640237E-03	
C1		1.2514863341E-06	
C2	C1	4.5016330897E-02	
C2	H3	1.5510683460E-02	
C2	H4	1.5764979497E-02	
C2	H5	1.5511431242E-02	
C2		9.1803425096E-02	
H3	C2	2.0775003155E-02	
H3		2.0775003155E-02	
H4	C2	1.6676940477E-02	
H4		1.6676940477E-02	
H5	C2	2.0775423296E-02	
H5		2.0775423296E-02	
C6	C1	-2.2528654007E-02	
C6	H7	-7.8823251073E-03	
C6	H8	-3.5987837311E-02	
C6	H9	2.0481734295E-02	
C6		-4.5917082130E-02	
H7	C6	-8.3383672144E-03	
H7		-8.3383672144E-03	
H8	C6	-4.5459963150E-02	
H8		-4.5459963150E-02	
H9	C6	2.4687250930E-02	
H9		2.4687250930E-02	
C10	C1	-2.2486649658E-02	
C10	H11	-3.5990504938E-02	
C10	H12	-7.8824132462E-03	

C10	H13	2.0481042871E-02
C10		-4.5878524971E-02
H11	C10	-4.5461376713E-02
H11		-4.5461376713E-02
H12	C10	-8.3384237941E-03
H12		-8.3384237941E-03
H13	C10	2.4686901284E-02
H13		2.4686901284E-02

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	C2	1.4890890805E-04	
C1	C6	1.4766261593E-04	
C1	C10	1.5021771994E-04	
C1		4.4678924391E-04	
C2	C1	-2.3343471278E-03	
C2	H3	1.4593788042E-02	
C2	H4	-8.2838412475E-02	
C2	H5	1.4594491620E-02	
C2		-5.5984479941E-02	
H3	C2	1.8422956330E-02	
H3		1.8422956330E-02	
H4	C2	-7.2305079220E-02	
H4		-7.2305079220E-02	
H5	C2	1.8423328905E-02	
H5		1.8423328905E-02	
C6	C1	-2.3364722775E-03	
C6	H7	-8.2836691689E-02	
C6	H8	1.4594184218E-02	
C6	H9	1.4597748264E-02	
C6		-5.5981231485E-02	
H7	C6	-7.2304163655E-02	

H7		-7.2304163655E-02
H8	C6	1.8423165345E-02
H8		1.8423165345E-02
H9	C6	1.8425052975E-02
H9		1.8425052975E-02
C10	C1	-2.3321159588E-03
C10	H11	1.4595266023E-02
C10	H12	-8.2837617955E-02
C10	H13	1.4597255472E-02
C10		-5.5977212419E-02
H11	C10	1.8423738207E-02
H11		1.8423738207E-02
H12	C10	-7.2304654272E-02
H12		-7.2304654272E-02
H13	C10	1.8424792021E-02
H13		1.8424792021E-02

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	C2	5.9572441965E-03	
C1	C6	5.9073863636E-03	
C1	C10	6.0096057812E-03	
C1		4.5547108061E-04	
C2	C1	4.5076814705E-02	
C2	H3	3.8939074630E-02	
C2	H4	8.4325186985E-02	
C2	H5	3.8940951913E-02	
C2		1.0752734934E-01	
H3	C2	4.9102556814E-02	
H3		4.9102556814E-02	
H4	C2	7.4203401706E-02	
H4		7.4203401706E-02	

H5	C2	4.9103549834E-02
H5		4.9103549834E-02
C6	C1	4.5117847256E-02
C6	H7	8.4323435205E-02
C6	H8	3.8940131074E-02
C6	H9	3.8949641267E-02
C6		1.0756368027E-01
H7	C6	7.4202462451E-02
H7		7.4202462451E-02
H8	C6	4.9103115525E-02
H8		4.9103115525E-02
H9	C6	4.9108144323E-02
H9		4.9108144323E-02
C10	C1	4.5033725683E-02
C10	H11	3.8943017543E-02
C10	H12	8.4324378096E-02
C10	H13	3.8948326402E-02
C10		1.0749054633E-01
H11	C10	4.9104642370E-02
H11		4.9104642370E-02
H12	C10	7.4202965950E-02
H12		7.4202965950E-02
H13	C10	4.9107448803E-02
H13		4.9107448803E-02

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle Rho*y*y \rangle(A) - \langle Rho*r*r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle Rho*y*z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle Rho*z*z \rangle(A) - \langle Rho*r*r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	9.9103901244E-02	2.3606577304E-03	-4.6799686170E-04	1.0097588906E-01	1.2688428772E-03	-2.0007979031E-01
C2	-1.2492680416E-01	-2.6338096651E-05	-4.5092427688E-04	9.1223731936E-01	4.2469252774E-02	-7.8731051520E-01
H3	2.1226778601E-01	1.7770582342E-01	1.9852774012E-01	-6.8614661971E-02	9.0609815525E-02	-1.4365312404E-01
H4	-2.0382824668E-01	9.0772730529E-07	-3.2089193433E-07	-1.3426761032E-01	-1.2060718363E-01	3.3809585700E-01
H5	2.1225853658E-01	-1.7770405260E-01	-1.9852654771E-01	-6.8612256666E-02	9.0600014596E-02	-1.4364627991E-01
C6	6.5193942303E-01	4.5095621959E-01	-3.9790822318E-02	1.3421953702E-01	-2.0551022850E-02	-7.8615896005E-01
H7	-1.5165158810E-01	3.0129036244E-02	1.0444597895E-01	-1.8644943183E-01	6.0300501060E-02	3.3810101993E-01
H8	-1.5229685677E-01	-3.2774340385E-02	2.0783642133E-02	2.9593954370E-01	-2.1723680675E-01	-1.4364268694E-01
H9	1.5549844804E-01	-2.1046630005E-01	-1.7772274427E-01	-1.1858692508E-02	1.2661020308E-01	-1.4363975554E-01
C10	6.5218616303E-01	-4.5179201821E-01	3.9377900914E-02	1.3436482631E-01	-2.0498076371E-02	-7.8655098935E-01
H11	-1.5228766636E-01	3.2778256846E-02	-2.0772265107E-02	2.9593212176E-01	-2.1723670646E-01	-1.4364445540E-01
H12	-1.5166039394E-01	-3.0120496722E-02	-1.0444618841E-01	-1.8643994777E-01	6.0306717675E-02	3.3810034171E-01
H13	1.5550540545E-01	2.1046716703E-01	1.7773054424E-01	-1.1856569444E-02	1.2661246786E-01	-1.4364883601E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$$Q\_EigVal\_n(A) = \text{nth Eigenvalue of } Q(A)$$

$$Q\_EigVal\_n\_X(A) = \text{X Component of the nth Eigenvector of } Q(A)$$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of Q(A)

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
C1	1	-2.0008590147E-01	1.5975500544E-03	-4.2270431889E-03	9.9998978992E-01
C1	2	9.7504513408E-02	8.2753483664E-01	-5.6140220886E-01	-3.6951374341E-03
C1	3	1.0258138806E-01	5.6141209640E-01	8.2753229060E-01	2.6011573655E-03
C2	1	-7.8837140422E-01	6.7846824669E-04	-2.4965171463E-02	9.9968809130E-01
C2	2	-1.2492650012E-01	9.999976919E-01	5.3130241795E-05	-6.7735295677E-04
C2	3	9.1329790434E-01	-3.6203437304E-05	9.9968832012E-01	2.4965201748E-02
H3	1	-2.3347253462E-01	-3.6646584755E-01	-1.1260272506E-01	9.2359266394E-01
H3	2	-1.5441239313E-01	-4.1226587882E-01	9.0953863293E-01	-5.2690799723E-02
H3	3	3.8788492775E-01	8.3411008131E-01	4.0007511985E-01	3.7973710739E-01
H4	1	-2.0382824670E-01	9.999999980E-01	-1.9577010222E-05	-3.7648004926E-06
H4	2	-1.6327996417E-01	1.9914561845E-05	9.7226527865E-01	2.3388079771E-01
H4	3	3.6710821087E-01	-9.1830196752E-07	-2.3388079774E-01	9.7226527885E-01
H5	1	-2.3346520959E-01	3.6651663020E-01	-1.1249641573E-01	9.2358546775E-01
H5	2	-1.5440973966E-01	4.1222251945E-01	9.0955196769E-01	-5.2799739864E-02
H5	3	3.8787494925E-01	8.3410919803E-01	-4.0007471117E-01	-3.7973947811E-01
C6	1	-7.8734277838E-01	2.4391661752E-02	1.0356580628E-02	9.9964883238E-01
C6	2	-1.2688464143E-01	-5.0095731555E-01	8.6546586274E-01	3.2570581785E-03
C6	3	9.1422741981E-01	8.6512820717E-01	5.0086084062E-01	-2.6298355411E-02
H7	1	-2.0384248191E-01	-4.9993682946E-01	8.6606187213E-01	-1.3974287723E-05
H7	2	-1.6326925839E-01	8.4204456378E-01	4.8606899204E-01	-2.3387579524E-01
H7	3	3.6711174030E-01	2.0254411660E-01	1.1693489053E-01	9.7226648210E-01
H8	1	-2.3346402975E-01	-8.5603546083E-02	3.7369067766E-01	9.2359477604E-01
H8	2	-1.5441875738E-01	9.9382651788E-01	9.7690695154E-02	5.2586884755E-02
H8	3	3.8788278713E-01	-7.0575387112E-02	9.2239460401E-01	-3.7974637487E-01
H9	1	-2.3345070786E-01	2.8076413618E-01	-2.6104354240E-01	9.2359502424E-01
H9	2	-1.5440845752E-01	5.8153202568E-01	8.1181668299E-01	5.2670450341E-02
H9	3	3.8785916538E-01	7.6353912994E-01	-5.2231211186E-01	-3.7973418974E-01

C10	1	-7.8771285149E-01	-2.4065260352E-02	1.0431368223E-02	9.9965596572E-01
C10	2	-1.2743978943E-01	5.0127612708E-01	8.6528204251E-01	3.0383101875E-03
C10	3	9.1515264092E-01	8.6495266209E-01	-5.0117678864E-01	2.6052233493E-02
H11	1	-2.3346439070E-01	8.5440969619E-02	3.7370818961E-01	9.2360274455E-01
H11	2	-1.5441170233E-01	9.9384045248E-01	-9.7630377072E-02	-5.2435336216E-02
H11	3	3.8787609303E-01	7.0576169646E-02	9.2239389552E-01	-3.7974795033E-01
H12	1	-2.0383017469E-01	4.9998697024E-01	8.6603292632E-01	-1.0831441598E-05
H12	2	-1.6328178452E-01	8.4201588538E-01	-4.8611828189E-01	2.3387660161E-01
H12	3	3.6711195921E-01	-2.0253957233E-01	1.1694437370E-01	9.7226628816E-01
H13	1	-2.3346277096E-01	-2.8078256070E-01	-2.6101851498E-01	9.2359649655E-01
H13	2	-1.5440583333E-01	-5.8151942604E-01	8.1182744739E-01	5.2643639703E-02
H13	3	3.8786860430E-01	7.6354195087E-01	5.2230788861E-01	3.7973432654E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)

C1	1.3791277360E+02	1.4938098243E+01	5.9482546616E+00	5.9384031620E+00	8.6406797081E+00
C2	1.3764841318E+02	1.5020046613E+01	6.0434475367E+00	6.1607743786E+00	9.4146947030E+00
H3	2.7618724081E+00	1.1754956965E+00	8.9115372334E-01	9.5958229306E-01	1.3616070768E+00
H4	2.6184233755E+00	1.1237446735E+00	8.5833624732E-01	9.2988719630E-01	1.3276173121E+00
H5	2.7618719762E+00	1.1754950124E+00	8.9115233061E-01	9.5957877675E-01	1.3615950872E+00

C6	1.3764841152E+02 9.4141454060E+00	1.5020040831E+01	6.0434206628E+00	6.1606513134E+00
H7	2.6184244916E+00 1.3276211907E+00	1.1237457666E+00	8.5833753053E-01	9.2988917847E-01
H8	2.7618726330E+00 1.3616056993E+00	1.1754955007E+00	8.9115293964E-01	9.5958083718E-01
H9	2.7618699072E+00 1.3615785220E+00	1.1754912656E+00	8.9114588441E-01	9.5956804549E-01
C10	1.3764841622E+02 9.4152814594E+00	1.5020058395E+01	6.0434898084E+00	6.1609301308E+00
H11	2.7618715654E+00 1.3615976172E+00	1.1754940876E+00	8.9115079821E-01	9.5957703808E-01
H12	2.6184236522E+00 1.3276201599E+00	1.1237449794E+00	8.5833684056E-01	9.2988854467E-01
H13	2.7618701247E+00 1.3615892758E+00	1.1754916503E+00	8.9114685989E-01	9.5957113176E-01

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3623763943E+02 2.0950663940E+01	-2.6831427068E+01	-1.2152908097E+01	-1.2737177013E+01	-
C2	-1.3602811909E+02 3.0081842184E+01	-2.7349173692E+01	-1.3456468302E+01	-1.6046373556E+01	-
H3	-2.0908428757E+00 5.0776661472E+00	-1.6588979522E+00	-1.8740972795E+00	-2.7639661792E+00	-
H4	-1.9782473943E+00 4.9703690846E+00	-1.5779684386E+00	-1.7973177107E+00	-2.6778106223E+00	-

H5 -2.0908418648E+00 -1.6588955852E+00 -1.8740911298E+00 -2.7639454832E+00 -
5.0775712620E+00

C6 -1.3602810585E+02 -2.7349107340E+01 -1.3456154831E+01 -1.6044957383E+01 -
3.0075587577E+01

H7 -1.9782481628E+00 -1.5779698454E+00 -1.7973209716E+00 -2.6778188183E+00 -
4.9703913733E+00

H8 -2.0908418650E+00 -1.6588959203E+00 -1.8740940076E+00 -2.7639619653E+00 -
5.0776621625E+00

H9 -2.0908346857E+00 -1.6588839483E+00 -1.8740722781E+00 -2.7639168236E+00 -
5.0775416370E+00

C10 -1.3602814112E+02 -2.7349244051E+01 -1.3456695582E+01 -1.6047118183E+01 -
3.0084256638E+01

H11 -2.0908398937E+00 -1.6588926577E+00 -1.8740876493E+00 -2.7639464422E+00 -
5.0776147898E+00

H12 -1.9782475631E+00 -1.5779695128E+00 -1.7973208077E+00 -2.6778181274E+00 -
4.9703883812E+00

H13 -2.0908351836E+00 -1.6588853566E+00 -1.8740771259E+00 -2.7639344721E+00 -
5.0776086435E+00

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
C1	2.9741273308E+00	2.9741273308E+00	5.9482546616E+00	0.0000000000E+00
C2	3.0217237683E+00	3.0217237683E+00	6.0434475367E+00	0.0000000000E+00
H3	4.4557686167E-01	4.4557686167E-01	8.9115372334E-01	0.0000000000E+00
H4	4.2916812366E-01	4.2916812366E-01	8.5833624732E-01	0.0000000000E+00
H5	4.4557616531E-01	4.4557616531E-01	8.9115233061E-01	0.0000000000E+00
C6	3.0217103314E+00	3.0217103314E+00	6.0434206628E+00	0.0000000000E+00
H7	4.2916876526E-01	4.2916876526E-01	8.5833753053E-01	0.0000000000E+00

H8	4.4557646982E-01	4.4557646982E-01	8.9115293964E-01	0.0000000000E+00
H9	4.4557294221E-01	4.4557294221E-01	8.9114588441E-01	0.0000000000E+00
C10	3.0217449042E+00	3.0217449042E+00	6.0434898084E+00	0.0000000000E+00
H11	4.4557539910E-01	4.4557539910E-01	8.9115079821E-01	0.0000000000E+00
H12	4.2916842028E-01	4.2916842028E-01	8.5833684056E-01	0.0000000000E+00
H13	4.4557342994E-01	4.4557342994E-01	8.9114685989E-01	0.0000000000E+00

Total	1.6000262912E+01	1.6000262912E+01	3.2000525824E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A').

For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies $E_{\text{IQA}}(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

Cyclopropane

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\cycloprop\cycloprop.wfn

Sum File: D:\calc\ellipticity\cycloprop\cycloprop.sum

SumViz File: D:\calc\ellipticity\cycloprop\cycloprop.sumviz

Wfn Title: cycloprop.wfn

Total memory allocated for AIMSum = 0.687 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs) = 24.0000003000

Number of Alpha electrons (from MO Occs) = 12.0000001500

Number of Beta electrons (from MO Occs) = 12.0000001500
 Number of electron pairs ($N*(N-1)/2$) = 276.0000070500
 Number of electron pairs (from Muller 2EDM) = 275.9999034500
 Number of electron pairs (from Muller 2EDM, no SOSI) = 276.2978683723

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	-1.4272162200E+00	-8.2400029000E-01	0.0000000000E+00
C2	6.0	0.0000000000E+00	1.6479850200E+00	0.0000000000E+00
C3	6.0	1.4272103600E+00	-8.2400167000E-01	0.0000000000E+00
H4	1.0	-2.3791849000E+00	-1.3735835600E+00	1.7276096400E+00
H5	1.0	-2.3791849000E+00	-1.3735835600E+00	-1.7276096400E+00
H6	1.0	1.4210000000E-05	2.7472052700E+00	1.7276086100E+00
H7	1.0	1.4210000000E-05	2.7472052700E+00	-1.7276086100E+00
H8	1.0	2.3791882600E+00	-1.3735709000E+00	-1.7276084700E+00
H9	1.0	2.3791882600E+00	-1.3735709000E+00	1.7276084700E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
C1	-4.3810549900E-02	3.2327994708E-05	3.7911200870E+01	-3.7965181871E+01	2.3121840598E-01
C2	-4.3719091200E-02	1.2363157396E-04	3.7911234344E+01	-3.7965215392E+01	2.3137319568E-01

C3	-4.3978817100E-02	-1.0339953606E-04	3.7911192690E+01	-3.7965173679E+01	2.3115829702E-01
H4	2.1954407140E-02	2.4817706910E-05	6.1301404741E-01	-6.1388690585E-01	1.5356192860E-01
H5	2.1955227240E-02	2.5191069761E-05	6.1301392801E-01	-6.1388678628E-01	1.5356220114E-01
H6	2.1952629590E-02	2.6163783381E-05	6.1301622864E-01	-6.1388909019E-01	1.5356322367E-01
H7	2.1952928240E-02	2.5789726656E-05	6.1301589108E-01	-6.1388875214E-01	1.5356316184E-01
H8	2.1955071280E-02	2.5143149195E-05	6.1301408176E-01	-6.1388694025E-01	1.5356295745E-01
H9	2.1956916170E-02	2.6777758393E-05	6.1301418015E-01	-6.1388703879E-01	1.5356380956E-01

Total 2.1872146000E-04 2.0644322690E-04 1.1741171626E+02 -1.1757889646E+02

Molecular charge q(Mol) from the wfn file: -2.9999999706E-07

Molecular energy E(Mol) from the wfn file: -1.1708856920E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0014238800E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR

C1	48	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
C2	48	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
C3	48	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H4	11	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H5	11	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H6	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H7	11	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H8	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H9	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 207

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -1.42721303064119E+00 -8.23998448758258E-01 8.40356104565346E-20

Type = (3,-3) NACP C1

Rho = 1.1936148909E+02 Rho at Nucleus = 1.1936148786E+02

GradRho = -1.9339232424E-11 -9.6818453442E-12 6.1984690732E-17

HessRho_EigVals = -1.8096066431E+05 -1.8095925606E+05 -1.8095922844E+05

HessRho_EigVec1 = 8.6604837520E-01 4.9996021022E-01 1.5807087800E-14

HessRho_EigVec2 = -1.2169270082E-14 -1.0536660940E-14 1.0000000000E+00

HessRho_EigVec3 = -4.9996021022E-01 8.6604837520E-01 3.0411072588E-15

DelSqRho = -5.4287914881E+05

Bond Ellipticity = NA

V = -1.3573505284E+05

G = 7.6328208275E+00

K = 1.3572742002E+05

L = 1.3571978720E+05
Vnuc = 1.6292514645E+06
Ven = -1.9446988090E+08
Vrep = 1.9433414585E+08
DelSqV = 4.6000389189E+09
DelSqVen = 8.8448664781E+11
DelSqVrep = -8.7988660889E+11
DelSqG = 2.0578527777E+08
DelSqK = -4.8058241966E+09
Stress_EigVals = -4.5245184948E+04 -4.5245035675E+04 -4.5244832220E+04
Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec2 = -4.9993899130E-01 8.6606062431E-01 0.0000000000E+00
Stress_EigVec3 = 8.6606062431E-01 4.9993899130E-01 0.0000000000E+00
-DivStress = -4.7738607157E+03 -2.7559868476E+03 -1.1906550036E-10

CP# 2 Coords = -1.71451309716394E-11 1.64798133751151E+00 -1.26101288367180E-18

Type = (3,-3) NACP C2

Rho = 1.1936149198E+02 Rho at Nucleus = 1.1936149075E+02

GradRho = -5.4581917211E-17 -2.3047154792E-12 3.1155984623E-17

HessRho_EigVals = -1.8096066848E+05 -1.8095926029E+05 -1.8095923259E+05

HessRho_EigVec1 = 1.2342908679E-05 9.9999999992E-01 1.1174354082E-13

HessRho_EigVec2 = -1.3792403198E-18 -1.1174354082E-13 1.0000000000E+00

HessRho_EigVec3 = 9.9999999992E-01 -1.2342908679E-05 0.0000000000E+00

DelSqRho = -5.4287916137E+05

Bond Ellipticity = NA

V = -1.3573505603E+05

G = 7.6328440772E+00

K = 1.3572742319E+05

L = 1.3571979034E+05

Vnuc = 1.6293391244E+06

Ven = -1.9448034883E+08

Vrep = 1.9434461377E+08

DelSqV = 4.6000390391E+09
DelSqVen = 8.8453425152E+11
DelSqVrep = -8.7993421248E+11
DelSqG = 2.0578528238E+08
DelSqK = -4.8058243215E+09
Stress_EigVals = -4.5245185998E+04 -4.5245036745E+04 -4.5244833286E+04
Stress_EigVec1 = -1.9891142187E-18 -1.4049027283E-13 1.0000000000E+00
Stress_EigVec2 = 9.999999990E-01 -1.4158376793E-05 0.0000000000E+00
Stress_EigVec3 = 1.4158376793E-05 9.999999990E-01 1.4049027285E-13
-DivStress = 2.5710610928E-02 5.5119815963E+03 1.7430169593E-09

CP# 3 Coords = 1.42720717068228E+00 -8.23999828760187E-01 -1.08180990243689E-19

Type = (3,-3) NACP C3

Rho = 1.1936148966E+02 Rho at Nucleus = 1.1936148843E+02

GradRho = 5.9901006516E-12 8.2685591482E-12 4.9568042946E-17

HessRho_EigVals = -1.8096066530E+05 -1.8095925706E+05 -1.8095922941E+05

HessRho_EigVec1 = 8.6605271395E-01 -4.9995269442E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 4.9995269442E-01 8.6605271395E-01 0.0000000000E+00

DelSqRho = -5.4287915178E+05

Bond Ellipticity = NA

V = -1.3573505360E+05

G = 7.6328267057E+00

K = 1.3572742077E+05

L = 1.3571978794E+05

Vnuc = 1.6292676356E+06

Ven = -1.9447181204E+08

Vrep = 1.9433607698E+08

DelSqV = 4.6000389557E+09

DelSqVen = 8.8449542554E+11

DelSqVrep = -8.7989538658E+11

DelSqG = 2.0578527905E+08

DelSqK = -4.8058242348E+09

Stress_EigVals = -4.5245185197E+04 -4.5245035930E+04 -4.5244832471E+04

Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec2 = 4.9993358172E-01 8.6606374700E-01 0.0000000000E+00

Stress_EigVec3 = 8.6606374700E-01 -4.9993358172E-01 0.0000000000E+00

-DivStress = 4.7737992730E+03 -2.7559839461E+03 1.5817307790E-10

CP# 4 Coords = -2.36582697686002E+00 -1.36587193809028E+00 1.70383323178715E+00

Type = (3,-3) NACP H4

Rho = 4.2911590714E-01 Rho at Nucleus = 4.2584397223E-01

GradRho = -8.0118232590E-16 -5.8475380088E-16 -1.7939729012E-16

HessRho_EigVals = -8.5750073995E+00 -8.5679016276E+00 -7.9034789742E+00

HessRho_EigVec1 = 7.2547808759E-01 4.1883355772E-01 5.4613184796E-01

HessRho_EigVec2 = -4.9997837007E-01 8.6603789146E-01 -4.3569004452E-06

HessRho_EigVec3 = -4.7297269888E-01 -2.7305095035E-01 8.3769923279E-01

DelSqRho = -2.5046388001E+01

Bond Ellipticity = NA

V = -6.2826443820E+00

G = 1.0523690827E-02

K = 6.2721206912E+00

L = 6.2615970003E+00

Vnuc = 4.2171849735E+01

Ven = -1.8096611555E+01

Vrep = 1.1813967173E+01

DelSqV = 1.6190244699E+03

DelSqVen = 1.0562525112E+03

DelSqVrep = 5.6277195872E+02

DelSqG = 1.2304341784E+02

DelSqK = -1.7420678878E+03

Stress_EigVals = -2.1507217011E+00 -2.1499067522E+00 -1.9820159287E+00

Stress_EigVec1 = -4.9995650501E-01 8.6605051409E-01 1.1829448625E-05

Stress_EigVec2 = 7.2532044648E-01 4.1870792232E-01 5.4643748563E-01

Stress_EigVec3 = -4.7323751227E-01 -2.7320355566E-01 8.3749989502E-01

-DivStress = -7.0141858730E+00 -4.0493379521E+00 1.2480436995E+01

CP# 5 Coords = -2.36582697686002E+00 -1.36587193809028E+00 -1.70383323178715E+00

Type = (3,-3) NACP H5

Rho = 4.2911590714E-01 Rho at Nucleus = 4.2584397223E-01

GradRho = -2.9824035367E-16 1.6714081602E-16 7.9171806944E-16

HessRho_EigVals = -8.5750073995E+00 -8.5679016276E+00 -7.9034789742E+00

HessRho_EigVec1 = 7.2547808759E-01 4.1883355772E-01 -5.4613184796E-01

HessRho_EigVec2 = -4.9997837007E-01 8.6603789146E-01 4.3569004261E-06

HessRho_EigVec3 = 4.7297269888E-01 2.7305095035E-01 8.3769923279E-01

DelSqRho = -2.5046388001E+01

Bond Ellipticity = NA

V = -6.2826443820E+00

G = 1.0523690827E-02

K = 6.2721206912E+00

L = 6.2615970003E+00

Vnuc = 4.2171849735E+01

Ven = -1.8096611555E+01

Vrep = 1.1813967173E+01

DelSqV = 1.6190244699E+03

DelSqVen = 1.0562525112E+03

DelSqVrep = 5.6277195872E+02

DelSqG = 1.2304341784E+02

DelSqK = -1.7420678878E+03

Stress_EigVals = -2.1507217011E+00 -2.1499067522E+00 -1.9820159287E+00

Stress_EigVec1 = -4.9995650501E-01 8.6605051409E-01 -1.1829448859E-05

Stress_EigVec2 = 7.2532044648E-01 4.1870792232E-01 -5.4643748563E-01

Stress_EigVec3 = 4.7323751227E-01 2.7320355566E-01 8.3749989502E-01

-DivStress = -7.0141858730E+00 -4.0493379521E+00 -1.2480436995E+01

CP# 6 Coords = 1.39823355709686E-05 2.73178118566140E+00 1.70383223804281E+00

Type = (3,-3) NACP H6

Rho = 4.2911673533E-01 Rho at Nucleus = 4.2584480437E-01

GradRho = 7.9096664534E-19 6.1402932831E-16 -7.4623692816E-16

HessRho_EigVals = -8.5750238836E+00 -8.5679180407E+00 -7.9034954922E+00

HessRho_EigVec1 = 9.8265211517E-06 8.3769929061E-01 -5.4613175921E-01

HessRho_EigVec2 = 9.999999992E-01 -1.2504781268E-05 -1.1878548268E-06

HessRho_EigVec3 = 7.8243233381E-06 5.4613175916E-01 8.3769929066E-01

DelSqRho = -2.5046437416E+01

Bond Ellipticity = NA

V = -6.2826568381E+00

G = 1.0523742011E-02

K = 6.2721330961E+00

L = 6.2616093541E+00

Vnuc = 4.2171921476E+01

Ven = -1.8096677266E+01

Vrep = 1.1814020428E+01

DelSqV = 1.6190277843E+03

DelSqVen = 1.0562563920E+03

DelSqVrep = 5.6277139237E+02

DelSqG = 1.2304366744E+02

DelSqK = -1.7420714518E+03

Stress_EigVals = -2.1507258531E+00 -2.1499108966E+00 -1.9820200884E+00

Stress_EigVec1 = 9.999999979E-01 -2.0258489626E-05 3.7484313685E-06

Stress_EigVec2 = 1.9014767848E-05 8.3749999819E-01 -5.4643732730E-01

Stress_EigVec3 = 7.9306836620E-06 5.4643732725E-01 8.3749999840E-01

-DivStress = 1.1964617015E-04 8.0991335020E+00 1.2480442460E+01

CP# 7 Coords = 1.39823355709065E-05 2.73178118566140E+00 -1.70383223804282E+00

Type = (3,-3) NACP H7

Rho = 4.2911673533E-01 Rho at Nucleus = 4.2584480437E-01

GradRho = -6.2390263138E-19 -1.1033308275E-15 3.0205900650E-16

HessRho_EigVals = -8.5750238836E+00 -8.5679180407E+00 -7.9034954922E+00

HessRho_EigVec1 = 9.8265211197E-06 8.3769929061E-01 5.4613175921E-01

HessRho_EigVec2 = 9.999999992E-01 -1.2504781242E-05 1.1878548452E-06

HessRho_EigVec3 = -7.8243233392E-06 -5.4613175916E-01 8.3769929066E-01

DelSqRho = -2.5046437416E+01

Bond Ellipticity = NA

V = -6.2826568381E+00

G = 1.0523742011E-02

K = 6.2721330961E+00

L = 6.2616093541E+00

Vnuc = 4.2171921476E+01

Ven = -1.8096677266E+01

Vrep = 1.1814020428E+01

DelSqV = 1.6190277843E+03

DelSqVen = 1.0562563920E+03

DelSqVrep = 5.6277139237E+02

DelSqG = 1.2304366744E+02

DelSqK = -1.7420714518E+03

Stress_EigVals = -2.1507258531E+00 -2.1499108966E+00 -1.9820200884E+00

Stress_EigVec1 = 9.999999979E-01 -2.0258489750E-05 -3.7484314470E-06

Stress_EigVec2 = 1.9014767995E-05 8.3749999819E-01 5.4643732730E-01

Stress_EigVec3 = -7.9306836640E-06 -5.4643732725E-01 8.3749999840E-01

-DivStress = 1.1964617018E-04 8.0991335020E+00 -1.2480442460E+01

CP# 8 Coords = 2.36583018469445E+00 -1.36585950619675E+00 -1.70383208531402E+00

Type = (3,-3) NACP H8

Rho = 4.2911616387E-01 Rho at Nucleus = 4.2584422932E-01

GradRho = -3.5743887755E-16 5.6663220595E-16 -5.1484806586E-16

HessRho_EigVals = -8.5750124429E+00 -8.5679066049E+00 -7.9034838979E+00

HessRho_EigVec1 = 7.2548309854E-01 -4.1882386347E-01 5.4613262595E-01

HessRho_EigVec2 = 4.9996603287E-01 8.6604501381E-01 6.2474466521E-06

HessRho_EigVec3 = -4.7297805416E-01 2.7304323000E-01 8.3769872558E-01

DelSqRho = -2.5046402946E+01

Bond Ellipticity = NA

V = -6.2826481624E+00

G = 1.0523712972E-02

K = 6.2721244494E+00

L = 6.2616007365E+00

Vnuc = 4.2171865215E+01

Ven = -1.8096629024E+01

Vrep = 1.1813980862E+01

DelSqV = 1.6190254588E+03

DelSqVen = 1.0562535291E+03

DelSqVrep = 5.6277192968E+02

DelSqG = 1.2304349186E+02

DelSqK = -1.7420689507E+03

Stress_EigVals = -2.1507229735E+00 -2.1499080209E+00 -1.9820171679E+00

Stress_EigVec1 = 4.9993721884E-01 8.6606164734E-01 -1.5028595053E-05

Stress_EigVec2 = 7.2533019450E-01 -4.1868999637E-01 5.4643828187E-01

Stress_EigVec3 = -4.7324294624E-01 2.7319573560E-01 8.3749937545E-01

-DivStress = 7.0142699973E+00 -4.0492204682E+00 -1.2480431996E+01

CP# 9 Coords = 2.36583018469445E+00 -1.36585950619675E+00 1.70383208531402E+00

Type = (3,-3) NACP H9

Rho = 4.2911616387E-01 Rho at Nucleus = 4.2584422932E-01

GradRho = 6.3986361731E-16 3.4372062310E-16 -8.0510723835E-16

HessRho_EigVals = -8.5750124429E+00 -8.5679066049E+00 -7.9034838979E+00

HessRho_EigVec1 = 7.2548309854E-01 -4.1882386347E-01 -5.4613262595E-01

HessRho_EigVec2 = 4.9996603287E-01 8.6604501381E-01 -6.2474466215E-06

HessRho_EigVec3 = 4.7297805416E-01 -2.7304323000E-01 8.3769872558E-01

DelSqRho = -2.5046402946E+01

Bond Ellipticity = NA

V = -6.2826481624E+00

G = 1.0523712972E-02

K = 6.2721244494E+00

L = 6.2616007365E+00
Vnuc = 4.2171865215E+01
Ven = -1.8096629024E+01
Vrep = 1.1813980862E+01
DelSqV = 1.6190254588E+03
DelSqVen = 1.0562535291E+03
DelSqVrep = 5.6277192968E+02
DelSqG = 1.2304349186E+02
DelSqK = -1.7420689507E+03
Stress_EigVals = -2.1507229735E+00 -2.1499080209E+00 -1.9820171679E+00
Stress_EigVec1 = 4.9993721884E-01 8.6606164734E-01 1.5028594993E-05
Stress_EigVec2 = 7.2533019450E-01 -4.1868999637E-01 -5.4643828187E-01
Stress_EigVec3 = 4.7324294624E-01 -2.7319573560E-01 8.3749937545E-01
-DivStress = 7.0142699973E+00 -4.0492204682E+00 1.2480431996E+01

CP# 10 Coords = -4.03853116164409E-06 -2.29264614272367E-05 -2.03167278616762E-15

Type = (3,+1) RCP C1 C2 C3
Rho = 1.9467611684E-01
GradRho = 1.7210576083E-17 4.4314918608E-17 2.6956452620E-19
HessRho_EigVals = -3.4860141930E-01 2.3008942280E-01 2.3010037371E-01
HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec2 = -6.5892307722E-02 9.9782674036E-01 0.0000000000E+00
HessRho_EigVec3 = 9.9782674036E-01 6.5892307722E-02 0.0000000000E+00
DelSqRho = 1.1158837722E-01
Bond Ellipticity = NA
V = -2.6611839530E-01
G = 1.4700774480E-01
K = 1.1911065050E-01
L = -2.7897094305E-02
Vnuc = 1.2771187028E+01
Ven = -2.4862450981E+00
Vrep = 2.2201267028E+00

DelSqV = -7.8308205297E-01

DelSqVen = -1.4251160356E+00

DelSqVrep = 6.4203398266E-01

DelSqG = -1.0252435258E-02

DelSqK = 7.9333448823E-01

Stress_EigVals = -1.2618388608E-01 -6.9969584912E-02 -6.9964924307E-02

Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec2 = -6.2355385509E-02 9.9805400951E-01 0.0000000000E+00

Stress_EigVec3 = 9.9805400951E-01 6.2355385509E-02 0.0000000000E+00

-DivStress = -4.2644833643E-07 -2.4018140287E-06 -2.0032136129E-15

CP# 11 Coords = -7.83262228904495E-01 4.52206246754633E-01 4.25877156284896E-16

Type = (3,-1) BCP C2 C1

Rho = 2.3331459709E-01

GradRho = 2.8928458829E-16 -1.3339943062E-16 -1.4106273501E-18

HessRho_EigVals = -4.3796465148E-01 -2.8753679511E-01 3.0948220841E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 8.6602225814E-01 -5.0000544838E-01 0.0000000000E+00

HessRho_EigVec3 = 5.0000544838E-01 8.6602225814E-01 0.0000000000E+00

DelSqRho = -4.1601923818E-01

Bond Ellipticity = 5.2316037089E-01

V = -2.9207567567E-01

G = 9.4035433061E-02

K = 1.9804024261E-01

L = 1.0400480954E-01

Vnuc = 1.2583946474E+01

Ven = -2.9360184014E+00

Vrep = 2.6439427257E+00

DelSqV = -1.5219684313E+00

DelSqVen = 5.2351638253E+00

DelSqVrep = -6.7571322567E+00

DelSqG = 9.9192157912E-01

DelSqK = 5.3004685222E-01

Stress_EigVals = -1.7627064616E-01 -1.6323416573E-01 4.7429136226E-02

Stress_EigVec1 = 8.6602329493E-01 -5.0000365262E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 5.0000365262E-01 8.6602329493E-01 0.0000000000E+00

-DivStress = 3.4761754590E-02 -2.0072227595E-02 -1.5260079243E-15

BPL = 2.8653200381E+00 = 1.4326610238E+00 + 1.4326590143E+00

GBL_I = 2.8544038079E+00

GBL_II = 2.8544101863E+00

GBL_III = 2.8589329642E+00 = 1.4294676586E+00 + 1.4294653056E+00

GBL_IV = 2.8589391252E+00 = 1.4294707390E+00 + 1.4294683862E+00

CP# 12 Coords = -3.41570858497766E-06 -9.04428248970183E-01 5.00331085716506E-16

Type = (3,-1) BCP C3 C1

Rho = 2.3330998509E-01

GradRho = -3.5642087629E-18 9.1151158767E-13 1.3469410045E-18

HessRho_EigVals = -4.3795350250E-01 -2.8752070224E-01 3.0948142414E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 5.7397850692E-07 1.0000000000E+00 0.0000000000E+00

HessRho_EigVec3 = 1.0000000000E+00 -5.7397850692E-07 0.0000000000E+00

DelSqRho = -4.1599278060E-01

Bond Ellipticity = 5.2320684769E-01

V = -2.9206691450E-01

G = 9.4034359674E-02

K = 1.9803255482E-01

L = 1.0399819515E-01

Vnuc = 1.2583906773E+01

Ven = -2.9359511017E+00

Vrep = 2.6438841872E+00

DelSqV = -1.5219424660E+00

DelSqVen = 5.2348143696E+00

DelSqVrep = -6.7567568355E+00

DelSqG = 9.9188535486E-01

DelSqK = 5.3005711110E-01

Stress_EigVals = -1.7626619277E-01 -1.6322948682E-01 4.7428765091E-02

Stress_EigVec1 = 7.6867254284E-07 1.0000000000E+00 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 1.0000000000E+00 -7.6867254284E-07 0.0000000000E+00

-DivStress = -8.4771564324E-07 4.0139640051E-02 -4.1140118719E-16

BPL = 2.8653358687E+00 = 1.4326683970E+00 + 1.4326674717E+00

GBL_I = 2.8544202013E+00

GBL_II = 2.8544265800E+00

GBL_III = 2.8589491169E+00 = 1.4294750046E+00 + 1.4294741123E+00

GBL_IV = 2.8589552782E+00 = 1.4294780852E+00 + 1.4294771930E+00

CP# 13 Coords = 7.83259130074438E-01 4.52205286063047E-01 -4.53116858772206E-16

Type = (3,-1) BCP C2 C3

Rho = 2.3331523337E-01

GradRho = -1.4108154300E-16 -4.4458006544E-17 1.2460422297E-18

HessRho_EigVals = -4.3796611354E-01 -2.8753920264E-01 3.0948262162E-01

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 8.6602338545E-01 5.0000349584E-01 0.0000000000E+00

HessRho_EigVec3 = -5.0000349584E-01 8.6602338545E-01 0.0000000000E+00

DelSqRho = -4.1602269456E-01

Bond Ellipticity = 5.2315270239E-01

V = -2.9207693229E-01

G = 9.4035629326E-02

K = 1.9804130297E-01

L = 1.0400567364E-01

Vnuc = 1.2583953399E+01

Ven = -2.9360280240E+00

Vrep = 2.6439510917E+00

DelSqV = -1.5219728539E+00

DelSqVen = 5.2352102012E+00

DelSqVrep = -6.7571830551E+00

DelSqG = 9.9192722281E-01

DelSqK = 5.3004563109E-01

Stress_EigVals = -1.7627120165E-01 -1.6323487241E-01 4.7429141774E-02

Stress_EigVec1 = 8.6602424442E-01 5.0000200808E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = -5.0000200808E-01 8.6602424442E-01 0.0000000000E+00

-DivStress = -3.4761785684E-02 -2.0071982564E-02 -1.0191646980E-15

BPL = 2.8653182787E+00 = 1.4326601512E+00 + 1.4326581275E+00

GBL_I = 2.8544020730E+00

GBL_II = 2.8544084514E+00

GBL_III = 2.8589312004E+00 = 1.4294667642E+00 + 1.4294644361E+00

GBL_IV = 2.8589373614E+00 = 1.4294698447E+00 + 1.4294675167E+00

CP# 14 Coords = -2.03181984595263E+00 -1.17304663661948E+00 1.11135190832013E+00

Type = (3,-1) BCP H4 C1

Rho = 2.7800754814E-01

GradRho = -9.6304072683E-18 -9.2719363075E-17 -5.3673195615E-17

HessRho_EigVals = -7.2504395423E-01 -7.0282295554E-01 4.8359042893E-01

HessRho_EigVec1 = 7.2570588083E-01 4.1894880211E-01 5.4574066711E-01

HessRho_EigVec2 = -4.9996844501E-01 8.6604362129E-01 3.8535841078E-06

HessRho_EigVec3 = -4.7263360918E-01 -2.7285590929E-01 8.3795413015E-01

DelSqRho = -9.4427648083E-01

Bond Ellipticity = 3.1616779894E-02

V = -3.3073114886E-01

G = 4.7331014328E-02

K = 2.8340013454E-01

L = 2.3606912021E-01

Vnuc = 1.0397803886E+01

Ven = -2.8906679645E+00

Vrep = 2.5599368156E+00

DelSqV = -2.5929222688E+00

DelSqVen = 9.8184016622E+00

DelSqVrep = -1.2411323931E+01

DelSqG = 1.5988094343E+00

DelSqK = 9.9411283453E-01

Stress_EigVals = -2.1946900736E-01 -2.1535011505E-01 1.0408797355E-01

Stress_EigVec1 = -4.9996377937E-01 8.6604631474E-01 6.6658723936E-06

Stress_EigVec2 = 7.2672554102E-01 4.1953047553E-01 5.4393397406E-01

Stress_EigVec3 = -4.7106921716E-01 -2.7195212966E-01 8.3912801873E-01

-DivStress = 5.3248951041E-02 3.0742391398E-02 -9.7230473190E-02

BPL = 2.0195854104E+00 = 7.0694871237E-01 + 1.3126366980E+00

GBL_I = 2.0193243177E+00

GBL_II = 2.0476623761E+00

GBL_III = 2.0193842717E+00 = 7.0694871033E-01 + 1.3124355614E+00

GBL_IV = 2.0477234298E+00 = 7.3528982739E-01 + 1.3124336024E+00

CP# 15 Coords = -2.03181984595263E+00 -1.17304663661948E+00 -1.11135190832014E+00

Type = (3,-1) BCP C1 H5

Rho = 2.7800754814E-01

GradRho = -7.0754806136E-17 1.3233987181E-16 1.9415093068E-16

HessRho_EigVals = -7.2504395423E-01 -7.0282295554E-01 4.8359042893E-01

HessRho_EigVec1 = 7.2570588083E-01 4.1894880211E-01 -5.4574066711E-01

HessRho_EigVec2 = -4.9996844501E-01 8.6604362129E-01 -3.8535841165E-06

HessRho_EigVec3 = 4.7263360918E-01 2.7285590929E-01 8.3795413015E-01

DelSqRho = -9.4427648083E-01

Bond Ellipticity = 3.1616779894E-02

V = -3.3073114886E-01

G = 4.7331014328E-02

K = 2.8340013454E-01

L = 2.3606912021E-01

Vnuc = 1.0397803886E+01

Ven = -2.8906679645E+00

Vrep = 2.5599368156E+00

DelSqV = -2.5929222688E+00

DelSqVen = 9.8184016622E+00

DelSqVrep = -1.2411323931E+01

DelSqG = 1.5988094343E+00

DelSqK = 9.9411283453E-01

Stress_EigVals = -2.1946900736E-01 -2.1535011505E-01 1.0408797355E-01

Stress_EigVec1 = -4.9996377937E-01 8.6604631474E-01 -6.6658723715E-06

Stress_EigVec2 = 7.2672554102E-01 4.1953047553E-01 -5.4393397406E-01

Stress_EigVec3 = 4.7106921716E-01 2.7195212966E-01 8.3912801873E-01

-DivStress = 5.3248951041E-02 3.0742391398E-02 9.7230473190E-02

BPL = 2.0195854104E+00 = 1.3126366980E+00 + 7.0694871237E-01

GBL_I = 2.0193243177E+00

GBL_II = 2.0476623761E+00

GBL_III = 2.0193842717E+00 = 1.3124355614E+00 + 7.0694871033E-01

GBL_IV = 2.0477234298E+00 = 1.3124336024E+00 + 7.3528982739E-01

CP# 16 Coords = 8.58310334529045E-06 2.34610933332521E+00 1.11134999523899E+00

Type = (3,-1) BCP H6 C2

Rho = 2.7800784090E-01

GradRho = 4.0038883457E-18 -7.4157711371E-17 1.0960586596E-16

HessRho_EigVals = -7.2504408276E-01 -7.0282267121E-01 4.8358897174E-01

HessRho_EigVec1 = 1.3724145019E-05 8.3795414916E-01 -5.4574063777E-01

HessRho_EigVec2 = 9.9999999988E-01 -1.5593178269E-05 1.2052915671E-06

HessRho_EigVec3 = 7.4998519836E-06 5.4574063772E-01 8.3795414927E-01

DelSqRho = -9.4427778223E-01

Bond Ellipticity = 3.1617380129E-02

V = -3.3073235356E-01

G = 4.7331454002E-02

K = 2.8340089956E-01

L = 2.3606944556E-01

Vnuc = 1.0397826825E+01

Ven = -2.8906773856E+00

Vrep = 2.5599450320E+00
DelSqV = -2.5929073943E+00
DelSqVen = 9.8184368541E+00
DelSqVrep = -1.2411344248E+01
DelSqG = 1.5988139047E+00
DelSqK = 9.9409348967E-01
Stress_EigVals = -2.1946941016E-01 -2.1535045821E-01 1.0408751480E-01
Stress_EigVec1 = 9.9999999986E-01 -1.6395989341E-05 1.4309615423E-06
Stress_EigVec2 = 1.4536684447E-05 8.3912814529E-01 -5.4393377867E-01
Stress_EigVec3 = 7.7175723326E-06 5.4393377862E-01 8.3912814541E-01
-DivStress = -3.9909715269E-07 -6.1488643804E-02 -9.7234002932E-02
BPL = 2.0195843377E+00 = 7.0694977801E-01 + 1.3126345597E+00
GBL_I = 2.0193232546E+00
GBL_II = 2.0476612678E+00
GBL_III = 2.0193832069E+00 = 7.0694977598E-01 + 1.3124334309E+00
GBL_IV = 2.0477223198E+00 = 7.3529084770E-01 + 1.3124314721E+00

CP# 17 Coords = 8.58310334515589E-06 2.34610933332513E+00 -1.11134999523882E+00

Type = (3,-1) BCP C2 H7
Rho = 2.7800784090E-01
GradRho = -2.1837899044E-18 -1.6470793887E-16 -2.7614198636E-16
HessRho_EigVals = -7.2504408276E-01 -7.0282267121E-01 4.8358897174E-01
HessRho_EigVec1 = 1.3724144961E-05 8.3795414916E-01 5.4574063777E-01
HessRho_EigVec2 = 9.9999999988E-01 -1.5593178220E-05 -1.2052915357E-06
HessRho_EigVec3 = -7.4998519832E-06 -5.4574063772E-01 8.3795414927E-01
DelSqRho = -9.4427778223E-01
Bond Ellipticity = 3.1617380129E-02
V = -3.3073235356E-01
G = 4.7331454002E-02
K = 2.8340089956E-01
L = 2.3606944556E-01
Vnuc = 1.0397826825E+01

Ven = -2.8906773856E+00
Vrep = 2.5599450320E+00
DelSqV = -2.5929073943E+00
DelSqVen = 9.8184368541E+00
DelSqVrep = -1.2411344248E+01
DelSqG = 1.5988139047E+00
DelSqK = 9.9409348967E-01
Stress_EigVals = -2.1946941016E-01 -2.1535045821E-01 1.0408751480E-01
Stress_EigVec1 = 9.9999999986E-01 -1.6395989406E-05 -1.4309615840E-06
Stress_EigVec2 = 1.4536684523E-05 8.3912814529E-01 5.4393377867E-01
Stress_EigVec3 = -7.7175723325E-06 -5.4393377862E-01 8.3912814541E-01
-DivStress = -3.9909715241E-07 -6.1488643804E-02 9.7234002933E-02
BPL = 2.0195843377E+00 = 1.3126345597E+00 + 7.0694977801E-01
GBL_I = 2.0193232546E+00
GBL_II = 2.0476612678E+00
GBL_III = 2.0193832069E+00 = 1.3124334309E+00 + 7.0694977598E-01
GBL_IV = 2.0477223198E+00 = 1.3124314721E+00 + 7.3529084770E-01

CP# 18 Coords = 2.03181925046661E+00 -1.17303945841207E+00 -1.11135087473345E+00

Type = (3,-1) BCP C3 H8
Rho = 2.7800765984E-01
GradRho = 5.5763672929E-17 -3.8936185526E-17 1.0866848434E-16
HessRho_EigVals = -7.2504411297E-01 -7.0282287990E-01 4.8359002362E-01
HessRho_EigVec1 = 7.2571297629E-01 -4.1893559161E-01 5.4574137293E-01
HessRho_EigVec2 = 4.9995333700E-01 8.6605234299E-01 -4.5324089024E-06
HessRho_EigVec3 = -4.7263869590E-01 2.7284850976E-01 8.3795367047E-01
DelSqRho = -9.4427696925E-01
Bond Ellipticity = 3.1617116770E-02
V = -3.3073158073E-01
G = 4.7331169209E-02
K = 2.8340041152E-01
L = 2.3606924231E-01

Vnuc = 1.0397808949E+01
Ven = -2.8906705333E+00
Vrep = 2.5599389526E+00
DelSqV = -2.5929187226E+00
DelSqVen = 9.8184115213E+00
DelSqVrep = -1.2411330244E+01
DelSqG = 1.5988109836E+00
DelSqK = 9.9410773896E-01
Stress_EigVals = -2.1946917681E-01 -2.1535025175E-01 1.0408784783E-01
Stress_EigVec1 = 4.9994880887E-01 8.6605495695E-01 -6.8769843752E-06
Stress_EigVec2 = 7.2673244053E-01 -4.1951757734E-01 5.4393470397E-01
Stress_EigVec3 = -4.7107446161E-01 2.7194450508E-01 8.3912754559E-01
-DivStress = -5.3249746455E-02 3.0742397007E-02 9.7231539838E-02
BPL = 2.0195849568E+00 = 1.3126359751E+00 + 7.0694898174E-01
GBL_I = 2.0193238590E+00
GBL_II = 2.0476619072E+00
GBL_III = 2.0193838150E+00 = 1.3124348353E+00 + 7.0694897970E-01
GBL_IV = 2.0477229630E+00 = 1.3124328764E+00 + 7.3529008668E-01

CP# 19 Coords = 2.03181925046661E+00 -1.17303945841207E+00 1.11135087473345E+00

Type = (3,-1) BCP H9 C3
Rho = 2.7800765984E-01
GradRho = -6.2058265927E-17 2.5938372306E-17 2.5217903659E-16
HessRho_EigVals = -7.2504411297E-01 -7.0282287990E-01 4.8359002362E-01
HessRho_EigVec1 = 7.2571297629E-01 -4.1893559161E-01 -5.4574137293E-01
HessRho_EigVec2 = 4.9995333700E-01 8.6605234299E-01 4.5324089131E-06
HessRho_EigVec3 = 4.7263869590E-01 -2.7284850976E-01 8.3795367047E-01
DelSqRho = -9.4427696925E-01
Bond Ellipticity = 3.1617116770E-02
V = -3.3073158073E-01
G = 4.7331169209E-02
K = 2.8340041152E-01

$$L = 2.3606924231E-01$$

$$V_{nuc} = 1.0397808949E+01$$

$$V_{en} = -2.8906705333E+00$$

$$V_{rep} = 2.5599389526E+00$$

$$DelSqV = -2.5929187226E+00$$

$$DelSqVen = 9.8184115213E+00$$

$$DelSqVrep = -1.2411330244E+01$$

$$DelSqG = 1.5988109836E+00$$

$$DelSqK = 9.9410773896E-01$$

$$Stress\_EigVals = -2.1946917681E-01 \ -2.1535025175E-01 \ 1.0408784783E-01$$

$$Stress\_EigVec1 = 4.9994880887E-01 \ 8.6605495695E-01 \ 6.8769843650E-06$$

$$Stress\_EigVec2 = 7.2673244053E-01 \ -4.1951757734E-01 \ -5.4393470397E-01$$

$$Stress\_EigVec3 = 4.7107446161E-01 \ -2.7194450508E-01 \ 8.3912754559E-01$$

$$-DivStress = -5.3249746455E-02 \ 3.0742397007E-02 \ -9.7231539838E-02$$

$$BPL = 2.0195849568E+00 = 7.0694898174E-01 + 1.3126359751E+00$$

$$GBL\_I = 2.0193238590E+00$$

$$GBL\_II = 2.0476619072E+00$$

$$GBL\_III = 2.0193838150E+00 = 7.0694897970E-01 + 1.3124348353E+00$$

$$GBL\_IV = 2.0477229630E+00 = 7.3529008668E-01 + 1.3124328764E+00$$

$$\text{Number of NACPs} = 9$$

$$\text{Number of NNACPs} = 0$$

$$\text{Number of BCPs} = 9$$

$$\text{Number of RCPs} = 1$$

$$\text{Number of CCPs} = 0$$

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
C3	C1	C2	75.30810674	59.99976981	59.99976980	66.45074697	66.45058521
C3	C2	C1	75.30860718	60.00040007	60.00040008	66.45145383	66.45129208
C2	C3	C1	75.30817592	59.99983012	59.99983012	66.45079593	66.45063417
H4	C1	C2	113.89079016	117.69739699	117.70317044	116.42122065	116.42113930
H4	C1	C3	113.89171524	117.69829634	117.70407201	116.42216396	116.42208260
H5	C1	C2	113.89079016	117.69739699	117.70317044	116.42122065	116.42113930
H5	C1	C3	113.89171524	117.69829634	117.70407201	116.42216396	116.42208260
H5	C1	H4	118.46559338	115.07950629	115.06551213	115.72757311	115.72784539
H6	C2	C1	113.89139381	117.69796188	117.70373678	116.42179329	116.42171193
H6	C2	C3	113.89099593	117.69754887	117.70332277	116.42137544	116.42129409
H7	C2	C1	113.89139381	117.69796188	117.70373678	116.42179329	116.42171193
H7	C2	C3	113.89099593	117.69754887	117.70332277	116.42137544	116.42129409
H7	C2	H6	118.46551895	115.07949607	115.06550224	115.72755521	115.72782748
H8	C3	C1	113.89199695	117.69861055	117.70438708	116.42247810	116.42239674
H8	C3	C2	113.89052400	117.69713073	117.70290367	116.42094492	116.42086357
H9	C3	C1	113.89199695	117.69861055	117.70438708	116.42247810	116.42239674
H9	C3	C2	113.89052400	117.69713073	117.70290367	116.42094492	116.42086357
H9	C3	H8	118.46554068	115.07942600	115.06543140	115.72750437	115.72777665

Total time for electron density critical point search, analysis and connectivity = 13 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$V_{ee}(A) = V_{ee}(A, Mol)$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$
C1	-3.7911200870E+01	3.7911200870E+01	-1.2614002563E+02	-8.9977314673E+01		
C2	-3.7911234344E+01	3.7911234344E+01	-1.2613954694E+02	-8.9977167538E+01		
C3	-3.7911192690E+01	3.7911192690E+01	-1.2614122724E+02	-8.9977662775E+01		
H4	-6.1301404741E-01	6.1301404741E-01	-7.5093012126E+00	-1.2543435571E+00		
H5	-6.1301392801E-01	6.1301392801E-01	-7.5092951341E+00	-1.2543429938E+00		
H6	-6.1301622864E-01	6.1301622864E-01	-7.5093279619E+00	-1.2543462466E+00		
H7	-6.1301589108E-01	6.1301589108E-01	-7.5093259191E+00	-1.2543458822E+00		
H8	-6.1301408176E-01	6.1301408176E-01	-7.5092974284E+00	-1.2543432396E+00		
H9	-6.1301418015E-01	6.1301418015E-01	-7.5092835492E+00	-1.2543421572E+00		
Total	-1.1741171626E+02	1.1741171626E+02	-4.2347663102E+02	-2.7745820906E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$E_e(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	$E_e(A)$	$W(A)$	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
C1	-3.7911200870E+01					
C2	-3.7911234344E+01					
C3	-3.7911192690E+01					
H4	-6.1301404741E-01					
H5	-6.1301392801E-01					
H6	-6.1301622864E-01					
H7	-6.1301589108E-01					
H8	-6.1301408176E-01					
H9	-6.1301418015E-01					
Total	-1.1741171626E+02					

IQA Atomic Energy Components:

$E_{IQA}(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$\text{Vee}(\text{A}) = \text{Vee}(\text{A}, \text{Mol}) = (1/2)[\text{Vee}(\text{A}, \text{Mol}) + \text{Vee}(\text{Mol}, \text{A})]$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$\text{Vnn}(\text{A}, \text{Mol})/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$\text{VeeC}(\text{A})$ = Coulomb Part of $\text{Vee}(\text{A})$

$\text{VeeX}(\text{A})$ = Exchange-Correlation Part of $\text{Vee}(\text{A})$

See "2EDM Note" and "DFT Note".

Atom A VeeC(A)	E_IQA(A) VeeX(A)	T(A)	Vne(A,Mol)/2	Ven(A,Mol)/2	Vee(A)	Vnn(A,Mol)/2
C1 1.8388449153E+01			3.7911200870E+01	-6.2644804298E+01	-6.3070012816E+01	
C2 1.8388510836E+01			3.7911234344E+01	-6.2644874381E+01	-6.3069773469E+01	
C3 1.8388459331E+01			3.7911192690E+01	-6.2644817069E+01	-6.3070613619E+01	
H4 3.4131337120E+00			6.1301404741E-01	-3.9673786720E+00	-3.7546506063E+00	
H5 3.4131337120E+00			6.1301392801E-01	-3.9673786720E+00	-3.7546475671E+00	
H6 3.4131413395E+00			6.1301622864E-01	-3.9673870297E+00	-3.7546639809E+00	
H7 3.4131413395E+00			6.1301589108E-01	-3.9673870297E+00	-3.7546629595E+00	
H8 3.4131351655E+00			6.1301408176E-01	-3.9673803672E+00	-3.7546487142E+00	
H9 3.4131351655E+00			6.1301418015E-01	-3.9673803672E+00	-3.7546417746E+00	
Total 7.5644239754E+01			1.1741171626E+02	-2.1173878789E+02	-2.1173831551E+02	

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$
C1	3.7911200870E+01	-8.9977314673E+01				
C2	3.7911234344E+01	-8.9977167538E+01				
C3	3.7911192690E+01	-8.9977662775E+01				
H4	6.1301404741E-01	-1.2543435571E+00				
H5	6.1301392801E-01	-1.2543429938E+00				
H6	6.1301622864E-01	-1.2543462466E+00				
H7	6.1301589108E-01	-1.2543458822E+00				
H8	6.1301408176E-01	-1.2543432396E+00				
H9	6.1301418015E-01	-1.2543421572E+00				
Total	1.1741171626E+02	-2.7745820906E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

= $Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$

= Interatomic ("Interaction") Contribution to $E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$V_{en}(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[V_{en}(A,Mol) - V_{en}(A,A)]$$

$V_{ee}(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= V_{ee}(A,Mol) - V_{ee}(A,A)$$

$V_{nn}(A) = V_{nn}(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A,A')$ = Coulomb Part of $V_{ee}(A,A')$

$V_{eeX}(A,A')$ = Exchange-Correlation Part of $V_{ee}(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E_{IQA\_Inter}(A)$	$V_{ne}(A,A')/2$	$V_{en}(A,A')/2$	$V_{ee}(A,A')$	$V_{nn}(A)$	$V_{eeC}(A,A')$
$V_{eeX}(A,A')$						
C1	-1.7656146962E+01	-1.8081355480E+01		1.8388449153E+01		
C2	-1.7656290612E+01	-1.8081189700E+01		1.8388510836E+01		
C3	-1.7655985681E+01	-1.8081782231E+01		1.8388459331E+01		
H4	-3.3402068934E+00	-3.1274788277E+00		3.4131337120E+00		
H5	-3.3402071751E+00	-3.1274760702E+00		3.4131337120E+00		
H6	-3.3402139064E+00	-3.1274908576E+00		3.4131413395E+00		
H7	-3.3402140886E+00	-3.1274900184E+00		3.4131413395E+00		
H8	-3.3402087474E+00	-3.1274770944E+00		3.4131351655E+00		
H9	-3.3402092886E+00	-3.1274706960E+00		3.4131351655E+00		
Total	-7.3009683354E+01	-7.3009210975E+01		7.5644239754E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$$\%Loc(A) = 100 * LI(A) / N(A)$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A)$$

$$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other
Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1 2.9053011965E+01	6.0438105500E+00		4.2879015478E+00	7.0946988035E+01	1.7559090023E+00
C2 2.9052987275E+01	6.0437190911E+00		4.2878381527E+00	7.0947012725E+01	1.7558809385E+00
C3 2.9052820819E+01	6.0439788165E+00		4.2880324806E+00	7.0947179181E+01	1.7559463359E+00
H4 4.9629722415E+01	9.7804559345E-01		4.9264428032E-01	5.0370277585E+01	4.8540131313E-01
H5 4.9629740613E+01	9.7804477319E-01		4.9264368918E-01	5.0370259387E+01	4.8540108401E-01
H6 4.9629647204E+01	9.7804737030E-01		4.9264591093E-01	5.0370352796E+01	4.8540145937E-01
H7 4.9629661583E+01	9.7804707191E-01		4.9264562000E-01	5.0370338417E+01	4.8540145192E-01
H8 4.9629746004E+01	9.7804492803E-01		4.9264371445E-01	5.0370253996E+01	4.8540121358E-01
H9 4.9629794379E+01	9.7804308311E-01		4.9264231203E-01	5.0370205621E+01	4.8540077109E-01
Total 3.4084242165E+01	2.3999781278E+01		1.5819637708E+01	6.5915757835E+01	8.1801435698E+00

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

$DI\_Bond(A,A')/2$ = Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$DI\_NonBond(A,A')/2$ = Non-Bonding Contribution to $DI(A,A')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	6.0438105500E+00	4.2879015478E+00	1.7559090023E+00	1.6888730821E+00	6.7035920190E-02
C2	6.0437190911E+00	4.2878381527E+00	1.7558809385E+00	1.6888264907E+00	6.7054447824E-02
C3	6.0439788165E+00	4.2880324806E+00	1.7559463359E+00	1.6889156352E+00	6.7030700709E-02
H4	9.7804559345E-01	4.9264428032E-01	4.8540131313E-01	4.2621222167E-01	5.9189091455E-02
H5	9.7804477319E-01	4.9264368918E-01	4.8540108401E-01	4.2621692076E-01	5.9184163257E-02
H6	9.7804737030E-01	4.9264591093E-01	4.8540145937E-01	4.2616010932E-01	5.9241350048E-02
H7	9.7804707191E-01	4.9264562000E-01	4.8540145192E-01	4.2623369873E-01	5.9167753187E-02
H8	9.7804492803E-01	4.9264371445E-01	4.8540121358E-01	4.2624166142E-01	5.9159552160E-02
H9	9.7804308311E-01	4.9264231203E-01	4.8540077109E-01	4.2622861376E-01	5.9172157331E-02
Total	2.3999781278E+01	1.5819637708E+01	8.1801435698E+00	7.6239084336E+00	5.5623513616E-01

Atomic Electron Pair Contributions:

$D2(A,A)$ = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

$D2(A,A')$ = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	$D2(A,A)$	$D2(A,A')$	$D2(A,Mol)$

C1	1.6119872209E+01	5.3383936081E+01	6.9503808290E+01
C2	1.6119351150E+01	5.3383405341E+01	6.9502756491E+01
C3	1.6120823727E+01	5.3384919657E+01	6.9505743384E+01
H4	2.3196445127E-01	1.1015549757E+01	1.1247514208E+01
H5	2.3196394459E-01	1.1015540831E+01	1.1247504776E+01
H6	2.3196537381E-01	1.1015569268E+01	1.1247534642E+01
H7	2.3196522744E-01	1.1015565983E+01	1.1247531210E+01
H8	2.3196408340E-01	1.1015542473E+01	1.1247506556E+01
H9	2.3196298020E-01	1.1015522359E+01	1.1247485340E+01

Total	4.9751833146E+01	2.2624555175E+02	2.7599738490E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A)$ = Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A)$ = Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	

C1	C2	3.6108877573E+01	8.3643126225E-01	6.9197342912E+00	6.9198390067E+00	(Bonded)
C1	C3	3.6110434627E+01	8.3645661705E-01	6.9199440495E+00	6.9197513959E+00	(Bonded)
C2	C3	3.6109893108E+01	8.3643410298E-01	6.9198625082E+00	6.9195651439E+00	(Bonded)
C1	H4	5.4849100544E+00	8.5242444334E-01	7.0520447016E+00	4.3577950202E+01	(Bonded)
C2	H4	5.8942791248E+00	3.3507400632E-02	2.7720845498E-01	1.7129774346E+00	
C3	H4	5.8945279492E+00	3.3517798439E-02	2.7728256052E-01	1.7135089950E+00	
C1	H5	5.4849003979E+00	8.5243384151E-01	7.0521224520E+00	4.3578467207E+01	(Bonded)
C2	H5	5.8942673601E+00	3.3521015381E-02	2.7732109051E-01	1.7136748900E+00	
C3	H5	5.8945226896E+00	3.3518402225E-02	2.7728755546E-01	1.7135412991E+00	
H4	H5	9.4187574288E-01	2.9393275473E-02	1.5026536426E+00	1.5026549029E+00	
C1	H6	5.8943766439E+00	3.3512742379E-02	2.7724845196E-01	1.7132474048E+00	
C2	H6	5.4848834546E+00	8.5232021864E-01	7.0512891631E+00	4.3572542830E+01	(Bonded)
C3	H6	5.8945392587E+00	3.3516657910E-02	2.7727312527E-01	1.7134475756E+00	
H4	H6	9.5385895170E-01	5.4319380214E-03	2.7769349700E-01	2.7769299251E-01	
H5	H6	9.5379916496E-01	5.5499069873E-03	2.8372458702E-01	2.8372383362E-01	
C1	H7	5.8943749667E+00	3.3512489919E-02	2.7724636338E-01	1.7132350211E+00	
C2	H7	5.4848080618E+00	8.5246739746E-01	7.0525067810E+00	4.3580080240E+01	(Bonded)
C3	H7	5.8945346965E+00	3.3522175326E-02	2.7731876917E-01	1.7137301613E+00	
H4	H7	9.5379967574E-01	5.5499062602E-03	2.8372431190E-01	2.8372388301E-01	
H5	H7	9.5385785267E-01	5.4319479090E-03	2.7769423537E-01	2.7769358270E-01	
H6	H7	9.4187974220E-01	2.9393249024E-02	1.5026495606E+00	1.5026500190E+00	
C1	H8	5.8943618944E+00	3.3512720098E-02	2.7724826764E-01	1.7132505439E+00	
C2	H8	5.8942727799E+00	3.3512047372E-02	2.7724689771E-01	1.7132161526E+00	

C3	H8	5.4850411652E+00	8.5248332285E-01	7.0523354625E+00	4.3580989912E+01 (Bonded)
H4	H8	9.5379758061E-01	5.5499028997E-03	2.8372414010E-01	2.8372433314E-01
H5	H8	9.5385594182E-01	5.4315759685E-03	2.7767522088E-01	2.7767517692E-01
H6	H8	9.5379935505E-01	5.5498296891E-03	2.8371988196E-01	2.8372059044E-01
H7	H8	9.5385790921E-01	5.4321376956E-03	2.7770328503E-01	2.7770389375E-01
C1	H9	5.8943512549E+00	3.3511698519E-02	2.7723981619E-01	1.7132015500E+00
C2	H9	5.8942740624E+00	3.3487182017E-02	2.7704118533E-01	1.7119482053E+00
C3	H9	5.4850430622E+00	8.5245722751E-01	7.0521195837E+00	4.3579738062E+01 (Bonded)
H4	H9	9.5385492228E-01	5.4316107140E-03	2.7767676427E-01	2.7767747698E-01
H5	H9	9.5379498264E-01	5.5498855033E-03	2.8372348871E-01	2.8372397899E-01
H6	H9	9.5385642860E-01	5.4320737523E-03	2.7769993138E-01	2.7770114865E-01
H7	H9	9.5379726930E-01	5.5498086955E-03	2.8371889528E-01	2.8372005238E-01
H8	H9	9.4187347516E-01	2.9393203341E-02	1.5026509774E+00	1.5026538119E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
C1	C2	3.5861486859E+01	2.8827182552E+01	2.3713383193E+01
C1	C3	3.5861191754E+01	2.8826921606E+01	2.3713154450E+01
C1	H4	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01
C1	H5	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01
C1	Total	1.5610704074E+02	1.2306377115E+02	9.9666496499E+01

C2	C1	3.5861486859E+01	2.8827182552E+01	2.3713383193E+01
C2	C3	3.5861528811E+01	2.8827219564E+01	2.3713415462E+01
C2	H6	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01
C2	H7	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01

C2	Total	1.5610291296E+02	1.2307073975E+02	9.9659980617E+01
C3	C1	3.5861191754E+01	2.8826921606E+01	2.3713154450E+01
C3	C2	3.5861528811E+01	2.8827219564E+01	2.3713415462E+01
C3	H8	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01
C3	H9	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01

C3	Total	1.5610262482E+02	1.2307294916E+02	9.9659752264E+01
H4	C1	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01

H4	Total	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01
H5	C1	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01

H5	Total	4.2192181065E+01	3.2704833496E+01	2.6119979428E+01
H6	C2	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01

H6	Total	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01
H7	C2	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01

H7	Total	4.2189948647E+01	3.2708168818E+01	2.6116590981E+01
H8	C3	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01

H8	Total	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01
H9	C3	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01
H9	Total	4.2189952129E+01	3.2709403994E+01	2.6116591176E+01
Total	Total	7.2145674221E+02	5.6545227268E+02	4.5569255255E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta \rho\_IAS(A B)$	$V\_IAS(A B)$
C1	C2	9.9487405478E-01	6.8717708883E-01	3.7596162769E-01	-3.1121546114E-01	1.2448618446E+00	-1.0631387165E+00
C1	C3	9.9485030350E-01	6.8715340361E-01	3.7594562465E-01	-3.1120777896E-01	1.2448311159E+00	-1.0630990283E+00
C1	H4	9.6328460150E-01	5.3280786397E-01	4.0724479048E-01	-1.2556307349E-01	5.0225229397E-01	-9.4005265445E-01
C1	H5	9.6328460150E-01	5.3280786397E-01	4.0724479048E-01	-1.2556307349E-01	5.0225229397E-01	-9.4005265445E-01

C1 Total 3.9162935613E+00 2.4399462204E+00 1.5663968333E+00 -8.7354938708E-01
3.4941975484E+00 -4.0063430537E+00

C2 C1 9.9487405478E-01 6.8717708883E-01 3.7596162769E-01 -3.1121546114E-01
1.2448618446E+00 -1.0631387165E+00

C2 C3 9.9487770588E-01 6.8718149450E-01 3.7596378500E-01 -3.1121770949E-01
1.2448708380E+00 -1.0631452795E+00

C2 H6 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

C2 H7 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

C2 Total 3.9163299389E+00 2.4399812379E+00 1.5664202128E+00 -8.7356102507E-01
3.4942441003E+00 -4.0064014507E+00

C3 C1 9.9485030350E-01 6.8715340361E-01 3.7594562465E-01 -3.1120777896E-01
1.2448311159E+00 -1.0630990283E+00

C3 C2 9.9487770588E-01 6.8718149450E-01 3.7596378500E-01 -3.1121770949E-01
1.2448708380E+00 -1.0631452795E+00

C3 H8 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

C3 H9 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

C3 Total 3.9163032475E+00 2.4399538216E+00 1.5664026456E+00 -8.7355117597E-01
3.4942047040E+00 -4.0063564673E+00

H4 C1 9.6328460150E-01 5.3280786397E-01 4.0724479048E-01 -1.2556307349E-01
5.0225229397E-01 -9.4005265445E-01

H4 Total 9.6328460150E-01 5.3280786397E-01 4.0724479048E-01 -1.2556307349E-01
5.0225229397E-01 -9.4005265445E-01

H5 C1 9.6328460150E-01 5.3280786397E-01 4.0724479048E-01 -1.2556307349E-01
5.0225229397E-01 -9.4005265445E-01

H5 Total 9.6328460150E-01 5.3280786397E-01 4.0724479048E-01 -1.2556307349E-01
5.0225229397E-01 -9.4005265445E-01

H6 C2 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

H6 Total 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

H7 C2 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

H7 Total 9.6328908910E-01 5.3281132729E-01 4.0724740007E-01 -1.2556392722E-01
5.0225570886E-01 -9.4005872736E-01

H8 C3 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

H8 Total 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

H9 C3 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

H9 Total 9.6328761907E-01 5.3280946176E-01 4.0724661800E-01 -1.2556284376E-01
5.0225137504E-01 -9.4005607976E-01

Total Total 1.7528649367E+01 1.0516738586E+01 7.1426973089E+00 -3.3740412771E+00
1.3496165108E+01 -1.7659435895E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP-_Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	2.9612300741E+01						

C2	3.0788646795E+01						

C3	2.9893191276E+01						

H4 5.0097853164E+01
H5 5.0399204072E+01
H6 5.0284786889E+01
H7 5.0194309683E+01
H8 5.0268104607E+01
H9 5.0526834129E+01

Total 3.9206523136E+02

0.001 IsoDensity Surface:

Atom A Area_IDS(A) ESP_Int_IDS(A) ESP_Max_IDS(A) ESP_Min_IDS(A) ESP_Avg_IDS(A)
ESP_MAD_IDS(A) ESP_Var_IDS(A)

C1 2.7848315802E+01 -2.7137025745E-01 1.5205574972E-02 -1.9562265408E-02 -9.7445841746E-
03 5.7590167992E-03 5.5255090353E-05

C2 2.7968384389E+01 -2.7490234302E-01 1.5127997654E-02 -1.9594890640E-02 -9.8290390750E-
03 5.6642669144E-03 5.4473312961E-05

C3 2.7772009792E+01 -2.7195275293E-01 1.5213547194E-02 -1.9572978032E-02 -9.7923324590E-
03 5.6676371803E-03 5.4192369640E-05

H4 4.2074320895E+01 2.6278302309E-01 1.6940146053E-02 -9.8263230048E-03 6.2456866206E-
03 5.9735272877E-03 4.8093393685E-05

H5 4.1940083341E+01 2.6273673794E-01 1.6943171280E-02 -1.0165535350E-02 6.2645735776E-
03 5.9855374354E-03 4.8306547910E-05

H6 4.1666530079E+01 2.6269141176E-01 1.6949352302E-02 -1.0117999023E-02 6.3046145494E-
03 5.9477661301E-03 4.7542389551E-05

H7 4.1861043197E+01 2.6283127761E-01 1.6945074006E-02 -1.0042270127E-02 6.2786604809E-
03 5.9429523142E-03 4.7733832287E-05

H8 4.1768585372E+01 2.6473938165E-01 1.6957778968E-02 -9.2891859041E-03 6.3382415107E-
03 5.9340753086E-03 4.7427475546E-05

H9 4.1850141209E+01 2.6300577051E-01 1.6942784920E-02 -1.0283408837E-02 6.2844655457E-
03 5.9728564562E-03 4.8123793779E-05

Total 3.3474941408E+02 7.6056224916E-01 1.6957778968E-02 -1.9594890640E-02 2.2720345942E-
03 9.7974027798E-05

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
C1	3.0602563626E-01 2.5913535774E+01	4.1831515220E-03 -2.8869794686E-01	1.9347800275E+00	1.7327689406E-02	
C2	3.0914889144E-01 2.6181889699E+01	4.2255564272E-03 -2.9202561723E-01	1.7864946901E+00	1.7123274208E-02	
C3	3.0568894426E-01 2.6001164692E+01	4.1680827901E-03 -2.8882084860E-01	1.7708450994E+00	1.6868095664E-02	
H4	3.3159709754E-01 9.2235507444E+00	3.6647572903E-03 -3.4407037227E-02	3.2850770150E+01	2.9719006031E-01	
H5	3.3157194564E-01 9.1163299479E+00	3.6719142717E-03 -3.4417603848E-02	3.2823753393E+01	2.9715434179E-01	
H6	3.2850257153E-01 8.9178327764E+00	3.6370945008E-03 -3.2905579888E-02	3.2748697302E+01	2.9559699165E-01	
H7	3.2978309451E-01 9.0069277207E+00	3.6484163712E-03 -3.3475908448E-02	3.2854115477E+01	2.9630718606E-01	
H8	3.3013267753E-01 8.6144543941E+00	3.6589606996E-03 -3.2696647940E-02	3.3154130978E+01	2.9743602959E-01	
H9	3.3087587851E-01 9.2008481237E+00	3.6668382682E-03 -3.3935054001E-02	3.2649293085E+01	2.9694082451E-01	
Total	2.9033267372E+00 1.3217653387E+02	3.4524772141E-02 -1.0713822440E+00	2.0257288020E+02	1.8319444932E+00	

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
C1	6.6815981847E-07 2.0575750885E-04	8.9558963603E-03	4.5659861759E-03	2.6138639869E-05
C2	1.4144202367E-04 2.0667184443E-04	9.5848447258E-03	4.2187716730E-03	2.3816426763E-05

C3	5.7043106793E-05	9.5254495547E-03	4.3178094022E-03	2.4148019036E-05
2.0343859550E-04				
H4	4.5279111903E-05	9.0466694982E-03	4.2334450342E-03	2.3768909735E-05
3.4694072442E-03				
H5	1.0320818941E-05	9.0530274899E-03	4.2473742153E-03	2.3866522559E-05
3.4735352758E-03				
H6	3.2976382791E-05	9.0262213766E-03	4.2609550697E-03	2.4026582998E-05
3.4549631787E-03				
H7	1.3943886735E-05	9.0188757713E-03	4.2461961552E-03	2.3844448047E-05
3.4557459509E-03				
H8	7.6927516350E-05	8.9713112911E-03	4.2904005628E-03	2.4362348024E-05
3.4761036880E-03				
H9	3.6790862018E-05	9.0948622912E-03	4.2217647646E-03	2.3618701710E-05
3.4717698220E-03				

Total	6.6815981847E-07	9.0433847382E-03	2.3944045386E-05	2.1417393108E-02

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-1.3568668542E-04	-1.1140816497E-02	4.5195557740E-03	2.9369329245E-05	
3.9773940132E-03					
C2	-6.2515079206E-05	-1.1153725747E-02	4.4814898783E-03	2.9093046604E-05	
4.0188845828E-03					
C3	-1.2738701679E-04	-1.1107996585E-02	4.4922440887E-03	2.9091896605E-05	
3.9646441946E-03					
H4	-7.3208530599E-06	-3.7303461736E-03	2.2862673351E-03	7.2640014917E-06	
1.9535004603E-04					
H5	-6.2232907089E-06	-3.7753793516E-03	2.3256824704E-03	7.5073505817E-06	
1.9837899584E-04					
H6	-6.1370344853E-05	-3.6898628527E-03	2.2119471928E-03	6.8081838714E-06	
1.8213132215E-04					
H7	-6.7405203011E-06	-3.7166844774E-03	2.3359838307E-03	7.5776150534E-06	
1.9267042038E-04					
H8	-1.1276351791E-06	-3.7955564502E-03	2.2061959947E-03	6.8205177017E-06	
1.8285701168E-04					

H9	-6.0153020822E-05	-3.6882528159E-03	2.3407616075E-03	7.5979286738E-06
	1.9506844626E-04			

Total	-1.1276351791E-06	-8.1056917794E-03	3.3463464771E-05	1.3107379033E-02

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

C1	2.6920033244E+01						

C2	2.7059948682E+01						

C3	2.6617201607E+01						

H4	3.5655799323E+01						

H5	3.5515379835E+01						

H6	3.5550321004E+01						

H7	3.5335176478E+01						

H8	3.5529467887E+01						

H9	3.5487547350E+01						

Total	2.9367087541E+02						

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an

Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1 9.9891733089E+01	1.8571934148E+02	9.1277794230E+01	6.0372671029E+00	6.6141684884E-02	
C2 9.9890853365E+01	1.8689155976E+02	9.1283942849E+01	6.0371225752E+00	6.6135646498E-02	
C3 9.9892050763E+01	1.8599581610E+02	9.1372165837E+01	6.0374543881E+00	6.6075421686E-02	
H4 9.8868556629E+01	9.2290034229E+01	6.8665391448E+01	9.6697956083E-01	1.4082488142E-02	
H5 9.8868855285E+01	9.2591385137E+01	6.8677693778E+01	9.6698167100E-01	1.4079996252E-02	
H6 9.8869670310E+01	9.2474735536E+01	6.8700542407E+01	9.6699221060E-01	1.4075466899E-02	
H7 9.8870072268E+01	9.2384258330E+01	6.8710517609E+01	9.6699584666E-01	1.4073476381E-02	
H8 9.8869127654E+01	9.2458056736E+01	6.8687893362E+01	9.6698448909E-01	1.4077946517E-02	
H9 9.8867273606E+01	9.2716786258E+01	6.8640309223E+01	9.6696453167E-01	1.4087415145E-02	
Total 9.9641501309E+01	1.1135219736E+03	6.8601625074E+02	2.3913742376E+01	3.4858856988E-02	

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1 9.9741764791E+01	1.5091208695E+02	7.7423506696E+01	6.0282033031E+00	7.7860117171E-02	
C2 9.9739896824E+01	1.5103912414E+02	7.7325350821E+01	6.0279991859E+00	7.7956312151E-02	
C3 9.9742161944E+01	1.5084495895E+02	7.7513982874E+01	6.0283951396E+00	7.7771711839E-02	

H4	7.4779154391E+01 9.7626765365E+01	4.9838568904E+01	9.5483427610E-01	1.9158541208E-02
H5	7.4644916837E+01 9.7624165960E+01	4.9810982229E+01	9.5480805212E-01	1.9168625259E-02
H6	7.4374698897E+01 9.7626807893E+01	4.9834722068E+01	9.5483642741E-01	1.9160063261E-02
H7	7.4569212015E+01 9.7632777481E+01	4.9893756825E+01	9.5489452123E-01	1.9138557246E-02
H8	7.4477989366E+01 9.7631486801E+01	4.9879705095E+01	9.5487980549E-01	1.9143653790E-02
H9	7.4559545203E+01 9.7625668520E+01	4.9824006865E+01	9.5482109900E-01	1.9163876193E-02

Total	9.0020168675E+02 9.9224536817E+01	5.3134458238E+02	2.3813671810E+01	4.4817755934E-02

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.2658652974E+02 9.9499878888E+01	6.7313465761E+01	6.0135841774E+00	8.9337016144E-02
C2	1.2671992930E+02 9.9500626726E+01	6.7316890266E+01	6.0135383733E+00	8.9331791019E-02
C3	1.2627695387E+02 9.9498650604E+01	6.7332106234E+01	6.0136773658E+00	8.9313667760E-02
H4	6.1775778751E+01 9.5746975310E+01	3.7040322885E+01	9.3644907232E-01	2.5281881997E-02
H5	6.1635359263E+01 9.5743837264E+01	3.7025441707E+01	9.3641759560E-01	2.5291193094E-02
H6	6.1666911985E+01 9.5750290766E+01	3.7056698610E+01	9.3648320100E-01	2.5271630667E-02
H7	6.1451767459E+01 9.5739725727E+01	3.7003818198E+01	9.3637958398E-01	2.5304944991E-02
H8	6.1646059063E+01 9.5746603325E+01	3.7039369478E+01	9.3644479824E-01	2.5282417370E-02
H9	6.1604138526E+01 9.5747585183E+01	3.7044753513E+01	9.3645263482E-01	2.5278954400E-02

Total	7.4936342796E+02	4.2417286665E+02	2.3659426802E+01	5.5777794061E-02

9.8581843429E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	C2	-2.9126942168E-05		
C1	C3	6.7455461057E-05		
C1	H4	-2.1930104756E-02		
C1	H5	-2.1930924856E-02		
C1		-4.3822701092E-02	-4.3810549900E-02	
C2	C1	4.1278134390E-05		
C2	C3	8.4432534499E-05		
C2	H6	-2.1928327206E-02		
C2	H7	-2.1928625856E-02		
C2		-4.3731242392E-02	-4.3719091200E-02	
C3	C1	-5.5304268835E-05		
C3	C2	-7.2281342277E-05		
C3	H8	-2.1930768896E-02		
C3	H9	-2.1932613786E-02		
C3		-4.3990968292E-02	-4.3978817100E-02	
H4	C1	2.1942255948E-02		
H4		2.1942255948E-02	2.1954407140E-02	
H5	C1	2.1943076048E-02		
H5		2.1943076048E-02	2.1955227240E-02	
H6	C2	2.1940478398E-02		

H6		2.1940478398E-02 2.1952629590E-02
H7	C2	2.1940777048E-02
H7		2.1940777048E-02 2.1952928240E-02
H8	C3	2.1942920088E-02
H8		2.1942920088E-02 2.1955071280E-02
H9	C3	2.1944764978E-02
H9		2.1944764978E-02 2.1956916170E-02

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	2.0030827748E-01	-2.6596054428E-02	1.7371222305E-01
C2	4.8145503217E-05	-3.3424521213E-05	1.4720982004E-05
C3	-2.0027331990E-01	2.6394714461E-02	-1.7387860544E-01
H4	8.0306904345E-02	-7.6219729232E-03	7.2684931422E-02
H5	8.0307503501E-02	-7.6222577973E-03	7.2685245704E-02
H6	-1.5948388754E-06	1.2345680450E-07	-1.4713820709E-06
H7	-1.6802352594E-06	1.2345848497E-07	-1.5567767744E-06
H8	-8.0308743201E-02	7.6222904172E-03	-7.2686452784E-02
H9	-8.0309671264E-02	7.6229312748E-03	-7.2686739989E-02

Total	7.5821390082E-05	-2.3352660114E-04	-1.5770521106E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	1.1549258146E-01	-1.5266934846E-02	1.0022564661E-01

C2	-2.3137118186E-01	3.0767927471E-02	-2.0060325439E-01
C3	1.1543279009E-01	-1.5222180065E-02	1.0021061003E-01
H4	4.6366111266E-02	-4.4002324998E-03	4.1965878766E-02
H5	4.6365842482E-02	-4.4003969601E-03	4.1965445522E-02
H6	-9.2735049412E-02	8.8002367340E-03	-8.3934812678E-02
H7	-9.2732990270E-02	8.8003565214E-03	-8.3932633749E-02
H8	4.6364912726E-02	-4.4002453979E-03	4.1964667328E-02
H9	4.6366643119E-02	-4.4006153563E-03	4.1966027763E-02

Total	-4.5034039900E-04	2.7791560188E-04	-1.7242479712E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	9.4146551606E-05	-9.1141970026E-07	9.3235131906E-05
C2	9.6413796143E-04	-3.3190467231E-07	9.6380605676E-04
C3	1.6305723611E-04	2.0503201153E-06	1.6510755623E-04
H4	-1.2240200470E-01	1.3522084878E-02	-1.0887991982E-01
H5	1.2240205534E-01	-1.3522590271E-02	1.0887946507E-01
H6	-1.2240046680E-01	1.3521008825E-02	-1.0887945798E-01
H7	1.2240194927E-01	-1.3521192870E-02	1.0888075640E-01
H8	1.2240254301E-01	-1.3522491166E-02	1.0888005184E-01
H9	-1.2240234767E-01	1.3523628094E-02	-1.0887871958E-01

Total	1.2230701991E-03	1.2544846131E-06	1.2243246838E-03

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	2.3121840598E-01	3.0666421564E-02	2.0055205152E-01
C2	2.3137319568E-01	3.0767945628E-02	2.0060557024E-01
C3	2.3115829702E-01	3.0469586830E-02	2.0068872178E-01
H4	1.5356192860E-01	1.6133917588E-02	1.3747389271E-01
H5	1.5356220114E-01	1.6134520600E-02	1.3747356646E-01

H6	1.5356322367E-01	1.6132632960E-02	1.3747650399E-01
H7	1.5356316184E-01	1.6132852555E-02	1.3747620203E-01
H8	1.5356295745E-01	1.6134411613E-02	1.3747443185E-01
H9	1.5356380956E-01	1.6135768143E-02	1.3747394383E-01

Total	1.3055481876E-03	3.6300596268E-04	1.2464237544E-03

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

C1	C2	1.8756410658E-05	
C1	C3	-9.6273297740E-05	
C1	H4	-1.3259020853E-02	
C1	H5	-1.3259516688E-02	
C1		-2.6596054428E-02	
C2	C1	3.2331603548E-05	
C2	C3	-6.6132553521E-05	
C2	H6	1.8821309859E-07	
C2	H7	1.8821566194E-07	
C2		-3.3424521213E-05	
C3	C1	-7.8931014337E-05	
C3	C2	-4.6545659260E-05	
C3	H8	1.3259537849E-02	
C3	H9	1.3260653286E-02	
C3		2.6394714461E-02	
H4	C1	-7.6219729232E-03	
H4		-7.6219729232E-03	

H5	C1	-7.6222577973E-03
H5		-7.6222577973E-03
H6	C2	1.2345680450E-07
H6		1.2345680450E-07
H7	C2	1.2345848497E-07
H7		1.2345848497E-07
H8	C3	7.6222904172E-03
H8		7.6222904172E-03
H9	C3	7.6229312748E-03
H9		7.6229312748E-03

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	C2	3.7171993991E-05	
C1	C3	5.4253050542E-06	
C1	H4	-7.6546229459E-03	
C1	H5	-7.6549091988E-03	
C1		-1.5266934846E-02	
C2	C1	4.9359516903E-05	
C2	C3	1.0096271364E-04	
C2	H6	1.5308698373E-02	
C2	H7	1.5308906868E-02	
C2		3.0767927471E-02	
C3	C1	-4.4479331448E-06	
C3	C2	9.2245951807E-05	
C3	H8	-7.6546670735E-03	
C3	H9	-7.6553110098E-03	
C3		-1.5222180065E-02	
H4	C1	-4.4002324998E-03	
H4		-4.4002324998E-03	
H5	C1	-4.4003969601E-03	
H5		-4.4003969601E-03	

H6	C2	8.8002367340E-03
H6		8.8002367340E-03
H7	C2	8.8003565214E-03
H7		8.8003565214E-03
H8	C3	-4.4002453979E-03
H8		-4.4002453979E-03
H9	C3	-4.4006153563E-03
H9		-4.4006153563E-03

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	C2	1.2404499302E-20	
C1	C3	-3.3750064068E-20	
C1	H4	2.4372063770E-02	
C1	H5	-2.4372975189E-02	
C1		-9.1141970026E-07	
C2	C1	-1.7579414491E-20	
C2	C3	3.8257804810E-20	
C2	H6	2.4370046335E-02	
C2	H7	-2.4370378240E-02	
C2		-3.3190467231E-07	
C3	C1	2.7670444871E-20	
C3	C2	-3.2751894760E-20	
C3	H8	-2.4372779196E-02	
C3	H9	2.4374829516E-02	
C3		2.0503201153E-06	
H4	C1	1.3522084878E-02	
H4		1.3522084878E-02	
H5	C1	-1.3522590271E-02	
H5		-1.3522590271E-02	
H6	C2	1.3521008825E-02	
H6		1.3521008825E-02	

H7	C2	-1.3521192870E-02
H7		-1.3521192870E-02
H8	C3	-1.3522491166E-02
H8		-1.3522491166E-02
H9	C3	1.3523628094E-02
H9		1.3523628094E-02

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	C2	4.1636043015E-05
C1	C3	9.6426043125E-05
C1	H4	2.8781806386E-02
C1	H5	2.8782882712E-02
C1		3.0666421564E-02
C2	C1	5.9005885273E-05
C2	C3	1.2069376198E-04
C2	H6	2.8779426754E-02
C2	H7	2.8779818712E-02
C2		3.0767945628E-02
C3	C1	7.9056240320E-05
C3	C2	1.0332383085E-04
C3	H8	2.8782662102E-02
C3	H9	2.8785083397E-02
C3		3.0469586830E-02
H4	C1	1.6133917588E-02
H4		1.6133917588E-02
H5	C1	1.6134520600E-02
H5		1.6134520600E-02
H6	C2	1.6132632960E-02
H6		1.6132632960E-02
H7	C2	1.6132852555E-02
H7		1.6132852555E-02

H8 C3 1.6134411613E-02
H8 1.6134411613E-02
H9 C3 1.6135768143E-02
H9 1.6135768143E-02

Atomic Traceless Quadrupole Moment Tensors:

 $Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$
C1	6.6824139097E-01	1.6610814209E+00	-1.1441400695E-04	-1.2481307388E+00	-1.5133296253E-04	5.7988934780E-01
C2	-2.2094994988E+00	-8.0288849272E-04	-2.4750284172E-04	1.6269150287E+00	-1.7129012744E-03	5.8258447002E-01
C3	6.6942300665E-01	-1.6616871039E+00	-9.8586051148E-05	-1.2476853100E+00	7.4411096566E-04	5.7826230333E-01
H4	-7.8732874077E-02	9.6517570286E-02	-2.4661698955E-01	-1.9019210544E-01	-1.4236767585E-01	2.6892497951E-01
H5	-7.8732553652E-02	9.6517004832E-02	2.4661571654E-01	-1.9019032524E-01	1.4236641935E-01	2.6892287889E-01
H6	-2.4591804349E-01	4.0191608723E-06	3.7998686587E-06	-2.3003515903E-02	2.8475380824E-01	2.6892155940E-01
H7	-2.4590428416E-01	2.3185094992E-06	-4.8276545158E-06	-2.3015159055E-02	-2.8475965929E-01	2.6891944322E-01
H8	-7.8727720715E-02	-9.6512344499E-02	-2.4661928903E-01	-1.9019236965E-01	1.4236574592E-01	2.6892009036E-01

H9 -7.8725127988E-02 -9.6513661659E-02 2.4661573942E-01 -1.9019314112E-01 -1.4236493016E-01 2.6891826911E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)

C1	1	-2.2075765544E+00	-5.0016420418E-01	8.6593057929E-01	2.6482135302E-05
C1	2	5.7988932060E-01	1.5767704064E-04	6.0492466575E-05	9.999998574E-01
C1	3	1.6276872338E+00	8.6593056534E-01	5.0016420122E-01	-1.6679353754E-04
C2	1	-2.2094996888E+00	9.9999997415E-01	2.0932057410E-04	8.8772890322E-05
C2	2	5.8258168272E-01	-8.9116082813E-05	1.6401156010E-03	9.999865104E-01
C2	3	1.6269180061E+00	-2.0917469393E-04	9.9999863310E-01	-1.6401342124E-03
C3	1	-2.2074717349E+00	5.0016051438E-01	8.6593268458E-01	-2.1360300298E-04
C3	2	5.7826223124E-01	4.8383109896E-04	-3.2785728000E-05	9.999988242E-01
C3	3	1.6292095037E+00	8.6593257576E-01	-5.0016055892E-01	-4.3536328899E-04
H4	1	-2.4591396597E-01	-5.0004669089E-01	8.6599844317E-01	-5.7928599799E-05
H4	2	-1.9703543968E-01	7.3892082012E-01	4.2670413700E-01	5.2145910775E-01
H4	3	4.4294940565E-01	-4.5160749386E-01	-2.6071109662E-01	8.5327627155E-01
H5	1	-2.4591206112E-01	-5.0005462584E-01	8.6599386089E-01	6.3874273356E-05
H5	2	-1.9703432816E-01	7.3891519620E-01	4.2671349821E-01	-5.2145941670E-01
H5	3	4.4294638928E-01	4.5160790958E-01	2.6071099584E-01	8.5327608232E-01
H6	1	-2.4591804358E-01	9.999999953E-01	-2.9310617252E-05	8.8307915731E-06
H6	2	-1.9702503048E-01	2.9614928601E-05	8.5327476868E-01	-5.2146156931E-01
H6	3	4.4294307405E-01	7.7492688328E-06	5.2146156932E-01	8.5327476914E-01
H7	1	-2.4590428421E-01	9.999999991E-01	5.3801132350E-06	1.2353148055E-05
H7	2	-1.9703928992E-01	-1.1032387873E-05	8.5327604845E-01	5.2145947592E-01

H7	3	4.4294357413E-01	-7.7351343302E-06	-5.2145947600E-01	8.5327604843E-01
H8	1	-2.4590835011E-01	5.0000169415E-01	8.6602442497E-01	3.4669951323E-05
H8	2	-1.9703821193E-01	7.3894741627E-01	-4.2665429338E-01	5.2146220374E-01
H8	3	4.4294656204E-01	-4.5161379722E-01	2.6070636603E-01	8.5327438077E-01
H9	1	-2.4590942118E-01	4.9998329788E-01	8.6603504629E-01	-2.0845476787E-05
H9	2	-1.9703350274E-01	7.3895972407E-01	-4.2663214562E-01	-5.2146288318E-01
H9	3	4.4294292392E-01	4.5161402552E-01	-2.6070732809E-01	8.5327396599E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
C1	1.3755544525E+02	1.4996219112E+01	6.0438105499E+00	6.2067735802E+00	9.6148527564E+00
C2	1.3755544880E+02	1.4996194590E+01	6.0437190912E+00	6.2065061345E+00	9.6142185316E+00
C3	1.3755546941E+02	1.4996277129E+01	6.0439788171E+00	6.2072989624E+00	9.6165315305E+00
H4	2.8883103023E+00	1.2543435571E+00	9.7804559286E-01	1.0935805279E+00	1.6328846672E+00
H5	2.8883098029E+00	1.2543429938E+00	9.7804477276E-01	1.0935789988E+00	1.6328814423E+00
H6	2.8883163804E+00	1.2543462466E+00	9.7804737041E-01	1.0935817507E+00	1.6328851457E+00
H7	2.8883160139E+00	1.2543458822E+00	9.7804707176E-01	1.0935815307E+00	1.6328844034E+00
H8	2.8883110118E+00	1.2543432396E+00	9.7804492872E-01	1.0935794508E+00	1.6328825683E+00

H9 2.8883104450E+00 1.2543421572E+00 9.7804308383E-01 1.0935765069E+00
1.6328784866E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3588550225E+02	-2.7168708279E+01	-1.3167380343E+01	-1.5649279572E+01	-
	2.9963765239E+01				
C2	-1.3588545441E+02	-2.7168554782E+01	-1.3166971767E+01	-1.5648475229E+01	-
	2.9963798788E+01				
C3	-1.3588558051E+02	-2.7168968374E+01	-1.3168253395E+01	-1.5652156529E+01	-
	2.9972823464E+01				
H4	-2.2158440431E+00	-1.8016092236E+00	-2.1078222316E+00	-3.2589470863E+00	-
	6.3603241274E+00				
H5	-2.2158435072E+00	-1.8016081680E+00	-2.1078198801E+00	-3.2589418470E+00	-
	6.3603158764E+00				
H6	-2.2158483685E+00	-1.8016119973E+00	-2.1078240820E+00	-3.2589478725E+00	-
	6.3603208326E+00				
H7	-2.2158479162E+00	-1.8016116785E+00	-2.1078238550E+00	-3.2589465296E+00	-
	6.3603100727E+00				
H8	-2.2158443221E+00	-1.8016087891E+00	-2.1078209151E+00	-3.2589438433E+00	-
	6.3603133903E+00				
H9	-2.2158422449E+00	-1.8016055265E+00	-2.1078159619E+00	-3.2589372793E+00	-
	6.3603125195E+00				

Atomic Electronic Spin Populations:

$$N_{\alpha}(A) = \text{Average number of Alpha electrons in Atom A}$$

$N_{\text{beta}}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\text{alpha}}(A) + N_{\text{beta}}(A)$

$N_{\text{spin}}(A) = N_{\text{alpha}}(A) - N_{\text{beta}}(A)$

Atom A	$N_{\text{alpha}}(A)$	$N_{\text{beta}}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$
C1	3.0219052750E+00	3.0219052750E+00	6.0438105499E+00	0.0000000000E+00
C2	3.0218595456E+00	3.0218595456E+00	6.0437190912E+00	0.0000000000E+00
C3	3.0219894085E+00	3.0219894085E+00	6.0439788171E+00	0.0000000000E+00
H4	4.8902279643E-01	4.8902279643E-01	9.7804559286E-01	0.0000000000E+00
H5	4.8902238638E-01	4.8902238638E-01	9.7804477276E-01	0.0000000000E+00
H6	4.8902368520E-01	4.8902368520E-01	9.7804737041E-01	0.0000000000E+00
H7	4.8902353588E-01	4.8902353588E-01	9.7804707176E-01	0.0000000000E+00
H8	4.8902246436E-01	4.8902246436E-01	9.7804492872E-01	0.0000000000E+00
H9	4.8902154191E-01	4.8902154191E-01	9.7804308383E-01	0.0000000000E+00
Total	1.1999890639E+01	1.1999890639E+01	2.3999781279E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron

Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

NH3

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\nh3\nh3pyr.wfn

Sum File: D:\calc\ellipticity\nh3\nh3pyr.sum

SumViz File: D:\calc\ellipticity\nh3\nh3pyr.sumviz

Wfn Title: nh3_as_pyr_mp2

Total memory allocated for AIMSum = 0.328 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Unknown

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	10.0000003000
Number of Alpha electrons (from MO Occs)	=	5.0000001500
Number of Beta electrons (from MO Occs)	=	5.0000001500
Number of electron pairs ($N*(N-1)/2$)	=	45.0000028500
Number of electron pairs (from Muller 2EDM)	=	44.9998035500
Number of electron pairs (from Muller 2EDM, no SOSI)	=	45.1151812898

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
N1	7.0	0.0000000000E+00	0.0000000000E+00	2.1121971000E-01
H2	1.0	0.0000000000E+00	1.7810570600E+00	-4.9284599000E-01
H3	1.0	-1.5424406600E+00	-8.9052853000E-01	-4.9284599000E-01
H4	1.0	1.5424406600E+00	-8.9052853000E-01	-4.9284599000E-01

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $

N1	-1.0436869446E+00	-1.7315006522E-04	5.4922723910E+01	-5.4994380489E+01

2.2679213293E-01

H2	3.4785225274E-01	2.5840326335E-05	4.8468516215E-01	-4.8531752119E-01	1.9938543065E-01

H3	3.4785120886E-01	2.4312884052E-05	4.8468466024E-01	-4.8531701862E-01	1.9938596166E-01

H4	3.4785126597E-01	2.4534525132E-05	4.8468486364E-01	-4.8531722229E-01	1.9938559940E-01

Total	-1.3221703000E-04	-9.8462329701E-05	5.6376778596E+01	-5.6450332251E+01

Molecular charge q(Mol) from the wfn file: -3.0000000073E-07

Molecular energy E(Mol) from the wfn file: -5.6214307647E+01

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0013046800E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	
N1	12	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

H3	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H4	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 21

Note: Total wall clock time is less than total of atomic times if more than one atom
was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 8.81905472512950E-16 -2.52948938039774E-15 2.11209247320283E-01

Type = (3,-3) NACP N1

Rho = 1.9391052560E+02 Rho at Nucleus = 1.9391050353E+02

GradRho = -5.2534030769E-17 1.4419848865E-16 -5.2598482431E-12

HessRho_EigVals = -4.0324237976E+05 -4.0324237976E+05 -4.0323077947E+05

HessRho_EigVec1 = 6.5436639901E-02 9.9785672627E-01 -1.1229848141E-10

HessRho_EigVec2 = 9.9785672627E-01 -6.5436639901E-02 3.6978281471E-12

HessRho_EigVec3 = 3.6585326004E-12 1.1229976848E-10 1.0000000000E+00

DelSqRho = -1.2097155390E+06

Bond Ellipticity = NA

V = -3.0247920316E+05

G = 2.5159207047E+01

K = 3.0245404395E+05

L = 3.0242888475E+05

Vnuc = 6.6904622699E+05

Ven = -1.2973510553E+08

Vrep = 1.2943262632E+08

DelSqV = 1.4125634462E+10

DelSqVen = 8.0935561574E+11

DelSqVrep = -7.9522998128E+11

DelSqG = 6.2901474585E+08

DelSqK = -1.4754649208E+10

Stress_EigVals = -1.0082800425E+05 -1.0082559945E+05 -1.0082559945E+05

Stress_EigVec1 = 1.2801851859E-11 -6.1999221389E-11 1.0000000000E+00

Stress_EigVec2 = 9.9691272107E-01 -7.8517683119E-02 -1.7630364190E-11

Stress_EigVec3 = 7.8517683119E-02 9.9691272107E-01 6.0802640752E-11

-DivStress = -3.7716556953E-06 1.1504818887E-05 4.8092125005E+04

CP# 2 Coords = -1.93814390551029E-14 1.74626278717887E+00 -4.80604781815523E-01

Type = (3,-3) NACP H2

Rho = 4.2717674452E-01 Rho at Nucleus = 4.2185282012E-01

GradRho = -4.7743374890E-19 -4.1249677615E-15 1.7250306662E-15

HessRho_EigVals = -8.5021170784E+00 -8.4822673054E+00 -7.4182888468E+00

HessRho_EigVec1 = 1.0000000000E+00 -1.4315881553E-10 -3.5543984067E-10

HessRho_EigVec2 = 3.8303150656E-10 3.4706579561E-01 9.3784078261E-01

HessRho_EigVec3 = 1.0899164498E-11 9.3784078261E-01 -3.4706579561E-01

DelSqRho = -2.4402673231E+01

Bond Ellipticity = NA

V = -6.1428655588E+00

G = 2.1098625580E-02

K = 6.1217669332E+00

L = 6.1006683077E+00

Vnuc = 3.1492891066E+01

Ven = -1.3453030681E+01

Vrep = 7.3101651222E+00

DelSqV = 1.5523580691E+03

DelSqVen = 7.6851072977E+02

DelSqVrep = 7.8384733937E+02

DelSqG = 1.1793178347E+02

DelSqK = -1.6702898526E+03

Stress_EigVals = -2.1407921355E+00 -2.1368811554E+00 -1.8651922678E+00

Stress_EigVec1 = -4.2933094641E-10 3.3736446578E-01 9.4137411120E-01

Stress_EigVec2 = 1.0000000000E+00 1.2964443429E-10 4.0960710148E-10

Stress_EigVec3 = 1.6142966866E-11 9.4137411120E-01 -3.3736446578E-01

-DivStress = 5.4977024017E-11 1.7808268084E+01 -6.2621273040E+00

CP# 3 Coords = -1.51230793584098E+00 -8.73131393528263E-01 -4.80604781676015E-01

Type = (3,-3) NACP H3

Rho = 4.2717675206E-01 Rho at Nucleus = 4.2185282762E-01

GradRho = 2.3006102975E-12 1.3283229170E-12 9.4853742234E-13

HessRho_EigVals = -8.5021171122E+00 -8.4822673389E+00 -7.4182888747E+00

HessRho_EigVec1 = 5.0000000117E-01 -8.6602540311E-01 -1.0459443553E-09

HessRho_EigVec2 = -3.0056779700E-01 -1.7353290018E-01 9.3784078178E-01

HessRho_EigVec3 = 8.1219394127E-01 4.6892039167E-01 3.4706579785E-01

DelSqRho = -2.4402673326E+01

Bond Ellipticity = NA

V = -6.1428655824E+00

G = 2.1098625465E-02

K = 6.1217669569E+00

L = 6.1006683315E+00

Vnuc = 3.1492891016E+01

Ven = -1.3453030897E+01

Vrep = 7.3101653148E+00

DelSqV = 1.5523580670E+03

DelSqVen = 7.6851073156E+02

DelSqVrep = 7.8384733546E+02

DelSqG = 1.1793178233E+02

DelSqK = -1.6702898493E+03

Stress_EigVals = -2.1407921439E+00 -2.1368811637E+00 -1.8651922747E+00

Stress_EigVec1 = -2.9216620008E-01 -1.6868223290E-01 9.4137411045E-01

Stress_EigVec2 = -5.0000000003E-01 8.6602540377E-01 -1.2680849943E-09

Stress_EigVec3 = 8.1525389389E-01 4.7068705563E-01 3.3736446785E-01

-DivStress = -1.5422412544E+01 -8.9041340653E+00 -6.2621273652E+00

CP# 4 Coords = 1.51230793598321E+00 -8.73131393635975E-01 -4.80604781748134E-01

Type = (3,-3) NACP H4

Rho = 4.2717675119E-01 Rho at Nucleus = 4.2185282678E-01

GradRho = -2.3018482072E-12 1.3292301624E-12 9.4897097086E-13

HessRho_EigVals = -8.5021171590E+00 -8.4822673859E+00 -7.4182889229E+00

HessRho_EigVec1 = -5.0000000034E-01 -8.6602540359E-01 3.9662000578E-10

HessRho_EigVec2 = 3.0056779763E-01 -1.7353289860E-01 9.3784078187E-01

HessRho_EigVec3 = 8.1219394155E-01 -4.6892039137E-01 -3.4706579760E-01

DelSqRho = -2.4402673468E+01

Bond Ellipticity = NA

V = -6.1428656180E+00

G = 2.1098625514E-02

K = 6.1217669925E+00

L = 6.1006683670E+00

Vnuc = 3.1492891156E+01

Ven = -1.3453030930E+01

Vrep = 7.3101653118E+00

DelSqV = 1.5523580823E+03

DelSqVen = 7.6851073944E+02

DelSqVrep = 7.8384734288E+02

DelSqG = 1.1793178391E+02

DelSqK = -1.6702898662E+03

Stress_EigVals = -2.1407921556E+00 -2.1368811755E+00 -1.8651922868E+00

Stress_EigVec1 = 2.9216620112E-01 -1.6868223093E-01 9.4137411048E-01

Stress_EigVec2 = 4.9999999924E-01 8.6602540422E-01 -3.3045884147E-09

Stress_EigVec3 = 8.1525389400E-01 -4.7068705549E-01 -3.3736446776E-01

-DivStress = 1.5422412613E+01 -8.9041340924E+00 -6.2621273888E+00

CP# 5 Coords = -4.81356831239245E-12 1.29985855302296E+00 -3.10279083500055E-01

Type = (3,-1) BCP H2 N1

Rho = 3.3380885856E-01

GradRho = 9.2337124869E-20 -2.6068354277E-15 -5.0544965298E-16

HessRho_EigVals = -1.2156339442E+00 -1.1651759388E+00 8.4949368670E-01

HessRho_EigVec1 = 1.0000000000E+00 -1.4808228532E-10 -3.4295248162E-10

HessRho_EigVec2 = 3.7336279364E-10 3.6661232706E-01 9.3037379673E-01

HessRho_EigVec3 = 1.2041270662E-11 9.3037379673E-01 -3.6661232706E-01

DelSqRho = -1.5313161963E+00

Bond Ellipticity = 4.3305052645E-02

V = -5.2058946333E-01

G = 6.8880207125E-02

K = 4.5170925620E-01

L = 3.8282904908E-01

Vnuc = 7.6857969488E+00

Ven = -2.5655871066E+00

Vrep = 2.0449976433E+00

DelSqV = -3.1913835206E+00

DelSqVen = 1.1769385349E+01

DelSqVrep = -1.4960768870E+01

DelSqG = 3.0836885502E+00

DelSqK = 1.0769497037E-01

Stress_EigVals = -3.5649117855E-01 -3.4487195459E-01 1.8077366982E-01

Stress_EigVec1 = -4.8478423910E-10 3.5645281108E-01 9.3431332725E-01

Stress_EigVec2 = 1.0000000000E+00 1.5537005299E-10 4.5959116116E-10

Stress_EigVec3 = 1.8658250174E-11 9.3431332725E-01 -3.5645281108E-01

-DivStress = 3.4512989569E-11 1.0654460779E+00 -4.1992497743E-01

BPL = 1.8784155873E+00 = 4.7780612836E-01 + 1.4006094589E+00

GBL_I = 1.8783078482E+00

GBL_II = 1.9151691207E+00

GBL_III = 1.8783595059E+00 = 4.7779449953E-01 + 1.4005650064E+00

GBL_IV = 1.9152364438E+00 = 5.1466754169E-01 + 1.4005689021E+00

CP# 6 Coords = -1.12571052235021E+00 -6.49929272386092E-01 -3.10279079382810E-01

Type = (3,-1) BCP N1 H3

Rho = 3.3380886361E-01

GradRho = 1.6622635131E-16 1.9105000179E-16 2.7696982112E-16

HessRho_EigVals = -1.2156339507E+00 -1.1651759437E+00 8.4949370289E-01
HessRho_EigVec1 = 5.0000000082E-01 -8.6602540331E-01 -1.3952892884E-09
HessRho_EigVec2 = -3.1749558878E-01 -1.8330616555E-01 9.3037379627E-01
HessRho_EigVec3 = 8.0572734240E-01 4.6518689845E-01 3.6661232824E-01
DelSqRho = -1.5313161915E+00
Bond Ellipticity = 4.3305053813E-02
V = -5.2058946516E-01
G = 6.8880208643E-02
K = 4.5170925652E-01
L = 3.8282904788E-01
Vnuc = 7.6857969474E+00
Ven = -2.5655871449E+00
Vrep = 2.0449976798E+00
DelSqV = -3.1913841809E+00
DelSqVen = 1.1769385310E+01
DelSqVrep = -1.4960769491E+01
DelSqG = 3.0836885691E+00
DelSqK = 1.0769561186E-01
Stress_EigVals = -3.5649118131E-01 -3.4487195700E-01 1.8077367315E-01
Stress_EigVec1 = -3.0869719198E-01 -1.7822640516E-01 9.3431332655E-01
Stress_EigVec2 = -4.9999999962E-01 8.6602540400E-01 -1.4354955953E-09
Stress_EigVec3 = 8.0913907583E-01 4.6715666337E-01 3.5645281292E-01
-DivStress = -9.2270333380E-01 -5.3272301911E-01 -4.1992496588E-01
BPL = 1.8784155876E+00 = 1.4006094508E+00 + 4.7780613682E-01
GBL_I = 1.8783078485E+00
GBL_II = 1.9151691211E+00
GBL_III = 1.8783595062E+00 = 1.4005649982E+00 + 4.7779450799E-01
GBL_IV = 1.9152364441E+00 = 1.4005688939E+00 + 5.1466755021E-01

CP# 7 Coords = 1.12571052404413E+00 -6.49929273574131E-01 -3.10279080316452E-01

Type = (3,-1) BCP H4 N1

Rho = 3.3380886290E-01

GradRho = -1.6043756933E-17 4.5950187430E-17 2.0355641679E-16
HessRho_EigVals = -1.2156339503E+00 -1.1651759439E+00 8.4949369632E-01
HessRho_EigVec1 = -5.0000000024E-01 -8.6602540365E-01 -3.2082031774E-10
HessRho_EigVec2 = 3.1749558932E-01 -1.8330616442E-01 9.3037379630E-01
HessRho_EigVec3 = 8.0572734254E-01 -4.6518689827E-01 -3.6661232815E-01
DelSqRho = -1.5313161980E+00
Bond Ellipticity = 4.3305053336E-02
V = -5.2058946599E-01
G = 6.8880208249E-02
K = 4.5170925774E-01
L = 3.8282904949E-01
Vnuc = 7.6857969474E+00
Ven = -2.5655871395E+00
Vrep = 2.0449976735E+00
DelSqV = -3.1913839612E+00
DelSqVen = 1.1769385360E+01
DelSqVrep = -1.4960769321E+01
DelSqG = 3.0836885612E+00
DelSqK = 1.0769539995E-01
Stress_EigVals = -3.5649118093E-01 -3.4487195677E-01 1.8077367172E-01
Stress_EigVec1 = 3.0869719228E-01 -1.7822640400E-01 9.3431332667E-01
Stress_EigVec2 = 4.9999999920E-01 8.6602540425E-01 -2.4877894692E-09
Stress_EigVec3 = 8.0913907598E-01 -4.6715666335E-01 -3.5645281259E-01
-DivStress = 9.2270334194E-01 -5.3272302327E-01 -4.1992496876E-01
BPL = 1.8784155878E+00 = 4.7780613475E-01 + 1.4006094530E+00
GBL_I = 1.8783078487E+00
GBL_II = 1.9151691211E+00
GBL_III = 1.8783595064E+00 = 4.7779450592E-01 + 1.4005650004E+00
GBL_IV = 1.9152364441E+00 = 5.1466754795E-01 + 1.4005688962E+00

Number of NACPs = 4

Number of NNACPs = 0

Number of BCPs = 3

Number of RCPs = 0

Number of CCPs = 0

NumNACP + NumNNACP - NumBCP + NumRCP - NumCCP = 1

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H3	N1	H2	105.78525701	107.24829204	107.29411687	106.98029671	106.97986611
H4	N1	H2	105.78525705	107.24829205	107.29411687	106.98029671	106.97986612
H4	N1	H3	105.78525717	107.24829207	107.29411689	106.98029679	106.97986619

Total time for electron density critical point search, analysis and connectivity = 1 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$E_e(A) = E(A) - W(A) = -T(A)$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{en}(A) = V_{en}(A, Mol)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{enO}(A) = V_{en}(A, A)$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$Vee(A) = Vee(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $Vnn(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)
N1	-5.4922723910E+01	5.4922723910E+01	-1.4569602687E+02	-1.3367937424E+02		
H2	-4.8468516215E-01	4.8468516215E-01	-3.3669659680E+00	-9.5957468010E-01		
H3	-4.8468466024E-01	4.8468466024E-01	-3.3669686241E+00	-9.5957487692E-01		
H4	-4.8468486364E-01	4.8468486364E-01	-3.3669694488E+00	-9.5957512720E-01		
Total	-5.6376778596E+01	5.6376778596E+01	-1.5579693091E+02	-1.3655809892E+02		

More Virial-Based Atomic Energy Components:

$$E(A) = Ee(A) + W(A)$$

= $T(A) + Ven(A) + Vee(A) + Vnn(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$Ee(A) = E(A) - W(A)$ = Contribution of Atom A to Electronic Energy of Molecule

Not additive to give molecular Ee unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$Vnn(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $Vnn(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	E(A)	Ee(A)	W(A)	Vnn(A)	VeeC(A)	VeeX(A)

N1	-5.4922723910E+01					
H2	-4.8468516215E-01					
H3	-4.8468466024E-01					
H4	-4.8468486364E-01					

Total	-5.6376778596E+01					

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$Vne(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$Ven(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$Vee(A) = Vee(A,Mol) = (1/2)[Vee(A,Mol) + Vee(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$Vnn(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$VeeC(A)$ = Coulomb Part of $Vee(A)$

$VeeX(A)$ = Exchange-Correlation Part of $Vee(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$Vne(A,Mol)/2$	$Ven(A,Mol)/2$	$Vee(A)$	$Vnn(A,Mol)/2$
VeeC(A)	$VeeX(A)$					

N1			5.4922723910E+01	-6.9867135314E+01	-7.2848013437E+01	
	5.4825445362E+00					
H2			4.8468516215E-01	-2.6770639448E+00	-1.6834829840E+00	
	2.1516764248E+00					

H3	4.8468466024E-01	-2.6770639537E+00	-1.6834843121E+00
2.1516764244E+00			
H4	4.8468486364E-01	-2.6770639524E+00	-1.6834847244E+00
2.1516764244E+00			

Total	5.6376778596E+01	-7.7898327165E+01	-7.7898465458E+01
1.1937573810E+01			

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$

N1	5.4922723910E+01	-1.3367937424E+02				

H2	4.8468516215E-01	-9.5957468010E-01				

H3	4.8468466024E-01	-9.5957487692E-01				

H4	4.8468486364E-01	-9.5957512720E-01				

Total	5.6376778596E+01	-1.3655809892E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= V_{ne}(A,A')/2 + V_{en}(A,A')/2 + V_{ee}(A,A') + V_{nn}(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$V_{ne}(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[V_{ne}(A,Mol) - V_{ne}(A,A)]$$

$V_{en}(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[V_{en}(A,Mol) - V_{en}(A,A)]$$

$V_{ee}(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= V_{ee}(A,Mol) - V_{ee}(A,A)$$

$V_{nn}(A) = V_{nn}(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A,A')$ = Coulomb Part of $V_{ee}(A,A')$

$V_{eeX}(A,A')$ = Exchange-Correlation Part of $V_{ee}(A,A')$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Inter(A)$	$V_{ne}(A,A')/2$	$V_{en}(A,A')/2$	$V_{ee}(A,A')$	$V_{nn}(A)$	$V_{eeC}(A,A')$
$V_{eeX}(A,A')$						
N1	-3.0274481927E+00	-6.0083263155E+00		5.4825445362E+00		
H2	-2.1972766047E+00	-1.2036956440E+00		2.1516764248E+00		
H3	-2.1972765153E+00	-1.2036968736E+00		2.1516764244E+00		
H4	-2.1972763888E+00	-1.2036971608E+00		2.1516764244E+00		
Total	-9.6192777015E+00	-9.6194159939E+00		1.1937573810E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$$\%Loc(A) = 100 * LI(A) / N(A)$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A,A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A

that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A)$$

$$\%Deloc(A,A') = 100 * (DI(A,A')/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
N1	8.0436869447E+00	6.8582934817E+00	8.5263058207E+01	1.1853934630E+00	1.4736941793E+01
H2	6.5214774759E-01	2.3936546810E-01	3.6704177694E+01	4.1278227949E-01	6.3295822306E+01
H3	6.5214879092E-01	2.3936603178E-01	3.6704205408E+01	4.1278275914E-01	6.3295794592E+01
H4	6.5214873415E-01	2.3936603600E-01	3.6704209250E+01	4.1278269814E-01	6.3295790750E+01
Total	1.0000132217E+01	7.5763910176E+00	7.5762908459E+01	2.4237411998E+00	2.4237091541E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

DI_Bond(A,A')/2 = Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

DI_NonBond(A,A')/2 = Non-Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
N1	8.0436869447E+00	6.8582934817E+00	1.1853934630E+00	1.1857875989E+00	-3.9413585874E-04
H2	6.5214774759E-01	2.3936546810E-01	4.1278227949E-01	3.9526236873E-01	1.7519910760E-02
H3	6.5214879092E-01	2.3936603178E-01	4.1278275914E-01	3.9526363259E-01	1.7519126547E-02
H4	6.5214873415E-01	2.3936603600E-01	4.1278269814E-01	3.9526159755E-01	1.7521100592E-02
Total	1.0000132217E+01	7.5763910176E+00	2.4237411998E+00	2.3715751977E+00	5.2166002041E-02

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
N1	2.8921303091E+01	7.2751440550E+00	3.6196447146E+01
H2	9.2965608295E-02	2.8416812361E+00	2.9346468444E+00

H3 9.2966006857E-02 2.8416855321E+00 2.9346515390E+00

H4 9.2965967723E-02 2.8416853156E+00 2.9346512834E+00

Total 2.9200200674E+01 1.5800196139E+01 4.5000396813E+01

Diatomic Electron Pair Contributions and Delocalization Data:

 $2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B
 $= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized
(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A Atom B 2*D2(A,B) DI(A,B) %Deloc(A,B) %Deloc(B,A)

N1 H2 4.8504099546E+00 7.9052473746E-01 4.9139452026E+00 6.0609328207E+01
(Bonded)
N1 H3 4.8504170829E+00 7.9052726518E-01 4.9139609150E+00 6.0609425041E+01
(Bonded)
H2 H3 4.1651436969E-01 1.7565990815E-02 1.3467799958E+00 1.3467778412E+00
N1 H4 4.8504186613E+00 7.9052319510E-01 4.9139356152E+00 6.0609118266E+01
(Bonded)
H2 H4 4.1651435374E-01 1.7565948669E-02 1.3467767644E+00 1.3467747271E+00
H3 H4 4.1651498152E-01 1.7566053912E-02 1.3467826788E+00 1.3467827960E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
N1	H2	3.4364702159E+01	2.6733107791E+01	2.1552497856E+01
N1	H3	3.4364702274E+01	2.6733107879E+01	2.1552497925E+01
N1	H4	3.4364702251E+01	2.6733107862E+01	2.1552497911E+01
N1	Total	1.0309410668E+02	8.0199323532E+01	6.4657493692E+01
H2	N1	3.4364702159E+01	2.6733107791E+01	2.1552497856E+01
H2	Total	3.4364702159E+01	2.6733107791E+01	2.1552497856E+01
H3	N1	3.4364702274E+01	2.6733107879E+01	2.1552497925E+01
H3	Total	3.4364702274E+01	2.6733107879E+01	2.1552497925E+01
H4	N1	3.4364702251E+01	2.6733107862E+01	2.1552497911E+01
H4	Total	3.4364702251E+01	2.6733107862E+01	2.1552497911E+01
Total	Total	2.0618821337E+02	1.6039864706E+02	1.2931498738E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta^2\rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta^2\rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta^2\rho\_IAS(A B)$	$V\_IAS(A B)$

N1	H2	8.7483415759E-01	5.6686388963E-01	4.4390921835E-01	-1.2295467128E-01	4.9181868512E-01	-1.0107731080E+00

N1	H3	8.7483417581E-01	5.6686390437E-01	4.4390922571E-01	-1.2295467865E-01	4.9181871461E-01	-1.0107731301E+00

N1	H4	8.7483417286E-01	5.6686390159E-01	4.4390922573E-01	-1.2295467586E-01	4.9181870344E-01	-1.0107731273E+00

N1	Total	2.6245025063E+00	1.7005916956E+00	1.3317276698E+00	-3.6886402579E-01	1.4754561032E+00	-3.0323193654E+00

H2	N1	8.7483415759E-01	5.6686388963E-01	4.4390921835E-01	-1.2295467128E-01	4.9181868512E-01	-1.0107731080E+00

H2	Total	8.7483415759E-01	5.6686388963E-01	4.4390921835E-01	-1.2295467128E-01	4.9181868512E-01	-1.0107731080E+00

H3	N1	8.7483417581E-01	5.6686390437E-01	4.4390922571E-01	-1.2295467865E-01	4.9181871461E-01	-1.0107731301E+00

H3	Total	8.7483417581E-01	5.6686390437E-01	4.4390922571E-01	-1.2295467865E-01	4.9181871461E-01	-1.0107731301E+00

H4	N1	8.7483417286E-01	5.6686390159E-01	4.4390922573E-01	-1.2295467586E-01
		4.9181870344E-01	-1.0107731273E+00		

H4	Total	8.7483417286E-01	5.6686390159E-01	4.4390922573E-01	-1.2295467586E-01
		4.9181870344E-01	-1.0107731273E+00		

Total	Total	5.2490050125E+00	3.4011833912E+00	2.6634553396E+00	-7.3772805158E-01
		2.9509122063E+00	-6.0646387308E+00		

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP-_{Min_IDS}(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{Avg_IDS}(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{MAD_IDS}(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-_{Var_IDS}(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP*ESP-_{Int_IDS}(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

N1	1.1508140013E+02						

H2	3.9633366923E+01						

H3	3.9760422652E+01						

H4	3.9914196734E+01						

Total	2.3438938644E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

N1	9.5130637925E+01	-1.8707170265E+00	2.3941831080E-02	-6.5156906110E-02	-1.9664716513E-02	2.4718433211E-02	7.7984754156E-04

H2	3.2070949425E+01	8.2756618820E-01	4.1851159214E-02	-5.7498551408E-03	2.5804231026E-02	8.2347599219E-03	1.0944382424E-04

H3	3.1943920602E+01	8.2611900079E-01	4.1831860006E-02	-6.2176438731E-03	2.5861540638E-02	8.2071131688E-03	1.0749407403E-04

H4	3.1930722716E+01	8.2469217930E-01	4.1836297640E-02	-7.0763382132E-03	2.5827545046E-02	8.2433887562E-03	1.0952812795E-04

Total	1.9107623067E+02	6.0766034179E-01	4.1851159214E-02	-6.5156906110E-02	3.1801984981E-03	9.6036167552E-04	

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP- _IDS(A)
N1	2.7106607340E+00	1.1097451411E-01	3.1270470769E+01	4.1997185375E-01	6.3860167155E+01
H2	8.3334251140E-01	2.4864676462E-02	3.1264678838E+01	8.3045434980E-01	8.0627058695E-01
H3	8.3042531181E-01	2.4798492277E-02	3.1198390811E+01	8.2827215630E-01	7.4552979029E-01
H4	8.2994922080E-01	2.4797086693E-02	3.1125572609E+01	8.2732070005E-01	8.0515010651E-01
Total	5.2043777780E+00	1.8543476954E-01	1.2485911303E+02	2.9060190599E+00	6.6217117639E+01

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)
N1	4.4642754445E-05	1.3430301605E-02	5.4345985805E-03	4.0009649853E-05
H2	2.1780927523E-04	2.6562062387E-02	7.6331486805E-03	8.9289451192E-05
H3	8.4122430985E-05	2.6548553780E-02	7.6621507876E-03	8.9754936176E-05
H4	1.5626822579E-04	2.6580095744E-02	7.6481452677E-03	8.9801357283E-05
Total	4.4642754445E-05	2.3274384940E-02	1.0957044690E-04	8.1316675059E-02

0.001 IsoDensity Surface:

Atom A	ESP- _{Max_IDS(A)}	ESP- _{Avg_IDS(A)}	ESP- _{MAD_IDS(A)}	ESP- _{Var_IDS(A)}	ESP- _{*ESP- _Int_IDS(A)}

N1	-3.2674204572E-05	-3.5870386538E-02	1.6045807591E-02	3.4317400457E-04	1.0408304487E-01
H2	-1.5573626906E-04	-3.5821244663E-03	2.0657389680E-03	5.1402645209E-06	1.4490198408E-05
H3	-7.6895816165E-05	-2.8880878250E-03	1.5840662681E-03	3.5361602811E-06	8.8548150481E-06
H4	-4.7788857259E-04	-3.2646344159E-03	1.6927133614E-03	3.8793376307E-06	1.1704608402E-05

Total	-3.2674204572E-05	-3.4709434660E-02	3.6762945308E-04	1.0411809449E-01	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)

N1	8.1871630709E+01
H2	2.6486881111E+01
H3	2.6737364608E+01
H4	2.6622384577E+01

Total	1.6171826100E+02

Atomic Surface Area and Volume Data:

$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$

$\text{Vol(A)} = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$
 $\text{Isosurface of the Electron Density Distribution (IsoDensity Surface)}$

$\text{N(Vol(A))} = \text{Average Number of Electrons in Vol(A)}$

$\text{N(Vol(A))}/\text{Vol(A)} = \text{Average Electron Density in Vol(A)}$

$$\%N(\text{Vol(A)}) = 100 * N(\text{Vol(A)}) / N(\text{A})$$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
N1	2.1817550681E+02	1.8806068010E+02	8.0135738923E+00	4.2611639435E-02	9.9625631225E+01
H2	7.3998069082E+01	4.7817504681E+01	6.4329619202E-01	1.3453152696E-02	9.8642707074E+01
H3	7.4125124926E+01	4.7845599254E+01	6.4330676524E-01	1.3445474093E-02	9.8644170468E+01
H4	7.4278898985E+01	4.7809634677E+01	6.4329277255E-01	1.3455295714E-02	9.8642033478E+01
Total	4.4057759980E+02	3.3153341871E+02	9.9434696221E+00	2.9992359928E-02	9.9433381539E+01

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
N1	1.7532996146E+02	1.4235295485E+02	7.9840844867E+00	5.6086538528E-02	9.9259015694E+01
H2	5.8804057216E+01	3.3886930790E+01	6.3431852789E-01	1.8718677469E-02	9.7266076676E+01
H3	5.8677028481E+01	3.3916406370E+01	6.3435229607E-01	1.8703405342E-02	9.7271098971E+01
H4	5.8663830578E+01	3.3929156544E+01	6.3436685748E-01	1.8696805995E-02	9.7273340325E+01
Total	3.5147487773E+02	2.4408544855E+02	9.8871221681E+00	4.0506807049E-02	9.8869914449E+01

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
N1	1.4652912440E+02	1.1307404528E+02	7.9422878245E+00	7.0239707128E-02	9.8739394996E+01
H2	4.8039378967E+01	2.5219646250E+01	6.2194096884E-01	2.4660971160E-02	9.5368108140E+01
H3	4.8289862533E+01	2.5210154486E+01	6.2191628068E-01	2.4669276860E-02	9.5364169823E+01
H4	4.8174882488E+01	2.5189489252E+01	6.2187847905E-01	2.4688014626E-02	9.5358381700E+01
Total	2.9103324839E+02	1.8869333527E+02	9.8080235531E+00	5.1978643226E-02	9.8078938757E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
N1	H2	-3.4789002903E-01		
N1	H3	-3.4788898515E-01		
N1	H4	-3.4788904226E-01		
N1		-1.0436680565E+00	-1.0436869446E+00	
H2	N1	3.4787114089E-01		
H2		3.4787114089E-01	3.4785225274E-01	
H3	N1	3.4787009701E-01		
H3		3.4787009701E-01	3.4785120886E-01	
H4	N1	3.4787015412E-01		
H4		3.4787015412E-01	3.4785126597E-01	

Atomic Dipole Moments:

$$\text{Mu\_Intra(A)} = \text{Intraatomic Dipole Moment Contribution of Atom A}$$
$$\text{Mu\_Bond(A)} = \text{Bonding Dipole Moment Contribution of Atom A}$$
$$\text{Mu(A)} = \text{Mu\_Intra(A)} + \text{Mu\_Bond(A)}$$
$$= \text{Total Dipole Moment Contribution of Atom A}$$

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

N1	7.3731304667E-05	6.4876949368E-08	7.3796181616E-05

H2	9.7444417860E-07	1.6745015006E-12	9.7444585310E-07

H3	1.5268940757E-01	-1.4496795341E-01	7.7214541600E-03

H4	-1.5268899817E-01	1.4496797662E-01	-7.7210215498E-03

Total	7.5115148846E-05	8.8088817657E-08	7.5203237663E-05

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

N1	-1.3971733239E-04	1.3222359342E-06	-1.3839509646E-04

H2	-1.7630919192E-01	1.6739507362E-01	-8.9141183047E-03

H3	8.8153568592E-02	-8.3697287086E-02	4.4562815060E-03

H4	8.8154278373E-02	-8.3697300413E-02	4.4569779597E-03

Total	-1.4106228739E-04	1.8083518931E-06	-1.3925393550E-04

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

N1	-2.2679207791E-01	-5.4427162971E-01	-7.7106370762E-01

H2	9.3110787774E-02	-6.3509758052E-02	2.9601029722E-02

H3	9.3110981446E-02	-6.3509568907E-02	2.9601412539E-02

H4	9.3110205097E-02	-6.3509579008E-02	2.9600626089E-02

Total 5.2539896407E-02 -7.3480053568E-01 -6.8226063928E-01

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

N1	2.2679213293E-01	5.4427162972E-01	7.7106372358E-01

H2	1.9938543065E-01	1.7903798490E-01	3.0914114360E-02

H3	1.9938596166E-01	1.7903745062E-01	3.0914768696E-02

H4	1.9938559940E-01	1.7903747923E-01	3.0914008008E-02

Total 5.2540139468E-02 7.3480053568E-01 6.8226065763E-01

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

N1	H2	-1.6745924200E-12	

N1	H3	-3.9162229120E-01	

N1	H4	3.9162235608E-01	

N1		6.4876949368E-08	

H2	N1	1.6745015006E-12	

H2		1.6745015006E-12	

H3	N1	-1.4496795341E-01	

H3		-1.4496795341E-01	

H4	N1	1.4496797662E-01	

H4		1.4496797662E-01	

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

N1	H2	4.5220782975E-01
N1	H3	-2.2610323499E-01
N1	H4	-2.2610327252E-01
N1		1.3222359342E-06
H2	N1	1.6739507362E-01
H2		1.6739507362E-01
H3	N1	-8.3697287086E-02
H3		-8.3697287086E-02
H4	N1	-8.3697300413E-02
H4		-8.3697300413E-02

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

N1	H2	-1.8142423041E-01	
N1	H3	-1.8142368460E-01	
N1	H4	-1.8142371471E-01	
N1		-5.4427162971E-01	
H2	N1	-6.3509758052E-02	
H2		-6.3509758052E-02	
H3	N1	-6.3509568907E-02	
H3		-6.3509568907E-02	
H4	N1	-6.3509579008E-02	
H4		-6.3509579008E-02	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

N1	H2	4.8724395601E-01	
N1	H3	4.8724249114E-01	
N1	H4	4.8724257191E-01	
N1		5.4427162972E-01	
H2	N1	1.7903798490E-01	
H2		1.7903798490E-01	

H3 N1 1.7903745062E-01
H3 1.7903745062E-01
H4 N1 1.7903747923E-01
H4 1.7903747923E-01

Atomic Traceless Quadrupole Moment Tensors:

 $Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$

N1	1.5229528133E+00	3.9123621944E-04	-1.1031517606E-03	1.5242463152E+00	7.4254332121E-04	-3.0471991285E+00

H2	-4.9603532918E-02	1.7141250928E-07	-2.1000310302E-06	1.3797624363E-01	-1.8787311057E-02	-8.8372710712E-02

H3	9.1084404619E-02	8.1226628393E-02	1.6271962362E-02	-2.7114057446E-03	9.3954917793E-03	-8.8372998875E-02

H4	9.1081779343E-02	-8.1226340729E-02	-1.6270957281E-02	-2.7092872606E-03	9.3941895696E-03	-8.8372492082E-02

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

 $Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
N1	1	-3.0471995154E+00	2.4139573287E-04	-1.6245139067E-04	9.9999995767E-01
N1	2	1.5228440341E+00	9.6325154005E-01	-2.6860080851E-01	-2.7615939802E-04
N1	3	1.5243554813E+00	2.6860084200E-01	9.6325156594E-01	9.1642463222E-05
H2	1	-8.9921489092E-02	5.1561351654E-05	8.2158763380E-02	9.9661925274E-01
H2	2	-4.9603532811E-02	9.9999999867E-01	-6.0456111336E-06	-5.1237873953E-05
H2	3	1.3952502190E-01	1.8155320882E-06	9.9661925406E-01	-8.2158763582E-02
H3	1	-8.9922139122E-02	-7.1148382598E-02	-4.1102486218E-02	9.9661852947E-01
H3	2	-4.9606776798E-02	-4.9999516584E-01	8.6602819449E-01	2.2139435874E-05
H3	3	1.3952891592E-01	8.6310065566E-01	4.9830287173E-01	8.2167549735E-02
H4	1	-8.9921397944E-02	7.1153086976E-02	-4.1082860243E-02	9.9661900283E-01
H4	2	-4.9605595138E-02	5.0000224254E-01	8.6602410905E-01	2.0513226538E-06
H4	3	1.3952699308E-01	8.6309616826E-01	-4.9831159042E-01	-8.2161811006E-02

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^2) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^2 \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
N1	1.9227440685E+02	1.9097053463E+01	8.0436869446E+00	8.9538349273E+00	1.5122531318E+01
H2	2.5728444818E+00	9.5957468010E-01	6.5214774726E-01	6.6458459069E-01	9.4777430353E-01
H3	2.5728439758E+00	9.5957487692E-01	6.5214879114E-01	6.6458720556E-01	9.4778221295E-01

H4 2.5728444284E+00 9.5957512720E-01 6.5214873403E-01 6.6458649290E-01 9.4778032151E-01

Atomic Radial Distortion Moments:

$$\text{Dot} = x*(d\rho/dx) + y*(d\rho/dy) + z*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot}*r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot}*r*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
N1	-1.9127138512E+02	-3.6476211743E+01	-2.1084640448E+01	-3.0171926675E+01	-6.4580544870E+01
H2	-1.8093007319E+00	-1.3174872711E+00	-1.4122608256E+00	-2.0613529006E+00	-3.9000207375E+00
H3	-1.8093021588E+00	-1.3174900595E+00	-1.4122666078E+00	-2.0613692255E+00	-3.9000979838E+00
H4	-1.8093023616E+00	-1.3174897650E+00	-1.4122648825E+00	-2.0613631035E+00	-3.9000767903E+00

Atomic Electronic Spin Populations:

$$N\_alpha(A) = \text{Average number of Alpha electrons in Atom A}$$

$$N\_beta(A) = \text{Average number of Beta electrons in Atom A}$$

$$N\_total(A) = N\_alpha(A) + N\_beta(A)$$

$$N\_spin(A) = N\_alpha(A) - N\_beta(A)$$

Atom A	N_alpha(A)	N_beta(A)	N_total(A)	N_spin(A)
N1	4.0218434723E+00	4.0218434723E+00	8.0436869446E+00	0.0000000000E+00
H2	3.2607387363E-01	3.2607387363E-01	6.5214774726E-01	0.0000000000E+00

H3	3.2607439557E-01	3.2607439557E-01	6.5214879114E-01	0.0000000000E+00
H4	3.2607436701E-01	3.2607436701E-01	6.5214873403E-01	0.0000000000E+00

Total	5.0000661085E+00	5.0000661085E+00	1.0000132217E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

PH3PO

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfx File: D:\calc\ellipticity\ph3po\ph3po.wfx

Sum File: D:\calc\ellipticity\ph3po\ph3po.sum

SumViz File: D:\calc\ellipticity\ph3po\ph3po.sumviz

Wfx Title: nh3_as_pyr_mp2

Total memory allocated for AIMSum = 0.429 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted MP2

Restricted, natural orbital wavefunction.

Number of electrons (from MO Occs)	=	25.9999999989
Number of Alpha electrons (from MO Occs)	=	12.9999999994
Number of Beta electrons (from MO Occs)	=	12.9999999994
Number of electron pairs ($N*(N-1)/2$)	=	324.9999999712
Number of electron pairs (from Muller 2EDM)	=	324.9995430306
Number of electron pairs (from Muller 2EDM, no SOSI)	=	325.2028626221

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
H1	1.0	-2.3666411000E+00	-1.9361852000E+00	0.0000000000E+00
H2	1.0	1.1834277700E+00	-1.9352177300E+00	2.0507183700E+00
H3	1.0	1.1834277700E+00	-1.9352177300E+00	-2.0507183700E+00
P4	15.0	-9.3232365100E-06	-7.2770147900E-01	0.0000000000E+00
O5	8.0	-9.3232365100E-06	2.0902678600E+00	0.0000000000E+00

Some Atomic Properties:

$q(A)$ = Net Charge of Atom A

$L(A)$ = Lagrangian of Atom A = $-(1/4)$ Times Atomic Integral of the Laplacian of the Electron Density

$K(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$K\_Scaled(A) = K(A) * E(Mol)/K(Mol)$ = Approximation to Virial-Based Total Energy of Atom A.

$|Mu\_Intra(A)|$ = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	$q(A)$	$L(A)$	$K(A)$	$K\_Scaled(A)$	$ Mu_Intra(A) $
H1	-6.1192647030E-01	3.4060212187E-05	8.7429404867E-01	-8.7424875575E-01	3.8191350041E-01
H2	-6.1169803540E-01	3.6381875959E-05	8.7396925944E-01	-8.7392398334E-01	3.8195756489E-01
H3	-6.1170050490E-01	3.4960398561E-05	8.7396961510E-01	-8.7392433898E-01	3.8196048556E-01
P4	3.2516036900E+00	-2.1762644015E-04	3.3943824165E+02	-3.3942065701E+02	8.2102861204E-02
O5	-1.4163583954E+00	7.0366220873E-06	7.5659602536E+01	-7.5655682980E+01	6.1853860856E-01
Total	-7.9716000000E-05	-1.0518733136E-04	4.1772007711E+02	-4.1769843707E+02	

Molecular charge q(Mol) from the wfx file: 1.1279184537E-09

Molecular energy E(Mol) from the wfx file: -4.1769846091E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfx file: 1.9999481949E+00

Full molecular virial ratio ((-V(Mol)+W(Mol))/T(Mol)) from the wfx file: 1.9999471640E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

H1	10	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H2	9	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	8	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
P4	18	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
O5	11	1	Proaim(5)	3074	(Very High)	1.00	1.00	1.00	13.00

Total 56

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = $(\text{HessRho\_EigVal}(1) / \text{HessRho\_EigVal}(2)) - 1$

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = $(-1/4)\text{DelSqRho}$

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = -2.34695071525818E+00 -1.92662029651809E+00 -1.32811199042858E-20

Type = (3,-3) NACP H1

Rho = 4.0545470445E-01 Rho at Nucleus = 4.0356092837E-01

GradRho = 7.4593109467E-15 3.0704605525E-15 2.1302046724E-20

HessRho_EigVals = -8.1542040611E+00 -8.1512355931E+00 -7.7662018839E+00

HessRho_EigVec1 = -4.4513184184E-01 8.9546504308E-01 0.0000000000E+00

HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec3 = 8.9546504308E-01 4.4513184184E-01 0.0000000000E+00

DelSqRho = -2.4071641538E+01

Bond Ellipticity = NA

V = -6.0284012317E+00

G = 5.2454235861E-03

K = 6.0231558081E+00

L = 6.0179103845E+00

Vnuc = 5.3582803025E+01

Ven = -2.1725399564E+01

Vrep = 1.5696998332E+01

DelSqV = 1.5713109182E+03

DelSqVen = 1.2898260270E+03

DelSqVrep = 2.8148489114E+02

DelSqG = 1.1999140789E+02

DelSqK = -1.6913023260E+03

Stress_EigVals = -2.0412111891E+00 -2.0408072007E+00 -1.9463828419E+00

Stress_EigVec1 = -4.4264730212E-01 8.9669580456E-01 0.0000000000E+00

Stress_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

Stress_EigVec3 = 8.9669580456E-01 4.4264730212E-01 0.0000000000E+00

-DivStress = -9.9120324653E+00 -4.8189641820E+00 6.8463541658E-18

CP# 2 Coords = 1.17358658220725E+00 -1.92566823496376E+00 2.03366112223429E+00

Type = (3,-3) NACP H2

Rho = 4.0533296949E-01 Rho at Nucleus = 4.0344055059E-01
GradRho = -1.7000290065E-15 1.0963452368E-15 -3.9981039313E-15
HessRho_EigVals = -8.1517826306E+00 -8.1488125569E+00 -7.7640518386E+00
HessRho_EigVec1 = 2.2272770071E-01 8.9575000890E-01 3.8473925311E-01
HessRho_EigVec2 = 8.6602595635E-01 -5.7922496028E-04 -4.9999870743E-01
HessRho_EigVec3 = 4.4765099605E-01 -4.4455774208E-01 7.7587176756E-01
DelSqRho = -2.4064647026E+01
Bond Ellipticity = NA
V = -6.0266454176E+00
G = 5.2418305521E-03
K = 6.0214035871E+00
L = 6.0161617565E+00
Vnuc = 5.3591584901E+01
Ven = -2.1722436248E+01
Vrep = 1.5695790830E+01
DelSqV = 1.5708660511E+03
DelSqVen = 1.2896625742E+03
DelSqVrep = 2.8120347685E+02
DelSqG = 1.1995746649E+02
DelSqK = -1.6908235175E+03
Stress_EigVals = -2.0406041130E+00 -2.0401985732E+00 -1.9458427314E+00
Stress_EigVec1 = 2.2293348645E-01 8.9698289228E-01 3.8173597103E-01
Stress_EigVec2 = 8.6565699258E-01 -2.0894813779E-03 -5.0063320431E-01
Stress_EigVec3 = 4.4826178937E-01 -4.4206031831E-01 7.7694532830E-01
-DivStress = 4.9525706537E+00 -4.8098214638E+00 8.5840595831E+00

CP# 3 Coords = 1.17358658220725E+00 -1.92566823496376E+00 -2.03366112223429E+00

Type = (3,-3) NACP H3

Rho = 4.0533296949E-01 Rho at Nucleus = 4.0344055059E-01
GradRho = -1.7034984534E-15 1.1084883011E-15 3.9950681652E-15
HessRho_EigVals = -8.1517826306E+00 -8.1488125569E+00 -7.7640518386E+00
HessRho_EigVec1 = 2.2272770071E-01 8.9575000890E-01 -3.8473925311E-01

HessRho_EigVec2 = 8.6602595635E-01 -5.7922496014E-04 4.9999870743E-01

HessRho_EigVec3 = -4.4765099605E-01 4.4455774208E-01 7.7587176756E-01

DelSqRho = -2.4064647026E+01

Bond Ellipticity = NA

V = -6.0266454176E+00

G = 5.2418305521E-03

K = 6.0214035871E+00

L = 6.0161617565E+00

Vnuc = 5.3591584901E+01

Ven = -2.1722436248E+01

Vrep = 1.5695790830E+01

DelSqV = 1.5708660511E+03

DelSqVen = 1.2896625742E+03

DelSqVrep = 2.8120347685E+02

DelSqG = 1.1995746649E+02

DelSqK = -1.6908235175E+03

Stress_EigVals = -2.0406041130E+00 -2.0401985732E+00 -1.9458427314E+00

Stress_EigVec1 = 2.2293348645E-01 8.9698289228E-01 -3.8173597103E-01

Stress_EigVec2 = 8.6565699258E-01 -2.0894813765E-03 5.0063320431E-01

Stress_EigVec3 = -4.4826178937E-01 4.4206031831E-01 7.7694532830E-01

-DivStress = 4.9525706537E+00 -4.8098214638E+00 -8.5840595831E+00

CP# 4 Coords = -9.32314514898941E-06 -7.27701538223167E-01 -2.71590823617317E-25

Type = (3,-3) NACP P4

Rho = 2.1167486212E+03 Rho at Nucleus = 2.1167486211E+03

GradRho = 5.1952886437E-13 1.1032739167E-09 6.6646992605E-17

HessRho_EigVals = -3.3421113636E+07 -3.3421113609E+07 -3.3421088537E+07

HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

HessRho_EigVec2 = 9.9999891387E-01 -1.4738577067E-03 0.0000000000E+00

HessRho_EigVec3 = 1.4738577067E-03 9.9999891387E-01 0.0000000000E+00

DelSqRho = -1.0026331578E+08

Bond Ellipticity = NA

V = -2.5078327366E+07
G = 6.2492099609E+03
K = 2.5072078156E+07
L = 2.5065828946E+07
Vnuc = 2.5327896486E+08
Ven = -5.3612789965E+11
Vrep = 5.3610282132E+11
DelSqV = 1.4053382790E+13
DelSqVen = 2.5394801591E+16
DelSqVrep = -2.5380748209E+16
DelSqG = 3.9600410263E+11
DelSqK = -1.4449386892E+13
Stress_EigVals = -8.3594465262E+06 -8.3594404231E+06 -8.3594404162E+06
Stress_EigVec1 = 1.5047196756E-03 9.9999886791E-01 0.0000000000E+00
Stress_EigVec2 = 9.9999886791E-01 -1.5047196756E-03 0.0000000000E+00
Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
-DivStress = -4.2177672076E+02 2.7350338641E+05 1.2524123477E-12

CP# 5 Coords = -9.32442227447606E-06 2.09025849388611E+00 1.10601989802846E-23

Type = (3,-3) NACP O5

Rho = 2.9532047770E+02 Rho at Nucleus = 2.9532044172E+02

GradRho = 7.1649500569E-16 -1.5480816629E-10 -7.0272224352E-18

HessRho_EigVals = -8.2034129496E+05 -8.2032475059E+05 -8.2032474503E+05

HessRho_EigVec1 = 2.6470679503E-04 9.9999996497E-01 0.0000000000E+00

HessRho_EigVec2 = 9.9999996497E-01 -2.6470679503E-04 0.0000000000E+00

HessRho_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

DelSqRho = -2.4609907906E+06

Bond Ellipticity = NA

V = -6.1538313571E+05

G = 6.7719031271E+01

K = 6.1531541668E+05

L = 6.1524769765E+05

Vnuc = 8.5414889301E+05
Ven = -2.5224765911E+08
Vrep = 2.5163227598E+08
DelSqV = 3.9138819201E+10
DelSqVen = 2.1020525568E+12
DelSqVrep = -2.0629137376E+12
DelSqG = 1.7094028342E+09
DelSqK = -4.0848222035E+10
Stress_EigVals = -2.0512914351E+05 -2.0512914213E+05 -2.0512485007E+05
Stress_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
Stress_EigVec2 = 9.9999996371E-01 -2.6941687565E-04 0.0000000000E+00
Stress_EigVec3 = 2.6941687565E-04 9.9999996371E-01 0.0000000000E+00
-DivStress = 1.5105254271E+01 1.1934919021E+05 -1.3155369695E-13

CP# 6 Coords = -1.11851075666349E+00 -1.29776700149654E+00 4.27418210970832E-19

Type = (3,-1) BCP P4 H1
Rho = 1.7266483636E-01
GradRho = 4.1078251911E-15 2.0764640007E-15 -8.6988004053E-19
HessRho_EigVals = -2.8795570365E-01 -2.7320489799E-01 5.9342166675E-01
HessRho_EigVec1 = -4.5763043060E-01 8.8914250207E-01 0.0000000000E+00
HessRho_EigVec2 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec3 = 8.8914250207E-01 4.5763043060E-01 0.0000000000E+00
DelSqRho = 3.2261065103E-02
Bond Ellipticity = 5.3991732086E-02
V = -3.5464071735E-01
G = 1.8135299181E-01
K = 1.7328772554E-01
L = -8.0652662757E-03
Vnuc = 1.5539240539E+01
Ven = -2.6830804247E+00
Vrep = 2.3284397073E+00
DelSqV = -3.2355634478E+00

DelSqVen = -5.0131245067E-01

DelSqVrep = -2.7342509971E+00

DelSqG = 6.6003082980E+00

DelSqK = -3.3647448502E+00

Stress_EigVals = -1.5101787775E-01 -1.0295687804E-01 -1.0066596155E-01

Stress_EigVec1 = 8.9340050393E-01 4.4926110401E-01 0.0000000000E+00

Stress_EigVec2 = -4.4926110401E-01 8.9340050393E-01 0.0000000000E+00

Stress_EigVec3 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00

-DivStress = 3.6530070988E-01 1.8576116747E-01 4.7076594431E-20

BPL = 2.6354657453E+00 = 1.2553970555E+00 + 1.3800686897E+00

GBL_I = 2.6354392588E+00

GBL_II = 2.6573255109E+00

GBL_III = 2.6354402991E+00 = 1.2553963873E+00 + 1.3800439118E+00

GBL_IV = 2.6573262091E+00 = 1.2553964141E+00 + 1.4019297950E+00

CP# 7 Coords = 5.59316173715760E-01 -1.29737455118211E+00 9.69067981964503E-01

Type = (3,-1) BCP H2 P4

Rho = 1.7260752614E-01

GradRho = 3.7296554734E-17 -8.6736173799E-17 6.9388939039E-17

HessRho_EigVals = -2.8775886505E-01 -2.7302727637E-01 5.9234676327E-01

HessRho_EigVec1 = 2.2785846353E-01 8.8934777626E-01 3.9641020858E-01

HessRho_EigVec2 = 8.6628959678E-01 7.1061183567E-04 -4.9954161944E-01

HessRho_EigVec3 = 4.4454792218E-01 -4.5723082562E-01 7.7027080757E-01

DelSqRho = 3.1560621852E-02

Bond Ellipticity = 5.3956472289E-02

V = -3.5436813394E-01

G = 1.8112914470E-01

K = 1.7323898924E-01

L = -7.8901554631E-03

Vnuc = 1.5537503603E+01

Ven = -2.6818900594E+00

Vrep = 2.3275219254E+00

DelSqV = -3.2304836746E+00

DelSqVen = -4.9037327574E-01

DelSqVrep = -2.7401103988E+00

DelSqG = 6.5917540581E+00

DelSqK = -3.3612703835E+00

Stress_EigVals = -1.5088306204E-01 -1.0289352926E-01 -1.0059154264E-01

Stress_EigVec1 = 4.4680865499E-01 -4.4913280813E-01 7.7371942362E-01

Stress_EigVec2 = -2.2657566277E-01 -8.9346269252E-01 -3.8779877014E-01

Stress_EigVec3 = -8.6546259010E-01 2.0341443141E-03 5.0096942760E-01

-DivStress = -1.8256473796E-01 1.8551928937E-01 -3.1630800265E-01

BPL = 2.6359760116E+00 = 1.3804017346E+00 + 1.2555742770E+00

GBL_I = 2.6359493765E+00

GBL_II = 2.6578308229E+00

GBL_III = 2.6359502472E+00 = 1.3803766305E+00 + 1.2555736166E+00

GBL_IV = 2.6578313828E+00 = 1.4022577393E+00 + 1.2555736436E+00

CP# 8 Coords = 5.59316173715760E-01 -1.29737455118211E+00 -9.69067981964503E-01

Type = (3,-1) BCP P4 H3

Rho = 1.7260752614E-01

GradRho = 3.0791341699E-17 -5.5511151231E-17 6.9388939039E-18

HessRho_EigVals = -2.8775886505E-01 -2.7302727637E-01 5.9234676327E-01

HessRho_EigVec1 = 2.2785846353E-01 8.8934777626E-01 -3.9641020858E-01

HessRho_EigVec2 = 8.6628959678E-01 7.1061183567E-04 4.9954161944E-01

HessRho_EigVec3 = -4.4454792218E-01 4.5723082562E-01 7.7027080757E-01

DelSqRho = 3.1560621852E-02

Bond Ellipticity = 5.3956472289E-02

V = -3.5436813394E-01

G = 1.8112914470E-01

K = 1.7323898924E-01

L = -7.8901554631E-03

Vnuc = 1.5537503603E+01

Ven = -2.6818900594E+00

Vrep = 2.3275219254E+00
DelSqV = -3.2304836746E+00
DelSqVen = -4.9037327574E-01
DelSqVrep = -2.7401103988E+00
DelSqG = 6.5917540581E+00
DelSqK = -3.3612703835E+00
Stress_EigVals = -1.5088306204E-01 -1.0289352926E-01 -1.0059154264E-01
Stress_EigVec1 = -4.4680865499E-01 4.4913280813E-01 7.7371942362E-01
Stress_EigVec2 = -2.2657566277E-01 -8.9346269252E-01 3.8779877014E-01
Stress_EigVec3 = -8.6546259010E-01 2.0341443141E-03 -5.0096942760E-01
-DivStress = -1.8256473796E-01 1.8551928937E-01 3.1630800265E-01
BPL = 2.6359760116E+00 = 1.2555742770E+00 + 1.3804017346E+00
GBL_I = 2.6359493765E+00
GBL_II = 2.6578308229E+00
GBL_III = 2.6359502472E+00 = 1.2555736166E+00 + 1.3803766305E+00
GBL_IV = 2.6578313828E+00 = 1.2555736436E+00 + 1.4022577393E+00

CP# 9 Coords = -2.75825471911585E-05 4.07255028554691E-01 9.28208424282889E-19

Type = (3,-1) BCP O5 P4
Rho = 2.2160946682E-01
GradRho = -8.4025668368E-19 -5.8286708793E-16 -1.1684949950E-21
HessRho_EigVals = -3.7482333054E-01 -3.7480161139E-01 2.1470173987E+00
HessRho_EigVec1 = 0.0000000000E+00 0.0000000000E+00 1.0000000000E+00
HessRho_EigVec2 = 9.9999999998E-01 7.0277506267E-06 0.0000000000E+00
HessRho_EigVec3 = -7.0277506267E-06 9.9999999998E-01 0.0000000000E+00
DelSqRho = 1.3973924567E+00
Bond Ellipticity = 5.7948404903E-05
V = -6.7783224693E-01
G = 5.1359018056E-01
K = 1.6424206637E-01
L = -3.4934811419E-01
Vnuc = 1.8870480774E+01

$$\text{Ven} = -4.1818771829\text{E}+00$$

$$\text{Vrep} = 3.5040449359\text{E}+00$$

$$\text{DelSqV} = -1.0394881611\text{E}+01$$

$$\text{DelSqVen} = -2.6369467488\text{E}+01$$

$$\text{DelSqVrep} = 1.5974585877\text{E}+01$$

$$\text{DelSqG} = 1.5695217190\text{E}+01$$

$$\text{DelSqK} = -5.3003355793\text{E}+00$$

$$\text{Stress\_EigVals} = -2.6065968678\text{E}-01 \ -2.0858648608\text{E}-01 \ -2.0858607407\text{E}-01$$

$$\text{Stress\_EigVec1} = -1.1849710101\text{E}-04 \ 9.9999999298\text{E}-01 \ 0.0000000000\text{E}+00$$

$$\text{Stress\_EigVec2} = 9.9999999298\text{E}-01 \ 1.1849710101\text{E}-04 \ 0.0000000000\text{E}+00$$

$$\text{Stress\_EigVec3} = 0.0000000000\text{E}+00 \ 0.0000000000\text{E}+00 \ 1.0000000000\text{E}+00$$

$$-\text{DivStress} = 6.1805811366\text{E}-06 \ -6.2155801966\text{E}-01 \ -3.8502642438\text{E}-19$$

$$\text{BPL} = 2.8179600341\text{E}+00 = 1.6830034672\text{E}+00 + 1.1349565669\text{E}+00$$

$$\text{GBL\_I} = 2.8179600321\text{E}+00$$

$$\text{GBL\_II} = 2.8179693390\text{E}+00$$

$$\text{GBL\_III} = 2.8179600324\text{E}+00 = 1.6830034654\text{E}+00 + 1.1349565669\text{E}+00$$

$$\text{GBL\_IV} = 2.8179693392\text{E}+00 = 1.6830128315\text{E}+00 + 1.1349565077\text{E}+00$$

$$\text{Number of NACPs} = 5$$

$$\text{Number of NNACPs} = 0$$

$$\text{Number of BCPs} = 4$$

$$\text{Number of RCPs} = 0$$

$$\text{Number of CCPs} = 0$$

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV
H2	P4	H1	100.94196413	100.93756260	100.94930540	101.00348811	101.00348513
H3	P4	H1	100.94196413	100.93756260	100.94930540	101.00348811	101.00348513
H3	P4	H2	100.97211042	100.97934730	100.99124083	101.03394167	101.03393869
O5	P4	H1	117.05572339	117.05990247	117.05042224	117.00560569	117.00560811
O5	P4	H2	117.03245971	117.03100383	117.02144570	116.98276829	116.98277069
O5	P4	H3	117.03245971	117.03100383	117.02144570	116.98276829	116.98277069

Total time for electron density critical point search, analysis and connectivity = 3 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$Ee(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular Ee unless molecular electronic virial theorem is satisfied.

T(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Ven(A) = Ven(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$VenO(A) = Ven(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$Vee(A) = Vee(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

Vnn(A) - W(A) = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus
the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of Vnn(A) - W(A) assumes satisfaction of the atomic virial theorem:

$$2T(A) + Ven(A) + Vee(A) + Vnn(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	Ee(A)	T(A)	Ven(A)	VenO(A)	Vee(A)	Vnn(A) - W(A)

H1	-8.7429404867E-01	8.7429404867E-01	-1.5085966899E+01	-1.6492630942E+00
H2	-8.7396925944E-01	8.7396925944E-01	-1.5082118373E+01	-1.6489068127E+00
H3	-8.7396961510E-01	8.7396961510E-01	-1.5082142124E+01	-1.6489079237E+00
P4	-3.3943824165E+02	3.3943824165E+02	-8.3687082130E+02	-7.9072671544E+02
O5	-7.5659602536E+01	7.5659602536E+01	-2.4209197410E+02	-1.8522625356E+02
Total	-4.1772007711E+02	4.1772007711E+02	-1.1242130228E+03	-9.8090004683E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

= $T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E(A)$	$E_e(A)$	$W(A)$	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$
H1	-8.7419322606E-01	-8.7429404867E-01	1.0082260845E-04			
H2	-8.7404157880E-01	-8.7396925944E-01	-7.2319357486E-05			
H3	-8.7404193446E-01	-8.7396961510E-01	-7.2319357483E-05			
P4	-3.3943842086E+02	-3.3943824165E+02	-1.7920538962E-04			
O5	-7.5659810118E+01	-7.5659602536E+01	-2.0758215007E-04			

Total -4.1772050771E+02 -4.1772007711E+02 -4.3060364621E-04

IQA Atomic Energy Components:

 $E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A, Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A, Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{ee}(A) = V_{ee}(A, Mol) = (1/2)[V_{ee}(A, Mol) + V_{ee}(Mol, A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$V_{ne}(A, Mol)/2$	$V_{en}(A, Mol)/2$	$V_{ee}(A)$	$V_{nn}(A, Mol)/2$
$V_{eeC}(A)$	$V_{eeX}(A)$					

H1			8.7429404867E-01	-4.4514628727E+00	-7.5429834494E+00	
3.9227456639E+00						
H2			8.7396925944E-01	-4.4509135258E+00	-7.5410591866E+00	
3.9222149928E+00						
H3			8.7396961510E-01	-4.4509135258E+00	-7.5410710621E+00	
3.9222149928E+00						
P4			3.3943824165E+02	-4.3535468454E+02	-4.1843541065E+02	
2.9758014605E+01						
O5			7.5659602536E+01	-1.1339824565E+02	-1.2104598705E+02	
2.3861372275E+01						

Total			4.1772007711E+02	-5.6210622011E+02	-5.6210651140E+02	
6.5386562529E+01						

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

$$= \text{Intraatomic ("Self") Contribution to } E\_IQA(A)$$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$

H1	8.7429404867E-01	-1.6492630942E+00				

H2	8.7396925944E-01	-1.6489068127E+00				

H3	8.7396961510E-01	-1.6489079237E+00				

P4	3.3943824165E+02	-7.9072671544E+02				

O5	7.5659602536E+01	-1.8522625356E+02				

Total	4.1772007711E+02	-9.8090004683E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[\text{Ven}(\text{A},\text{Mol}) - \text{Ven}(\text{A},\text{A})]$$

$\text{Vee}(\text{A},\text{A}') = \text{Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule}$

$$= \text{Vee}(\text{A},\text{Mol}) - \text{Vee}(\text{A},\text{A})$$

$\text{Vnn}(\text{A}) = \text{Vnn}(\text{A},\text{Mol})/2 = \text{Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule}$

$\text{VeeC}(\text{A},\text{A}') = \text{Coulomb Part of Vee}(\text{A},\text{A}')$

$\text{VeeX}(\text{A},\text{A}') = \text{Exchange-Correlation Part of Vee}(\text{A},\text{A}')$

See "2EDM Note" and "DFT Note".

Atom A	E_IQA_Inter(A)	Vne(A,A')/2	Ven(A,A')/2	Vee(A,A')	Vnn(A)	VeeC(A,A')
H1	-3.6268313256E+00	-6.7183519023E+00		3.9227456639E+00		
H2	-3.6264601194E+00	-6.7166057803E+00		3.9222149928E+00		
H3	-3.6264595639E+00	-6.7166171002E+00		3.9222149928E+00		
P4	-3.9991326824E+01	-2.3072052931E+01		2.9758014605E+01		
O5	-2.0785118874E+01	-2.8432860273E+01		2.3861372275E+01		
Total	-7.1656196707E+01	-7.1656487987E+01		6.5386562529E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(\text{A}) = \text{Average Number of Electrons in Atom A}$

$\text{LI}(\text{A}) = \text{Electron Localization Index of Atom A} = \text{Average Number of Electrons Localized in Atom A}$

$$\% \text{Loc}(\text{A}) = 100 * \text{LI}(\text{A}) / N(\text{A})$$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$\text{DI}(\text{A},\text{A}')/2 = \text{Electron Delocalization Index of Atom A} = \text{Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule}$

$$= N(\text{A}) - \text{LI}(\text{A})$$

$$\% \text{Deloc}(\text{A},\text{A}') = 100 * (\text{DI}(\text{A},\text{A}')/2) / N(\text{A})$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
H1	1.6119264700E+00	1.1721844273E+00	7.2719472575E+01	4.3974204273E-01	
	2.7280527425E+01				
H2	1.6116980351E+00	1.1719705123E+00	7.2716506860E+01	4.3972752284E-01	
	2.7283493140E+01				
H3	1.6117005047E+00	1.1719727426E+00	7.2716533824E+01	4.3972776206E-01	
	2.7283466176E+01				
P4	1.1748396310E+01	1.0474483354E+01	8.9156707667E+01	1.2739129563E+00	
	1.0843292333E+01				
O5	9.4163583955E+00	8.7983547328E+00	9.3436914392E+01	6.1800366270E-01	
	6.5630856084E+00				
Total	2.6000079716E+01	2.2788965769E+01	8.7649599610E+01	3.2111139467E+00	
	1.2350400390E+01				

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= LI(A) + DI(A,A')/2 = LI(A) + DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

LI(A) = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

DI(A,A')/2 = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= N(A) - LI(A) = DI\_Bond(A,A')/2 + DI\_NonBond(A,A')/2$$

DI_Bond(A,A')/2 = Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

DI_NonBond(A,A')/2 = Non-Bonding Contribution to DI(A,A')/2 = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= DI(A,A')/2 - DI\_Bond(A,A')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2

H1	1.6119264700E+00		1.1721844273E+00	4.3974204273E-01	2.8111942319E-01
	1.5862261954E-01				
H2	1.6116980351E+00		1.1719705123E+00	4.3972752284E-01	2.8109630390E-01
	1.5863121894E-01				
H3	1.6117005047E+00		1.1719727426E+00	4.3972776206E-01	2.8111695362E-01
	1.5861080844E-01				
P4	1.1748396310E+01	1.0474483354E+01	1.2739129563E+00	1.2739983018E+00	-
	8.5345445826E-05				
O5	9.4163583955E+00	8.7983547328E+00	6.1800366270E-01	4.3066562106E-01	
	1.8733804163E-01				

Total	2.6000079716E+01	2.2788965769E+01	3.2111139467E+00	2.5479966036E+00	
	6.6311734311E-01				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)

H1	7.1306125872E-01	1.9435962882E+01	2.0149024141E+01
H2	7.1280002205E-01	1.9433368682E+01	2.0146168704E+01
H3	7.1280288711E-01	1.9433396686E+01	2.0146199573E+01
P4	6.3775166256E+01	8.3079753576E+01	1.4685491983E+02
O5	3.9934725350E+01	7.7769502022E+01	1.1770422737E+02

Total 1.0584855577E+02 2.1915198385E+02 3.2500053962E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B

$= N(A) * N(B) - DI(A,B) / 2$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$
H1	H2	2.5498593453E+00	9.6158758348E-02	2.9827278147E+00	2.9831505733E+00
H1	H3	2.5498629359E+00	9.6159538742E-02	2.9827520216E+00	2.9831702125E+00
H2	H3	2.5495460763E+00	9.6056920619E-02	2.9799912430E+00	2.9799866768E+00
H1	P4	1.8656431570E+01	5.6223884638E-01	1.7439965682E+01	2.3928323131E+00 (Bonded)
H2	P4	1.8653770945E+01	5.6219260780E-01	1.7441003077E+01	2.3926355264E+00 (Bonded)
H3	P4	1.8653779309E+01	5.6223390725E-01	1.7442257591E+01	2.3928112927E+00 (Bonded)
H1	O5	1.5115864085E+01	1.2522652714E-01	3.8843746742E+00	6.6494138114E-01
H2	O5	1.5113699215E+01	1.2525421809E-01	3.8857842897E+00	6.6508841757E-01
H3	O5	1.5113722346E+01	1.2525446567E-01	3.8857860162E+00	6.6508973219E-01
P4	O5	1.1019644461E+02	8.6133124213E-01	3.6657396438E+00	4.5735899482E+00 (Bonded)

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002
H1	P4	4.6416731020E+01	3.6874176225E+01	3.0424586660E+01
H1	Total	4.6416731020E+01	3.6874176225E+01	3.0424586660E+01
H2	P4	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
H2	Total	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
H3	P4	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
H3	Total	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
P4	H1	4.6416731020E+01	3.6874176225E+01	3.0424586660E+01
P4	H2	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
P4	H3	4.6415137101E+01	3.6867850686E+01	3.0422072810E+01
P4	O5	5.4311264224E+01	4.3407209265E+01	3.6056081506E+01
P4	Total	1.9355826945E+02	1.5401708686E+02	1.2732481379E+02
O5	P4	5.4311264224E+01	4.3407209265E+01	3.6056081506E+01
O5	Total	5.4311264224E+01	4.3407209265E+01	3.6056081506E+01

Total	Total	3.8711653889E+02	3.0803417372E+02	2.5464962757E+02

Some Properties of Interatomic Surfaces:

$N\_IAS(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G\_IAS(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K\_IAS(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L\_IAS(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta\rho\_IAS(A|B)$ = Integral of Laplacian of Electron Density $\Delta\rho(r)$ Over Interatomic Surface Between Atoms A and B

$V\_IAS(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N\_IAS(A B)$	$G\_IAS(A B)$	$K\_IAS(A B)$	$L\_IAS(A B)$	$\Delta\rho\_IAS(A B)$	$V\_IAS(A B)$

H1	P4	9.5346313513E-01	7.1240271902E-01	4.7241061698E-01	-2.3999210203E-01	9.5996840814E-01	-1.1848133360E+00

H1	Total	9.5346313513E-01	7.1240271902E-01	4.7241061698E-01	-2.3999210203E-01	9.5996840814E-01	-1.1848133360E+00

H2	P4	9.5320555867E-01	7.1185315379E-01	4.7219462481E-01	-2.3965852898E-01	9.5863411590E-01	-1.1840477786E+00

H2	Total	9.5320555867E-01	7.1185315379E-01	4.7219462481E-01	-2.3965852898E-01	9.5863411590E-01	-1.1840477786E+00

H3	P4	9.5320555867E-01	7.1185315379E-01	4.7219462481E-01	-2.3965852898E-01	9.5863411590E-01	-1.1840477786E+00

H3	Total	9.5320555867E-01	7.1185315379E-01	4.7219462481E-01	-2.3965852898E-01	9.5863411590E-01	-1.1840477786E+00

P4 H1 9.5346313513E-01 7.1240271902E-01 4.7241061698E-01 -2.3999210203E-01
9.5996840814E-01 -1.1848133360E+00

P4 H2 9.5320555867E-01 7.1185315379E-01 4.7219462481E-01 -2.3965852898E-01
9.5863411590E-01 -1.1840477786E+00

P4 H3 9.5320555867E-01 7.1185315379E-01 4.7219462481E-01 -2.3965852898E-01
9.5863411590E-01 -1.1840477786E+00

P4 O5 1.3096968823E+00 1.4402935079E+00 6.9345391634E-01 -7.4683959156E-01
2.9873583662E+00 -2.1337474242E+00

P4 Total 4.1695711348E+00 3.5764025345E+00 2.1102537829E+00 -1.4661487516E+00
5.8645950061E+00 -5.6866563174E+00

O5 P4 1.3096968823E+00 1.4402935079E+00 6.9345391634E-01 -7.4683959156E-01
2.9873583662E+00 -2.1337474242E+00

O5 Total 1.3096968823E+00 1.4402935079E+00 6.9345391634E-01 -7.4683959156E-01
2.9873583662E+00 -2.1337474242E+00

Total Total 8.3391422695E+00 7.1528050690E+00 4.2205075659E+00 -2.9322975031E+00
1.1729190012E+01 -1.1373312635E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

$|ESP|_{Int\_IDS}(A)$ = Surface Integral of $|ESP|$ Over Atom A's Part of IDS

$ESP*ESP_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Atom A's Part of IDS

$Area\_ESP+_{IDS}(A)$ = Surface Area of Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Int\_IDS}(A)$ = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

$Area\_ESP-_{IDS}(A)$ = Surface Area of Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Int\_IDS}(A)$ = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

$ESP+_{Min\_IDS}(A)$ = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Avg\_IDS}(A)$ = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+_{Var\_IDS}(A)$ = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

$ESP+*ESP+_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Positive Regions of Atom A's Part of IDS

$ESP-_{Min\_IDS}(A)$ = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Avg\_IDS}(A)$ = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{MAD\_IDS}(A)$ = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-_{Var\_IDS}(A)$ = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

$ESP-*ESP-_{Int\_IDS}(A)$ = Surface Integral of $ESP*ESP$ Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

H1	6.9393504952E+01						

H2	6.8916736283E+01						

H3	6.9228139661E+01						

P4	1.1810771041E+01						

O5	1.2730224419E+02						

Total	3.4665139613E+02						

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

H1	5.7679418314E+01	1.9953535317E+00	6.8720079266E-02	9.5998312158E-03	3.4593856699E-02
	8.5363143128E-03	1.1338400923E-04			

H2	5.7502374838E+01	1.9855553013E+00	6.8938831163E-02	7.5110886666E-03	3.4529970404E-02
	8.4980853518E-03	1.1217458251E-04			

H3	5.7493620693E+01	1.9862692272E+00	6.8990959790E-02	7.1640016012E-03	3.4547645516E-02
	8.5367158691E-03	1.1315973764E-04			

P4	1.1906041531E+01	4.3227347532E-01	6.9970739393E-02	5.2074580787E-03	3.6307069331E-02
	1.2347755345E-02	2.3557826098E-04			

O5	1.0792185045E+02	-4.6633762420E+00	2.8791658642E-02	-7.5331585737E-02	-4.3210677195E-02
	2.2453030649E-02	7.0751679891E-04			

Total	2.9250330583E+02	1.7360752935E+00	6.9970739393E-02	-7.5331585737E-02	5.9352330690E-03
	1.7496034753E-03				

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)
	ESP-_Int_IDS(A)				

H1	1.9953535317E+00	7.5566897837E-02	5.7679418314E+01	1.9953535317E+00	0.0000000000E+00
	NULL				

H2	1.9855553013E+00	7.5011470679E-02	5.7502374838E+01	1.9855553013E+00	0.0000000000E+00
	NULL				

H3	1.9862692272E+00	7.5126888194E-02	5.7493620693E+01	1.9862692272E+00	0.0000000000E+00
	NULL				

P4	4.3227347532E-01	1.8499387597E-02	1.1906041531E+01	4.3227347532E-01	0.0000000000E+00
	NULL				

O5	4.8652433380E+00	2.7786416759E-01	9.9877998951E+00	1.0093354801E-01	9.7934050552E+01
	-4.7643097900E+00				

Total	1.1264694874E+01	5.2206881190E-01	1.9456925527E+02	6.5003850835E+00	9.7934050552E+01
	-4.7643097900E+00				

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)	ESP+*ESP+_Int_IDS(A)
H1	9.5998312158E-03	3.4593856699E-02	8.5363143128E-03	1.1338400923E-04	7.5566897837E-02
H2	7.5110886666E-03	3.4529970404E-02	8.4980853518E-03	1.1217458251E-04	7.5011470679E-02
H3	7.1640016012E-03	3.4547645516E-02	8.5367158691E-03	1.1315973764E-04	7.5126888194E-02
P4	5.2074580787E-03	3.6307069331E-02	1.2347755345E-02	2.3557826098E-04	1.8499387597E-02
O5	3.9169478332E-06	1.0105683841E-02	6.2313395433E-03	5.5037408579E-05	1.5697051487E-03
Total	3.9169478332E-06	3.3409107078E-02	1.4700312292E-04	2.4577434946E-01	

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)
H1	NULL	NULL	NULL	NULL	NULL
H2	NULL	NULL	NULL	NULL	NULL
H3	NULL	NULL	NULL	NULL	NULL
P4	NULL	NULL	NULL	NULL	NULL
O5	-7.7991009415E-05	-4.8648143961E-02	1.8120274681E-02	4.5458789515E-04	2.7629446245E-01
Total	-7.7991009415E-05	-4.8648143962E-02	4.5458789519E-04	2.7629446245E-01	

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)	ESP_MAD_IDS(A)	ESP_Var_IDS(A)

H1	4.9414418382E+01
H2	4.9393556520E+01
H3	4.9083604917E+01
P4	1.2867681950E+01
O5	9.4196741439E+01

Total	2.5495600321E+02

Atomic Surface Area and Volume Data:

$\text{Area(A)} = \text{Area\_IAS(A|Total)} + \text{Area\_IDS(A)}$

$\text{Vol(A)} = \text{Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an}$
 $\text{Isosurface of the Electron Density Distribution (IsoDensity Surface)}$

$\text{N(Vol(A))} = \text{Average Number of Electrons in Vol(A)}$

$\text{N(Vol(A))}/\text{Vol(A)} = \text{Average Electron Density in Vol(A)}$

$\% \text{N(Vol(A))} = 100 * \text{N(Vol(A))} / \text{N(A)}$

= Percentage of Atom A's Electron Population in Vol(A)

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
H1	1.1581023597E+02	1.0124044230E+02	1.5955042172E+00	1.5759553999E-02	9.8981203336E+01
H2	1.1533187338E+02	1.0127902886E+02	1.5952839139E+00	1.5751374513E-02	9.8981563473E+01
H3	1.1564327676E+02	1.0128960225E+02	1.5952896622E+00	1.5749787015E-02	9.8981768471E+01
P4	2.0536904049E+02	5.0019666520E+01	1.1745929165E+01	2.3482621901E-01	9.9979000155E+01
O5	1.8161350841E+02	2.0400889937E+02	9.3881140121E+00	4.6018159213E-02	9.9700049827E+01

Total	7.3376793502E+02	5.5783763930E+02	2.5920120970E+01	4.6465349672E-02
	9.9692467307E+01			

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

H1	9.4553594539E+01	7.5181995813E+01	1.5786045076E+00	2.0997108290E-02
	9.7932786432E+01			
H2	9.4370225524E+01	7.5230669041E+01	1.5784110245E+00	2.0980951581E-02
	9.7934662066E+01			
H3	9.4361471379E+01	7.5206976022E+01	1.5783894817E+00	2.0987274920E-02
	9.7933175357E+01			
P4	1.6592312839E+02	4.4738525550E+01	1.1742461800E+01	2.6246868121E-01
	9.9949486638E+01			
O5	1.5132905971E+02	1.5661998530E+02	9.3574004327E+00	5.9745890122E-02
	9.9373877244E+01			

Total	6.0053747955E+02	4.2697815173E+02	2.5835267246E+01	6.0507234719E-02
	9.9366107831E+01			

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

H1	7.9839005042E+01	5.8671511431E+01	1.5550424813E+00	2.6504217182E-02
	9.6471055594E+01			
H2	7.9815629330E+01	5.8618047412E+01	1.5546856434E+00	2.6522303490E-02
	9.6462588478E+01			
H3	7.9505677727E+01	5.8657615979E+01	1.5547681073E+00	2.6505818236E-02
	9.6467557252E+01			
P4	1.4019249574E+02	4.0773496233E+01	1.1736670300E+01	2.8785047602E-01
	9.9900190548E+01			
O5	1.3025282294E+02	1.2650451604E+02	9.3145086979E+00	7.3629851247E-02
	9.8918374883E+01			

Total	5.0960563078E+02	3.4322518710E+02	2.5715675230E+01	7.4923625062E-02

9.8906139947E+01

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$
H1	P4	-6.1191761297E-01		
H1		-6.1191761297E-01	-6.1192647030E-01	
H2	P4	-6.1168917807E-01		
H2		-6.1168917807E-01	-6.1169803540E-01	
H3	P4	-6.1169164757E-01		
H3		-6.1169164757E-01	-6.1170050490E-01	
P4	H1	6.1190875563E-01		
P4	H2	6.1168032073E-01		
P4	H3	6.1168279023E-01		
P4	O5	1.4163406807E+00		
P4		3.2516125473E+00	3.2516036900E+00	
O5	P4	-1.4163495381E+00		
O5		-1.4163495381E+00	-1.4163583954E+00	

Atomic Dipole Moments:

$\mu_{\text{Intra}}(A)$ = Intraatomic Dipole Moment Contribution of Atom A

$\mu_{\text{Bond}}(A)$ = Bonding Dipole Moment Contribution of Atom A

$\mu(A) = \mu_{\text{Intra}}(A) + \mu_{\text{Bond}}(A)$

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

H1	-3.3822210962E-01	7.6375294037E-01	4.2553083075E-01
H2	1.6902574621E-01	-3.8176230935E-01	-2.1273656314E-01
H3	1.6903081501E-01	-3.8176385060E-01	-2.1273303559E-01
P4	-9.7870750090E-05	1.8850171242E-04	9.0630962329E-05
O5	1.1632864162E-04	-2.5861566249E-05	9.0467075371E-05

Total	-1.4709050847E-04	3.8942056236E-04	2.4233005389E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

H1	-1.7738017464E-01	3.9065934010E-01	2.1327916546E-01
H2	-1.7698183489E-01	3.9016176979E-01	2.1317993490E-01
H3	-1.7698341505E-01	3.9016334494E-01	2.1317992989E-01
P4	8.2102665714E-02	-5.6173996619E-01	-4.7963730048E-01
O5	6.1853859762E-01	-2.3837344464E+00	-1.7651958488E+00

Total	1.6929583875E-01	-1.7744899577E+00	-1.6051941190E+00

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

H1	-5.3983484508E-07	2.6154473140E-19	-5.3983484508E-07
H2	2.9325638716E-01	-6.6163383681E-01	-3.6837744965E-01
H3	-2.9325631605E-01	6.6163650795E-01	3.6838019190E-01
P4	1.5007274123E-04	2.3931133815E-06	1.5246585461E-04
O5	-4.9455501400E-07	1.3146675730E-18	-4.9455501400E-07

Total	1.4910946137E-04	5.0642490150E-06	1.5417371039E-04

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

H1	3.8191350041E-01	8.5786553371E-01	4.7598790986E-01
H2	3.8195756489E-01	8.5774588397E-01	4.7581979294E-01
H3	3.8196048556E-01	8.5774934684E-01	4.7582033660E-01
P4	8.2102861204E-02	5.6173999783E-01	4.7963733328E-01
O5	6.1853860856E-01	2.3837344465E+00	1.7651958511E+00

Total 1.6929596832E-01 1.7744900005E+00 1.6051941447E+00

Bond Contributions to Atomic Dipole Moments:

$\text{Mu\_Bond}(A|B)$ = Contribution of Bond Between Atom A and Atom B to $\text{Mu\_Bond}(A)$

$\text{Mu\_Bond}(A)$ = Sum of $\text{Mu\_Bond}(A|B)$ Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	$\text{Mu\_Bond\_X}(A B)$	$\text{Mu\_Bond\_X}(A)$

H1	P4	7.6375294037E-01	
H1		7.6375294037E-01	
H2	P4	-3.8176230935E-01	
H2		-3.8176230935E-01	
H3	P4	-3.8176385060E-01	
H3		-3.8176385060E-01	
P4	H1	6.8442082030E-01	
P4	H2	-3.4212839937E-01	
P4	H3	-3.4212978062E-01	
P4	O5	2.5861404520E-05	
P4		1.8850171242E-04	
O5	P4	-2.5861566249E-05	
O5		-2.5861566249E-05	

Atom A	Atom B	$\text{Mu\_Bond\_Y}(A B)$	$\text{Mu\_Bond\_Y}(A)$

H1	P4	3.9065934010E-01	
H1		3.9065934010E-01	
H2	P4	3.9016176979E-01	
H2		3.9016176979E-01	
H3	P4	3.9016334494E-01	
H3		3.9016334494E-01	
P4	H1	3.4882808450E-01	
P4	H2	3.4845780751E-01	
P4	H3	3.4845921431E-01	
P4	O5	-1.6074850725E+00	
P4		-5.6173996619E-01	
O5	P4	-2.3837344464E+00	
O5		-2.3837344464E+00	

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

H1	P4	2.6154473140E-19	
H1		2.6154473140E-19	
H2	P4	-6.6163383681E-01	
H2		-6.6163383681E-01	
H3	P4	6.6163650795E-01	
H3		6.6163650795E-01	
P4	H1	-2.6154094561E-19	
P4	H2	-5.9275981402E-01	
P4	H3	5.9276220713E-01	
P4	O5	-1.3146593515E-18	
P4		2.3931133815E-06	
O5	P4	1.3146675730E-18	
O5		1.3146675730E-18	

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

H1	P4	8.5786553371E-01
H1		8.5786553371E-01
H2	P4	8.5774588397E-01
H2		8.5774588397E-01
H3	P4	8.5774934684E-01
H3		8.5774934684E-01
P4	H1	7.6818805757E-01
P4	H2	7.6800968899E-01
P4	H3	7.6801278963E-01
P4	O5	1.6074850727E+00
P4		5.6173999783E-01
O5	P4	2.3837344465E+00
O5		2.3837344465E+00

Atomic Traceless Quadrupole Moment Tensors:

$Q(A)$ = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	$Q_{XX}(A)$	$Q_{XY}(A)$	$Q_{XZ}(A)$	$Q_{YY}(A)$	$Q_{YZ}(A)$	$Q_{ZZ}(A)$
H1	2.1264216909E-01	1.2768503157E-01	-2.1980682613E-06	-2.2627746688E-02	1.1552270445E-06	-1.9001442240E-01
H2	-8.9253435356E-02	-6.3729893245E-02	1.7443350913E-01	-2.2281660458E-02	-1.1054974671E-01	1.1153509581E-01

H3 -8.9267648766E-02 -6.3717382547E-02 -1.7443561040E-01 -2.2273055410E-02 1.1055539788E-01 1.1154070418E-01

P4 -5.9890857741E-01 2.3334439640E-03 7.2771201902E-04 1.1907044846E+00 3.6034268127E-04 -5.9179590722E-01

O5 -4.3202063990E-01 -1.8248587535E-04 -1.3706476391E-06 8.6381678200E-01 2.3117842396E-06 -4.3179614210E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

Q_EigVal_n(A) = nth Eigenvalue of Q(A)

Q_EigVal_n_X(A) = X Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Y(A) = Y Component of the nth Eigenvector of Q(A)

Q_EigVal_n_Z(A) = Z Component of the nth Eigenvector of Q(A)

Atom A	n	Q_EigVal_n(A)	Q_EigVec_n_X(A)	Q_EigVec_n_Y(A)	Q_EigVec_n_Z(A)
H1	1	-1.9001442244E-01	1.0087555600E-05	-1.4596483792E-05	9.999999984E-01
H1	2	-7.8605722054E-02	-4.0151572445E-01	9.1585212929E-01	1.7418532959E-05
H1	3	2.6862014449E-01	9.1585212940E-01	4.0151572456E-01	-3.3779915114E-06
H2	1	-1.9012056349E-01	8.6547420989E-01	-1.3316696588E-03	-5.0095171291E-01
H2	2	-7.8294228611E-02	2.0240808486E-01	9.1566515543E-01	3.4725824731E-01
H2	3	2.6841479210E-01	4.5824159479E-01	-4.0193973403E-01	7.9275411762E-01
H3	1	-1.9013166210E-01	8.6546949120E-01	-1.4198841594E-03	5.0095962286E-01
H3	2	-7.8285580015E-02	2.0248298445E-01	9.1566347145E-01	-3.4721902032E-01
H3	3	2.6841724211E-01	-4.5821741654E-01	4.0194326837E-01	7.9276630112E-01
P4	1	-5.9898518582E-01	9.9492170254E-01	-1.2769408133E-03	-1.0064380374E-01
P4	2	-5.9172241457E-01	1.0064345729E-01	-3.3289382582E-04	9.9492250135E-01
P4	3	1.1907076004E+00	1.3039608489E-03	9.9999912930E-01	2.0268755375E-04
O5	1	-4.3202067396E-01	9.9998136719E-01	1.4081115319E-04	6.1029048934E-03
O5	2	-4.3179613374E-01	-6.1029045816E-03	-2.6438722790E-06	9.9998137710E-01
O5	3	8.6381680770E-01	-1.4082466618E-04	9.9999999008E-01	1.7844659842E-06

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho}/(r^*r) \rangle(A)$$

$$R-1(A) = \langle \text{Rho}/r \rangle(A)$$

$$R0(A) = \langle \text{Rho} \rangle(A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle(A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle(A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)
H1 3.4765222231E+00	3.0647573417E+00		1.6492630942E+00	1.6119264703E+00	2.1349494696E+00
H2 3.4765537167E+00	3.0639180340E+00		1.6489068127E+00	1.6116980354E+00	2.1348109636E+00
H3 3.4765680069E+00	3.0639185450E+00		1.6489079237E+00	1.6117005049E+00	2.1348166642E+00
P4 7.0106478844E+00	9.9036293660E+02		5.2715114362E+01	1.1748396310E+01	6.7481030057E+00
O5 1.6637476897E+01	2.5679647702E+02		2.3153281694E+01	9.4163583954E+00	1.0205109549E+01

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\text{Rho}/dx) + y^*(d\text{Rho}/dy) + z^*(d\text{Rho}/dz)$$

$$GR-2(A) = \langle \text{Dot}/(r^*r) \rangle(A)$$

$$GR-1(A) = \langle \text{Dot}/r \rangle(A)$$

$$GR0(A) = \langle \text{Dot} \rangle(A)$$

$$GR+1(A) = \langle \text{Dot} * r \rangle(A)$$

$$GR+2(A) = \langle \text{Dot} * r^*r \rangle(A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
H1 1.1438030450E+01	-2.6030814045E+00	-2.4711677919E+00	-3.3047655236E+00	-5.5944220797E+00	-
H2 1.1438255666E+01	-2.6023874900E+00	-2.4706342209E+00	-3.3042859738E+00	-5.5940664792E+00	-

H3 -2.6023886892E+00 -2.4706369658E+00 -3.3042925072E+00 -5.5940832003E+00 -
1.1438305585E+01

P4 -9.8875138375E+02 -1.0301350434E+02 -3.1439804935E+01 -2.0602168528E+01 -
2.3389578887E+01

O5 -2.5630381618E+02 -4.5231169648E+01 -2.5823981018E+01 -3.5145463942E+01 -
6.9330282381E+01

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

H1	8.0596323513E-01	8.0596323513E-01	1.6119264703E+00	0.0000000000E+00
H2	8.0584901772E-01	8.0584901772E-01	1.6116980354E+00	0.0000000000E+00
H3	8.0585025246E-01	8.0585025246E-01	1.6117005049E+00	0.0000000000E+00
P4	5.8741981552E+00	5.8741981552E+00	1.1748396310E+01	0.0000000000E+00
O5	4.7081791977E+00	4.7081791977E+00	9.4163583954E+00	0.0000000000E+00

Total	1.3000039858E+01	1.3000039858E+01	2.6000079716E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed to be the Hartree-Fock exchange functional and the atomic energies E_IQA(A) will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)

C2H6

AIMSum (Version 14.04.17, Standard)

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AIMSum is a component of the AIMAll package (<http://aim.tkgristmill.com>)

Much of the Quantum Theory of Atoms in Molecules (QTAIM) is described in the book:

"Atoms in Molecules - A Quantum Theory"

R.F.W. Bader, Oxford University Press, Oxford, 1990

For additional references see: <http://aim.tkgristmill.com/references.html>

Wfn File: D:\calc\ellipticity\propane\propane.wfn

Sum File: D:\calc\ellipticity\propane\propane.sum

SumViz File: D:\calc\ellipticity\propane\propane.sumviz

Wfn Title: c2h6_mp2

Total memory allocated for AIMSum = 0.512 Megabytes

Atomic units (a.u.) used throughout, except where stated otherwise

Model: Restricted SCF

Restricted, closed-shell, single-determinant wavefunction.

Number of electrons (from MO Occs)	=	26.0000000000
Number of Alpha electrons (from MO Occs)	=	13.0000000000
Number of Beta electrons (from MO Occs)	=	13.0000000000
Number of electron pairs ($N*(N-1)/2$)	=	325.0000000000
Number of electron pairs (from Muller 2EDM)	=	325.0000000000

Nuclear Charges and Cartesian Coordinates:

Atom	Charge	X	Y	Z
C1	6.0	1.7872000000E-04	1.1188185100E+00	0.0000000000E+00
H2	1.0	3.4343000000E-04	2.3569521200E+00	1.6603556800E+00
H3	1.0	3.4349000000E-04	2.3569527700E+00	-1.6603552000E+00
C4	6.0	2.3967915400E+00	-4.9399277000E-01	0.0000000000E+00
H5	1.0	4.1022357700E+00	6.7452075000E-01	-1.1000000000E-07
H6	1.0	2.4577284400E+00	-1.7123665800E+00	1.6715278900E+00
H7	1.0	2.4577281500E+00	-1.7123665300E+00	-1.6715279600E+00
C8	6.0	-2.3969282400E+00	-4.9383829000E-01	0.0000000000E+00
H9	1.0	-2.4581777200E+00	-1.7123886900E+00	1.6716619400E+00
H10	1.0	-4.1022761500E+00	6.7515992000E-01	-3.0000000000E-08

H11 1.0 -2.4581774900E+00 -1.7123884500E+00 -1.6716621500E+00

Some Atomic Properties:

q(A) = Net Charge of Atom A

L(A) = Lagrangian of Atom A = -(1/4) Times Atomic Integral of the Laplacian of the Electron Density

K(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

K_Scaled(A) = K(A) * E(Mol)/K(Mol) = Approximation to Virial-Based Total Energy of Atom A.

|Mu_Intra(A)| = Magnitude of Intraatomic Dipole Moment of Atom A

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	Mu_Intra(A)
C1	1.6191117940E-01	1.4255855812E-04	3.7673949711E+01	-3.7716719439E+01	3.8461038878E-03
H2	-6.2763994800E-02	4.9853171282E-05	6.4885293891E-01	-6.4958955570E-01	1.3160630021E-01
H3	-6.2765065400E-02	4.9059510587E-05	6.4885294396E-01	-6.4958956075E-01	1.3160565066E-01
C4	1.3372916470E-01	-2.4344522583E-04	3.7680549022E+01	-3.7723326243E+01	2.0741914975E-02
H5	-4.8165594000E-02	3.5703700444E-05	6.3588475021E-01	-6.3660664474E-01	1.3044311071E-01
H6	-5.1854552300E-02	5.2811682306E-05	6.3743237540E-01	-6.3815602688E-01	1.3313286902E-01
H7	-5.1852139500E-02	5.5723511472E-05	6.3743311660E-01	-6.3815676892E-01	1.3313245991E-01
C8	1.3354845740E-01	-1.3998248004E-04	3.7680282413E+01	-3.7723059331E+01	2.0582874125E-02
H9	-5.1774159600E-02	5.4976211100E-05	6.3732141783E-01	-6.3804494335E-01	1.3312841260E-01
H10	-4.8094546900E-02	3.6511230613E-05	6.3578889639E-01	-6.3651068210E-01	1.3044537898E-01
H11	-5.1772658900E-02	5.5969846853E-05	6.3732140009E-01	-6.3804492559E-01	1.3312874031E-01

Total 1.4609010000E-04 1.4973971691E-04 1.1815366899E+02 -1.1828780412E+02

Molecular charge q(Mol) from the wfn file: 0.0000000000E+00

Molecular energy E(Mol) from the wfn file: -1.1876743302E+02

Molecular virial ratio (-V(Mol)/T(Mol)) from the wfn file: 2.0011352600E+00

Note. $K\_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)$

Use K_Scaled(A) with caution.

Some Information About the Atomic Calculations:

Time(sec) = "Elapsed User Time", in Seconds, for Atom A by AIMInt

NProc = Number of Processors Used for AIMInt Job

BIM = Basin Integration Method

OAQ = Angular Quadrature Outside of Beta Sphere

ORQ = Multiple of Default for Radial Quadrature Outside of Beta Sphere

IAQ = Multiple of Default for Angular Quadrature Inside of Beta Sphere

IRQ = Multiple of Default for Radial Quadrature Inside of Beta Sphere

MIR = Maximum Integration Radius

Atom A	Time(sec)	NProc	BIM	OAQ	ORQ	IAQ	IRQ	MIR	

C1	15	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H2	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H3	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C4	14	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H5	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H6	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H7	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
C8	14	1	Proaim(5)	4334	(Very High)	1.00	1.00	1.00	13.00
H9	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H10	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00
H11	3	1	Proaim(5)	2030	(Very High)	1.00	1.00	1.00	13.00

Total 67

Note: Total wall clock time is less than total of atomic times if more than one atom was calculated at a time

Electron Density Critical Point Analysis of Molecular Structure:

NACP = Nuclear Attractor Critical Point

NNACP = Non-Nuclear Attractor Critical Point

BCP = Bond Critical Point

RCP = Ring Critical Point

CCP = Cage Critical Point

Rho = Electron Density

GradRho = Gradient of Electron Density

HessRho_EigVals = Eigenvalues of the Hessian of Rho, Ascending Order

HessRho_EigVecs = Eigenvectors of the Hessian of Rho

DelSqRho = Laplacian of Rho = Trace of Hessian of Rho

Bond Ellipticity = (HessRho_EigVal(1) / HessRho_EigVal(2)) - 1

V = Virial Field = Potential Energy Density = Trace of Stress Tensor

G = Lagrangian Form of Kinetic Energy Density

K = Hamiltonian Form of Kinetic Energy Density

L = K - G = Lagrangian Density = (-1/4)DelSqRho

Vnuc = Electrostatic Potential from Nuclei

Ven = Electron-nuclear attractive contribution to Virial Field V

Vrep = V - Ven = Repulsive contribution to Virial Field V

DelSqV = Laplacian of V

DelSqVen = Laplacian of Ven

DelSqVrep = Laplacian of Vrep

DelSqG = Laplacian of G

DelSqK = Laplacian of K

Stress_EigVals = Eigenvalues of Stress Tensor, Ascending Order

Stress_EigVecs = Eigenvectors of Stress Tensor

-DivStress = Ehrenfest Force Density = Minus Divergence of Stress Tensor

BP = Bond Path

BPL = Bond Path Length

GBL = Geometric Bond Length

GBL_I = Distance Between Nuclear Attractors

GBL_II = Distance Between Nuclei

GBL_III = Sum of Distances Between BCP and Nuclear Attractors

GBL_IV = Sum of Distances Between BCP and Nuclei

CP# 1 Coords = 1.78717412366156E-04 1.11881793743983E+00 3.21081789615703E-13

Type = (3,-3) NACP C1

Rho = 1.1935541729E+02 Rho at Nucleus = 1.1935541726E+02

GradRho = -3.8397063307E-13 -6.8424987898E-11 2.9318245524E-17

HessRho_EigVals = -1.8095658352E+05 -1.8095634810E+05 -1.8095604687E+05

HessRho_EigVec1 = 9.9999562539E-01 2.9579038463E-03 -2.4942366351E-08

HessRho_EigVec2 = -2.9579038463E-03 9.9999562539E-01 -4.1851308528E-07

HessRho_EigVec3 = 2.3704335773E-08 4.1858503157E-07 1.0000000000E+00

DelSqRho = -5.4286897848E+05

Bond Ellipticity = NA

V = -1.3573119845E+05

G = 6.9769135961E+00

K = 1.3572422153E+05

L = 1.3571724462E+05

Vnuc = 1.0479147492E+07

Ven = -1.2507430218E+09

Vrep = 1.2506072906E+09

DelSqV = 4.5999458680E+09

DelSqVen = 5.6888000512E+12

DelSqVrep = -5.6842001053E+12

DelSqG = 2.0578461506E+08

DelSqK = -4.8057304831E+09

Stress_EigVals = -4.5243800132E+04 -4.5243728023E+04 -4.5243670292E+04

Stress_EigVec1 = -1.2845888079E-09 8.2432011158E-08 1.0000000000E+00

Stress_EigVec2 = -3.3351409879E-03 9.9999443840E-01 -8.2435836989E-08

Stress_EigVec3 = 9.9999443840E-01 3.3351409879E-03 1.0096592844E-09

-DivStress = 3.8750809657E+00 8.5824522413E+02 -4.8208098658E-04

CP# 2 Coords = 3.40676066225899E-04 2.33942348875119E+00 1.63728509447024E+00

Type = (3,-3) NACP H2

Rho = 4.3628391749E-01 Rho at Nucleus = 4.3287164930E-01

GradRho = 2.1684043450E-18 -1.7178099221E-15 -7.9797279895E-16

HessRho_EigVals = -8.5590886294E+00 -8.5573443594E+00 -7.8771977360E+00

HessRho_EigVec1 = 9.9999999046E-01 2.3791855086E-05 -1.3604671871E-04

HessRho_EigVec2 = -1.0116902525E-04 7.9675899542E-01 -6.0429718928E-01

HessRho_EigVec3 = 9.4019095773E-05 6.0429719728E-01 7.9675899023E-01

DelSqRho = -2.4993630725E+01

Bond Ellipticity = NA

V = -6.2610203381E+00

G = 6.3063284329E-03

K = 6.2547140096E+00

L = 6.2484076812E+00

Vnuc = 4.1904829056E+01

Ven = -1.8282402982E+01

Vrep = 1.2021382644E+01

DelSqV = 1.6086800732E+03

DelSqVen = 1.0473538230E+03

DelSqVrep = 5.6132625019E+02

DelSqG = 1.1975037781E+02

DelSqK = -1.7284304510E+03

Stress_EigVals = -2.1447534166E+00 -2.1445228336E+00 -1.9717440879E+00

Stress_EigVec1 = 9.9999943745E-01 -8.9969996625E-04 5.6181519118E-04

Stress_EigVec2 = 1.0563481925E-03 7.9676358806E-01 -6.0429021907E-01

Stress_EigVec3 = 9.6046002153E-05 6.0429047260E-01 7.9676409024E-01

-DivStress = 1.4460402411E-03 9.1741186384E+00 1.2075259285E+01

CP# 3 Coords = 3.40734970268987E-04 2.33942412813069E+00 -1.63728462148623E+00

Type = (3,-3) NACP H3

Rho = 4.3628390929E-01 Rho at Nucleus = 4.3287164099E-01

GradRho = -3.4694469520E-18 1.9559007192E-16 9.2634233617E-16

HessRho_EigVals = -8.5590884381E+00 -8.5573441646E+00 -7.8771975336E+00

HessRho_EigVec1 = 9.9999999046E-01 2.3782471664E-05 1.3608544323E-04

HessRho_EigVec2 = -1.0118499073E-04 7.9675873403E-01 6.0429753393E-01

HessRho_EigVec3 = -9.4055576492E-05 -6.0429754193E-01 7.9675872883E-01

DelSqRho = -2.4993630136E+01

Bond Ellipticity = NA

V = -6.2610201892E+00

G = 6.3063275564E-03

K = 6.2547138616E+00

L = 6.2484075341E+00

Vnuc = 4.1904827821E+01

Ven = -1.8282402100E+01

Vrep = 1.2021381911E+01

DelSqV = 1.6086800319E+03

DelSqVen = 1.0473537675E+03

DelSqVrep = 5.6132626448E+02

DelSqG = 1.1975037440E+02

DelSqK = -1.7284304064E+03

Stress_EigVals = -2.1447533674E+00 -2.1445227851E+00 -1.9717440367E+00

Stress_EigVec1 = 9.9999943714E-01 -8.9995432117E-04 -5.6196159351E-04

Stress_EigVec2 = 1.0566392809E-03 7.9676332353E-01 6.0429056735E-01

Stress_EigVec3 = -9.6083520384E-05 -6.0429082101E-01 7.9676382600E-01

-DivStress = 1.4466150999E-03 9.1741239874E+00 -1.2075255319E+01

CP# 4 Coords = 2.39679160973245E+00 -4.93992783484095E-01 -2.15846569145559E-13

Type = (3,-3) NACP C4

Rho = 1.1937141877E+02 Rho at Nucleus = 1.1937141877E+02

GradRho = 4.2893466556E-13 -1.5207834991E-12 -1.1951370188E-18

HessRho_EigVals = -1.8098005813E+05 -1.8097975191E+05 -1.8097972459E+05

HessRho_EigVec1 = 7.4740834015E-01 -6.6436493968E-01 1.8051595304E-07

HessRho_EigVec2 = 2.9325930435E-07 6.0162777874E-07 1.0000000000E+00

HessRho_EigVec3 = 6.6436493968E-01 7.4740834015E-01 -6.4449281954E-07

DelSqRho = -5.4293953463E+05

Bond Ellipticity = NA

V = -1.3574902043E+05

G = 7.0683887650E+00

K = 1.3574195205E+05

L = 1.3573488366E+05

Vnuc = 8.4478271926E+07

Ven = -1.0084291175E+10

Vrep = 1.0084155426E+10

DelSqV = 4.6005429079E+09

DelSqVen = 4.5866492625E+13

DelSqVrep = -4.5861892082E+13

DelSqG = 2.0581085061E+08

DelSqK = -4.8063537585E+09

Stress_EigVals = -4.5249703201E+04 -4.5249694294E+04 -4.5249622940E+04

Stress_EigVec1 = 6.9767246870E-01 7.1641686637E-01 -5.8483995913E-07

Stress_EigVec2 = 4.3481758728E-07 3.9289931993E-07 1.0000000000E+00

Stress_EigVec3 = 7.1641686637E-01 -6.9767246870E-01 -3.7395614838E-08

-DivStress = -1.0329938944E+02 1.9283724676E+01 3.2455045499E-04

CP# 5 Coords = 4.07800790318993E+00 6.58232441088895E-01 -1.08424301348718E-07

Type = (3,-3) NACP H5

Rho = 4.3212681915E-01 Rho at Nucleus = 4.2869404123E-01

GradRho = 1.6757428778E-15 -2.6714741530E-16 7.4029356101E-19

HessRho_EigVals = -8.4825642246E+00 -8.4808181109E+00 -7.8016806243E+00

HessRho_EigVec1 = -5.5841737124E-01 8.2956014821E-01 -2.5780138734E-07

HessRho_EigVec2 = -9.9664125809E-08 2.4367998950E-07 1.0000000000E+00

HessRho_EigVec3 = 8.2956014821E-01 5.5841737124E-01 -5.3397752182E-08

DelSqRho = -2.4765062960E+01

Bond Ellipticity = NA

V = -6.2039978805E+00

G = 6.3660702817E-03

K = 6.1976318102E+00

L = 6.1912657399E+00

Vnuc = 4.0999351157E+01

Ven = -1.7716919203E+01

Vrep = 1.1512921322E+01

DelSqV = 1.5936900254E+03

DelSqVen = 1.0153515127E+03

DelSqVrep = 5.7833851267E+02

DelSqG = 1.1870723448E+02

DelSqK = -1.7123972599E+03

Stress_EigVals = -2.1256967611E+00 -2.1255799325E+00 -1.9527211869E+00

Stress_EigVec1 = -5.5872175781E-01 8.2935516960E-01 -2.2630960624E-07

Stress_EigVec2 = -8.2650983386E-08 2.1719368266E-07 1.0000000000E+00

Stress_EigVec3 = 8.2935516960E-01 5.5872175781E-01 -5.2803815816E-08

-DivStress = 1.2568073662E+01 8.4505442995E+00 -8.1623843267E-07

CP# 6 Coords = 2.45660618386457E+00 -1.69513363320006E+00 1.64810977317247E+00

Type = (3,-3) NACP H6

Rho = 4.3191974310E-01 Rho at Nucleus = 4.2851232194E-01

GradRho = -9.7838404045E-16 3.7643499429E-16 -8.3179990673E-16

HessRho_EigVals = -8.4749903718E+00 -8.4729645182E+00 -7.7975208734E+00

HessRho_EigVec1 = 8.9225411222E-01 -3.4316024988E-01 -2.9346829835E-01

HessRho_EigVec2 = 4.5000469989E-01 7.2924626628E-01 5.1545674231E-01

HessRho_EigVec3 = 3.7126396349E-02 -5.9198051152E-01 8.0509670517E-01

DelSqRho = -2.4745475763E+01

Bond Ellipticity = NA

V = -6.1991244226E+00

G = 6.3777408636E-03

K = 6.1927466817E+00
L = 6.1863689408E+00
Vnuc = 4.1415684672E+01
Ven = -1.7888251884E+01
Vrep = 1.1689127461E+01
DelSqV = 1.5926246906E+03
DelSqVen = 1.0248508213E+03
DelSqVrep = 5.6777386934E+02
DelSqG = 1.1857653834E+02
DelSqK = -1.7112012290E+03
Stress_EigVals = -2.1238072217E+00 -2.1235870585E+00 -1.9517301424E+00
Stress_EigVec1 = 8.3269157113E-01 -4.2741509443E-01 -3.5205267279E-01
Stress_EigVec2 = 5.5251183336E-01 6.8358110126E-01 4.7691461710E-01
Stress_EigVec3 = 3.6816047667E-02 -5.9163604949E-01 8.0536411863E-01
-DivStress = 5.8107897183E-01 -8.9317082027E+00 1.2138891228E+01

CP# 7 Coords = 2.45660589875715E+00 -1.69513358469816E+00 -1.64810984249191E+00

Type = (3,-3) NACP H7

Rho = 4.3191974390E-01 Rho at Nucleus = 4.2851232288E-01

GradRho = 1.5491080640E-15 8.3440199194E-16 -4.5189546549E-16

HessRho_EigVals = -8.4749903253E+00 -8.4729644719E+00 -7.7975208498E+00

HessRho_EigVec1 = 8.9225411737E-01 -3.4316035297E-01 2.9346816213E-01

HessRho_EigVec2 = 4.5000470319E-01 7.2924625052E-01 -5.1545676173E-01

HessRho_EigVec3 = -3.7126232584E-02 5.9198047118E-01 8.0509674239E-01

DelSqRho = -2.4745475647E+01

Bond Ellipticity = NA

V = -6.1991243936E+00

G = 6.3777409422E-03

K = 6.1927466527E+00

L = 6.1863689117E+00

Vnuc = 4.1415685407E+01

Ven = -1.7888252234E+01

Vrep = 1.1689127841E+01
DelSqV = 1.5926246779E+03
DelSqVen = 1.0248508346E+03
DelSqVrep = 5.6777384329E+02
DelSqG = 1.1857653700E+02
DelSqK = -1.7112012149E+03
Stress_EigVals = -2.1238072103E+00 -2.1235870466E+00 -1.9517301367E+00
Stress_EigVec1 = 8.3269181694E-01 -4.2741489879E-01 3.5205232891E-01
Stress_EigVec2 = 5.5251147402E-01 6.8358125962E-01 -4.7691480641E-01
Stress_EigVec3 = -3.6815880732E-02 5.9163600786E-01 8.0536415685E-01
-DivStress = 5.8107642767E-01 -8.9317073449E+00 -1.2138891475E+01

CP# 8 Coords = -2.39692830946817E+00 -4.93838303518798E-01 -2.90351632409758E-13

Type = (3,-3) NACP C8

Rho = 1.1937137186E+02 Rho at Nucleus = 1.1937137186E+02

GradRho = 1.2264661509E-11 3.1336044870E-12 3.0116785835E-17

HessRho_EigVals = -1.8098000676E+05 -1.8097970040E+05 -1.8097967290E+05

HessRho_EigVec1 = 7.4728305655E-01 6.6450585655E-01 -2.0353611578E-07

HessRho_EigVec2 = -2.7290412893E-07 6.1319662328E-07 1.0000000000E+00

HessRho_EigVec3 = -6.6450585655E-01 7.4728305655E-01 -6.3957783886E-07

DelSqRho = -5.4293938007E+05

Bond Ellipticity = NA

V = -1.3574898000E+05

G = 7.0674922362E+00

K = 1.3574191251E+05

L = 1.3573484502E+05

Vnuc = 8.4780074160E+07

Ven = -1.0120313759E+10

Vrep = 1.0120178010E+10

DelSqV = 4.6005415972E+09

DelSqVen = 4.6027553898E+13

DelSqVrep = -4.6022953357E+13

DelSqG = 2.0581081150E+08

DelSqK = -4.8063524087E+09

Stress_EigVals = -4.5249689770E+04 -4.5249680807E+04 -4.5249609426E+04

Stress_EigVec1 = -6.9764158321E-01 7.1644694247E-01 -7.7054226514E-07

Stress_EigVec2 = -5.8338546674E-07 5.0743227858E-07 1.0000000000E+00

Stress_EigVec3 = 7.1644694247E-01 6.9764158321E-01 6.3958875729E-08

-DivStress = 1.0290305065E+02 1.9335488287E+01 4.3742613373E-04

CP# 9 Coords = -2.45705079980364E+00 -1.69515682859478E+00 1.64824747663991E+00

Type = (3,-3) NACP H9

Rho = 4.3184978064E-01 Rho at Nucleus = 4.2844364268E-01

GradRho = 1.8669961410E-15 -3.6429192996E-16 -3.0357660830E-17

HessRho_EigVals = -8.4737036993E+00 -8.4716787325E+00 -7.7964683535E+00

HessRho_EigVec1 = 8.9221628717E-01 3.4311529510E-01 2.9363581386E-01

HessRho_EigVec2 = -4.5006637892E-01 7.2924268575E-01 5.1540795477E-01

HessRho_EigVec3 = -3.7287417036E-02 -5.9201097924E-01 8.0506685995E-01

DelSqRho = -2.4741850785E+01

Bond Ellipticity = NA

V = -6.1982115029E+00

G = 6.3744032634E-03

K = 6.1918370996E+00

L = 6.1854626963E+00

Vnuc = 4.1419013289E+01

Ven = -1.7886791803E+01

Vrep = 1.1688580300E+01

DelSqV = 1.5924051533E+03

DelSqVen = 1.0247830465E+03

DelSqVrep = 5.6762210686E+02

DelSqG = 1.1856082963E+02

DelSqK = -1.7109659830E+03

Stress_EigVals = -2.1234823839E+00 -2.1232626606E+00 -1.9514664584E+00

Stress_EigVec1 = 8.3244722980E-01 4.2761521784E-01 3.5238733671E-01

Stress_EigVec2 = -5.5286905922E-01 6.8342790413E-01 4.7672015190E-01

Stress_EigVec3 = -3.6978547368E-02 -5.9166842516E-01 8.0533288875E-01

-DivStress = -5.8341538936E-01 -8.9298637119E+00 1.2135248985E+01

CP# 10 Coords = -4.07805466241614E+00 6.58867436979101E-01 -2.94856911768525E-08

Type = (3,-3) NACP H10

Rho = 4.3206684975E-01 Rho at Nucleus = 4.2863518856E-01

GradRho = 1.0963452368E-15 -5.3429483060E-16 6.6534438007E-19

HessRho_EigVals = -8.4814614639E+00 -8.4797157295E+00 -7.8007795605E+00

HessRho_EigVec1 = 5.5861415502E-01 8.2942764954E-01 -2.7164365794E-07

HessRho_EigVec2 = 1.3766397038E-07 2.3479156448E-07 1.0000000000E+00

HessRho_EigVec3 = 8.2942764954E-01 -5.5861415502E-01 1.6975588021E-08

DelSqRho = -2.4761956754E+01

Bond Ellipticity = NA

V = -6.2032156317E+00

G = 6.3632216230E-03

K = 6.1968524101E+00

L = 6.1904891885E+00

Vnuc = 4.1002329294E+01

Ven = -1.7715747250E+01

Vrep = 1.1512531619E+01

DelSqV = 1.5935020824E+03

DelSqVen = 1.0152979048E+03

DelSqVrep = 5.7820417762E+02

DelSqG = 1.1869378011E+02

DelSqK = -1.7121958625E+03

Stress_EigVals = -2.1254185400E+00 -2.1253015255E+00 -1.9524955662E+00

Stress_EigVec1 = 5.5891983279E-01 8.2922169564E-01 -4.2052865224E-09

Stress_EigVec2 = -1.1361399994E-08 1.2729283813E-08 1.0000000000E+00

Stress_EigVec3 = 8.2922169564E-01 -5.5891983279E-01 1.6535768548E-08

-DivStress = -1.2563214832E+01 8.4516685257E+00 -2.6614218018E-07

CP# 11 Coords = -2.45705057402403E+00 -1.69515659314483E+00 -1.64824768415702E+00

Type = (3,-3) NACP H11

Rho = 4.3184977759E-01 Rho at Nucleus = 4.2844363984E-01

GradRho = 5.7722923663E-16 8.8991314318E-16 8.0404433112E-16

HessRho_EigVals = -8.4737036613E+00 -8.4716786947E+00 -7.7964683473E+00

HessRho_EigVec1 = 8.9221623849E-01 3.4311550617E-01 -2.9363571514E-01

HessRho_EigVec2 = -4.5006648695E-01 7.2924269792E-01 -5.1540784323E-01

HessRho_EigVec3 = 3.7287278100E-02 5.9201084193E-01 8.0506696736E-01

DelSqRho = -2.4741850703E+01

Bond Ellipticity = NA

V = -6.1982114826E+00

G = 6.3744033810E-03

K = 6.1918370792E+00

L = 6.1854626758E+00

Vnuc = 4.1419014413E+01

Ven = -1.7886792162E+01

Vrep = 1.1688580679E+01

DelSqV = 1.5924051513E+03

DelSqVen = 1.0247830709E+03

DelSqVrep = 5.6762208045E+02

DelSqG = 1.1856082967E+02

DelSqK = -1.7109659810E+03

Stress_EigVals = -2.1234823747E+00 -2.1232626508E+00 -1.9514664571E+00

Stress_EigVec1 = 8.3244746786E-01 4.2761506174E-01 -3.5238696377E-01

Stress_EigVec2 = -5.5286871032E-01 6.8342812246E-01 -4.7672024353E-01

Stress_EigVec3 = 3.6978404660E-02 5.9166828579E-01 8.0533299770E-01

-DivStress = -5.8341319576E-01 -8.9298613234E+00 -1.2135250238E+01

CP# 12 Coords = 2.71757209620979E-04 1.88464170928695E+00 1.03656013486829E+00

Type = (3,-1) BCP H2 C1

Rho = 2.7972355996E-01

GradRho = -4.3368086899E-18 8.4428991576E-15 1.4280243654E-14

HessRho_EigVals = -6.9576866305E-01 -6.9187154585E-01 3.8782172872E-01
HessRho_EigVec1 = 9.9999925493E-01 9.1668156007E-04 -8.0611693678E-04
HessRho_EigVec2 = -1.2174009228E-03 7.9748763039E-01 -6.0333406775E-01
HessRho_EigVec3 = 8.9803071253E-05 6.0333459960E-01 7.9748815218E-01
DelSqRho = -9.9981848017E-01
Bond Ellipticity = 5.6327178350E-03
V = -3.3612299635E-01
G = 4.3084188153E-02
K = 2.9303880820E-01
L = 2.4995462004E-01
Vnuc = 1.0994758420E+01
Ven = -3.0754929661E+00
Vrep = 2.7393699697E+00
DelSqV = -1.6742364660E+00
DelSqVen = 1.0992762653E+01
DelSqVrep = -1.2666999119E+01
DelSqG = 1.5944507508E+00
DelSqK = 7.9785715155E-02
Stress_EigVals = -2.1263016622E-01 -2.1229808565E-01 8.8805255528E-02
Stress_EigVec1 = -3.5009589502E-03 7.9772438192E-01 -6.0301206769E-01
Stress_EigVec2 = 9.9999386716E-01 2.7358550218E-03 -2.1864889507E-03
Stress_EigVec3 = 9.4461953190E-05 6.0301602433E-01 7.9772906772E-01
-DivStress = -1.0552225115E-05 -1.2753897765E-01 -1.7349655757E-01
BPL = 2.0422953166E+00 = 7.5345672895E-01 + 1.2888385876E+00
GBL_I = 2.0421998969E+00
GBL_II = 2.0711725779E+00
GBL_III = 2.0422324314E+00 = 7.5345666682E-01 + 1.2887757646E+00
GBL_IV = 2.0712062592E+00 = 7.8243083485E-01 + 1.2887754244E+00

CP# 13 Coords = 2.71790233236671E-04 1.88464210286728E+00 -1.03655986493493E+00

Type = (3,-1) BCP C1 H3

Rho = 2.7972355901E-01

GradRho = 6.9388939039E-18 8.5226964375E-15 -1.4231671397E-14
HessRho_EigVals = -6.9576867483E-01 -6.9187154228E-01 3.8782173953E-01
HessRho_EigVec1 = 9.9999925471E-01 9.1680567314E-04 8.0625228029E-04
HessRho_EigVec2 = -1.2175815961E-03 7.9748737997E-01 6.0333439839E-01
HessRho_EigVec3 = -8.9835619368E-05 -6.0333493041E-01 7.9748790190E-01
DelSqRho = -9.9981847758E-01
Bond Ellipticity = 5.6327400644E-03
V = -3.3612298218E-01
G = 4.3084181391E-02
K = 2.9303880079E-01
L = 2.4995461940E-01
Vnuc = 1.0994758163E+01
Ven = -3.0754928838E+00
Vrep = 2.7393699016E+00
DelSqV = -1.6742366434E+00
DelSqVen = 1.0992762368E+01
DelSqVrep = -1.2666999011E+01
DelSqG = 1.5944507063E+00
DelSqK = 7.9785937134E-02
Stress_EigVals = -2.1263016297E-01 -2.1229807968E-01 8.8805260472E-02
Stress_EigVec1 = -3.5014289771E-03 7.9772412479E-01 6.0301240512E-01
Stress_EigVec2 = 9.9999386551E-01 2.7362080581E-03 2.1868013130E-03
Stress_EigVec3 = -9.4496761462E-05 -6.0301636288E-01 7.9772881180E-01
-DivStress = -1.0556249043E-05 -1.2753901199E-01 1.7349648461E-01
BPL = 2.0422953202E+00 = 1.2888386048E+00 + 7.5345671542E-01
GBL_I = 2.0421998998E+00
GBL_II = 2.0711725817E+00
GBL_III = 2.0422324346E+00 = 1.2887757814E+00 + 7.5345665329E-01
GBL_IV = 2.0712062633E+00 = 1.2887754411E+00 + 7.8243082217E-01

CP# 14 Coords = 1.18908178263537E+00 3.13479689550470E-01 -4.59603653449448E-09

Type = (3,-1) BCP C4 C1

Rho = 2.5313590722E-01
GradRho = 9.0115415130E-14 -5.7738536174E-14 2.5138862540E-18
HessRho_EigVals = -4.8232423337E-01 -4.7803733355E-01 2.8359472664E-01
HessRho_EigVec1 = 5.5568309863E-01 8.3139418683E-01 -9.9780220070E-07
HessRho_EigVec2 = 5.4366911287E-07 8.3678052414E-07 1.0000000000E+00
HessRho_EigVec3 = 8.3139418683E-01 -5.5568309863E-01 1.2981454529E-08
DelSqRho = -6.7676684027E-01
Bond Ellipticity = 8.9677092533E-03
V = -2.7193012934E-01
G = 5.1369209636E-02
K = 2.2056091971E-01
L = 1.6919171007E-01
Vnuc = 1.2292823967E+01
Ven = -3.1117551472E+00
Vrep = 2.8398250179E+00
DelSqV = -1.3361473614E+00
DelSqVen = 8.3193756343E+00
DelSqVrep = -9.6555229957E+00
DelSqG = 1.1099158687E+00
DelSqK = 2.2623149270E-01
Stress_EigVals = -1.6610558182E-01 -1.6596157790E-01 6.0137030375E-02
Stress_EigVec1 = 3.5582812438E-06 5.3865668451E-06 9.9999999998E-01
Stress_EigVec2 = 5.5407426819E-01 8.3246723977E-01 -6.4556925097E-06
Stress_EigVec3 = 8.3246723979E-01 -5.5407426820E-01 2.2405517339E-08
-DivStress = -1.1457075626E-02 8.5999997674E-03 1.3694083734E-09
BPL = 2.8888051679E+00 = 1.4527839210E+00 + 1.4360212469E+00
GBL_I = 2.8887560951E+00
GBL_II = 2.8887563473E+00
GBL_III = 2.8887692848E+00 = 1.4527817528E+00 + 1.4359875320E+00
GBL_IV = 2.8887695383E+00 = 1.4527816873E+00 + 1.4359878509E+00

CP# 15 Coords = 3.45796064396014E+00 2.40184811536265E-01 -6.82398939414719E-08

Type = (3,-1) BCP H5 C4

Rho = 2.7831744499E-01

GradRho = 8.1670781249E-15 6.0854099537E-15 1.3204515729E-18

HessRho_EigVals = -6.9342384613E-01 -6.8873261754E-01 3.9154782459E-01

HessRho_EigVec1 = -5.5935216429E-01 8.2893012752E-01 -1.5554103367E-07

HessRho_EigVec2 = -4.2129199249E-08 1.5921242395E-07 1.0000000000E+00

HessRho_EigVec3 = 8.2893012752E-01 5.5935216429E-01 -5.4133651413E-08

DelSqRho = -9.9060863909E-01

Bond Ellipticity = 6.8113930842E-03

V = -3.3292443126E-01

G = 4.2636135742E-02

K = 2.9028829551E-01

L = 2.4765215977E-01

Vnuc = 1.0259138070E+01

Ven = -2.8552970953E+00

Vrep = 2.5223726640E+00

DelSqV = -1.7601241563E+00

DelSqVen = 1.0162790801E+01

DelSqVrep = -1.1922914958E+01

DelSqG = 1.5929706128E+00

DelSqK = 1.6715354355E-01

Stress_EigVals = -2.1199831845E-01 -2.1148631967E-01 9.0560206865E-02

Stress_EigVec1 = -3.9855937498E-08 1.5298788625E-07 1.0000000000E+00

Stress_EigVec2 = -5.5968552842E-01 8.2870507979E-01 -1.4908862992E-07

Stress_EigVec3 = 8.2870507979E-01 5.5968552842E-01 -5.2596288095E-08

-DivStress = -1.6774914726E-01 -1.1713736984E-01 1.0751337262E-08

BPL = 2.0382567077E+00 = 7.4781181032E-01 + 1.2904448974E+00

GBL_I = 2.0381636817E+00

GBL_II = 2.0673567346E+00

GBL_III = 2.0381979243E+00 = 7.4781175723E-01 + 1.2903861671E+00

GBL_IV = 2.0673921019E+00 = 7.7700588510E-01 + 1.2903862168E+00

CP# 16 Coords = 2.42916956659139E+00 -1.25117607936537E+00 1.04420732501351E+00

Type = (3,-1) BCP H6 C4

Rho = 2.7765843081E-01

GradRho = -4.7132436842E-15 -1.4789905411E-13 1.9250052941E-13

HessRho_EigVals = -6.8918796003E-01 -6.8505235665E-01 3.8875167513E-01

HessRho_EigVec1 = 8.7080209799E-01 -3.7629234490E-01 -3.1639813100E-01

HessRho_EigVec2 = 4.9026491386E-01 7.1263930433E-01 5.0178235935E-01

HessRho_EigVec3 = 3.6660883336E-02 -5.9207203370E-01 8.0505073539E-01

DelSqRho = -9.8548864156E-01

Bond Ellipticity = 6.0369157728E-03

V = -3.3263906201E-01

G = 4.3133450812E-02

K = 2.8950561120E-01

L = 2.4637216039E-01

Vnuc = 1.0498792336E+01

Ven = -2.9150782056E+00

Vrep = 2.5824391436E+00

DelSqV = -1.7264329419E+00

DelSqVen = 1.0346440598E+01

DelSqVrep = -1.2072873540E+01

DelSqG = 1.5865483876E+00

DelSqK = 1.3988455430E-01

Stress_EigVals = -2.1124013434E-01 -2.1095017680E-01 8.9551249123E-02

Stress_EigVec1 = 3.8321174585E-01 7.5240463568E-01 5.3575742837E-01

Stress_EigVec2 = 9.2300045279E-01 -2.9001279857E-01 -2.5290856216E-01

Stress_EigVec3 = 3.4913063419E-02 -5.9142188061E-01 8.0560613027E-01

-DivStress = -4.7490512910E-03 1.2102455904E-01 -1.6780044062E-01

BPL = 2.0403774427E+00 = 7.5003286803E-01 + 1.2903445747E+00

GBL_I = 2.0402409046E+00

GBL_II = 2.0693364960E+00

GBL_III = 2.0402823448E+00 = 7.5003282894E-01 + 1.2902495159E+00

GBL_IV = 2.0693794110E+00 = 7.7912988544E-01 + 1.2902495256E+00

CP# 17 Coords = 2.42916939873770E+00 -1.25117605045893E+00 -1.04420735593674E+00

Type = (3,-1) BCP C4 H7

Rho = 2.7765842691E-01

GradRho = -4.8069187519E-15 -1.4782272628E-13 -1.9252308081E-13

HessRho_EigVals = -6.8918793788E-01 -6.8505234047E-01 3.8875166718E-01

HessRho_EigVec1 = 8.7080205074E-01 -3.7629251429E-01 3.1639805961E-01

HessRho_EigVec2 = 4.9026500911E-01 7.1263924500E-01 -5.0178235055E-01

HessRho_EigVec3 = -3.6660732002E-02 5.9207199746E-01 8.0505076893E-01

DelSqRho = -9.8548861117E-01

Bond Ellipticity = 6.0369071967E-03

V = -3.3263905688E-01

G = 4.3133452045E-02

K = 2.8950560484E-01

L = 2.4637215279E-01

Vnuc = 1.0498792412E+01

Ven = -2.9150781854E+00

Vrep = 2.5824391285E+00

DelSqV = -1.7264327461E+00

DelSqVen = 1.0346440353E+01

DelSqVrep = -1.2072873099E+01

DelSqG = 1.5865483448E+00

DelSqK = 1.3988440135E-01

Stress_EigVals = -2.1124012963E-01 -2.1095017349E-01 8.9551246243E-02

Stress_EigVec1 = 3.8321174639E-01 7.5240462858E-01 -5.3575743795E-01

Stress_EigVec2 = 9.2300045858E-01 -2.9001289762E-01 2.5290842745E-01

Stress_EigVec3 = -3.4912904415E-02 5.9142184107E-01 8.0560616619E-01

-DivStress = -4.7490298008E-03 1.2102456351E-01 1.6780045298E-01

BPL = 2.0403774613E+00 = 1.2903445783E+00 + 7.5003288305E-01

GBL_I = 2.0402409236E+00

GBL_II = 2.0693365146E+00

GBL_III = 2.0402823637E+00 = 1.2902495197E+00 + 7.5003284396E-01

$$\text{GBL\_IV} = 2.0693794293\text{E}+00 = 1.2902495294\text{E}+00 + 7.7912989994\text{E}-01$$

CP# 18 Coords = -1.18893595529052E+00 3.13569686496646E-01 -5.16269508392387E-09

Type = (3,-1) BCP C1 C8

Rho = 2.5305613494E-01

GradRho = -8.5778606440E-14 -5.5119103726E-14 2.0656354257E-18

HessRho_EigVals = -4.8211537504E-01 -4.7783592854E-01 2.8360845373E-01

HessRho_EigVec1 = -5.5557775238E-01 8.3146458798E-01 -1.0611667816E-06

HessRho_EigVec2 = -5.7642018166E-07 8.9110295655E-07 1.0000000000E+00

HessRho_EigVec3 = 8.3146458798E-01 5.5557775238E-01 -1.5804008891E-08

DelSqRho = -6.7634284985E-01

Bond Ellipticity = 8.9558910010E-03

V = -2.7176693606E-01

G = 5.1340611798E-02

K = 2.2042632426E-01

L = 1.6908571246E-01

Vnuc = 1.2291887316E+01

Ven = -3.1105374953E+00

Vrep = 2.8387705592E+00

DelSqV = -1.3356976509E+00

DelSqVen = 8.3135300970E+00

DelSqVrep = -9.6492277480E+00

DelSqG = 1.1092932874E+00

DelSqK = 2.2640436350E-01

Stress_EigVals = -1.6602449093E-01 -1.6588264092E-01 6.0140195796E-02

Stress_EigVec1 = -4.2296202700E-06 6.4072150806E-06 9.999999997E-01

Stress_EigVec2 = -5.5397644995E-01 8.3253233741E-01 -7.6773237694E-06

Stress_EigVec3 = 8.3253233744E-01 5.5397644997E-01 -2.8150614666E-08

-DivStress = 1.1495248333E-02 8.6233637681E-03 1.6258036743E-09

BPL = 2.8891288627E+00 = 1.4361458646E+00 + 1.4529829981E+00

GBL_I = 2.8890798275E+00

GBL_II = 2.8890800841E+00

$$\text{GBL\_III} = 2.8890930643\text{E}+00 = 1.4361122695\text{E}+00 + 1.4529807948\text{E}+00$$

$$\text{GBL\_IV} = 2.8890933222\text{E}+00 = 1.4361125926\text{E}+00 + 1.4529807295\text{E}+00$$

CP# 19 Coords = -2.42949484100290E+00 -1.25116012593522E+00 1.04434042087280E+00

Type = (3,-1) BCP H9 C8

Rho = 2.7759411590E-01

GradRho = 4.1997655353E-15 -1.5143095111E-13 1.9716173139E-13

HessRho_EigVals = -6.8898417326E-01 -6.8484621659E-01 3.8876461281E-01

HessRho_EigVec1 = 8.7083506382E-01 3.7614653006E-01 3.1648077279E-01

HessRho_EigVec2 = -4.9019478782E-01 7.1269580064E-01 5.0177063061E-01

HessRho_EigVec3 = -3.6815236168E-02 -5.9209668440E-01 8.0502556153E-01

DelSqRho = -9.8506577704E-01

Bond Ellipticity = 6.0421691216E-03

V = -3.3247352088E-01

G = 4.3103538310E-02

K = 2.8936998257E-01

L = 2.4626644426E-01

Vnuc = 1.0497650942E+01

Ven = -2.9140861323E+00

Vrep = 2.5816126114E+00

DelSqV = -1.7259795518E+00

DelSqVen = 1.0340876682E+01

DelSqVrep = -1.2066856234E+01

DelSqG = 1.5856919641E+00

DelSqK = 1.4028758774E-01

Stress_EigVals = -2.1116121013E-01 -2.1087033849E-01 8.9558027740E-02

Stress_EigVec1 = -3.8341493358E-01 7.5235410783E-01 5.3568300807E-01

Stress_EigVec2 = 9.2291007927E-01 2.9008352830E-01 2.5315712945E-01

Stress_EigVec3 = -3.5070989237E-02 -5.9145147142E-01 8.0557754603E-01

-DivStress = 4.7694864798E-03 1.2090732432E-01 -1.6763540418E-01

$$\text{BPL} = 2.0406026813\text{E}+00 = 7.5006412668\text{E}-01 + 1.2905385546\text{E}+00$$

$$\text{GBL\_I} = 2.0404657941\text{E}+00$$

GBL_II = 2.0695579764E+00

GBL_III = 2.0405073584E+00 = 7.5006408717E-01 + 1.2904432713E+00

GBL_IV = 2.0696010212E+00 = 7.7915774027E-01 + 1.2904432810E+00

CP# 20 Coords = -3.45808392371075E+00 2.40662155516391E-01 -1.67872012109745E-08

Type = (3,-1) BCP C8 H10

Rho = 2.7826231172E-01

GradRho = -7.9519724139E-15 5.9049987122E-15 1.0193512125E-18

HessRho_EigVals = -6.9324886872E-01 -6.8856088647E-01 3.9156521158E-01

HessRho_EigVec1 = 5.5954118180E-01 8.2880254939E-01 -2.1221858666E-07

HessRho_EigVec2 = 1.0449952232E-07 1.8550473881E-07 1.0000000000E+00

HessRho_EigVec3 = 8.2880254939E-01 -5.5954118180E-01 1.7188070272E-08

DelSqRho = -9.9024454361E-01

Bond Ellipticity = 6.8083772268E-03

V = -3.3278042901E-01

G = 4.2609646553E-02

K = 2.9017078246E-01

L = 2.4756113590E-01

Vnuc = 1.0258187657E+01

Ven = -2.8544670115E+00

Vrep = 2.5216865825E+00

DelSqV = -1.7597572104E+00

DelSqVen = 1.0158114355E+01

DelSqVrep = -1.1917871565E+01

DelSqG = 1.5922231252E+00

DelSqK = 1.6753408513E-01

Stress_EigVals = -2.1192961029E-01 -2.1141831663E-01 9.0567497908E-02

Stress_EigVec1 = 1.5354058864E-07 2.5560146887E-07 1.0000000000E+00

Stress_EigVec2 = 5.5987667173E-01 8.2857595455E-01 -2.9774902479E-07

Stress_EigVec3 = 8.2857595455E-01 -5.5987667173E-01 1.5885259890E-08

-DivStress = 1.6757745905E-01 -1.1706976786E-01 2.2290969174E-09

BPL = 2.0384540061E+00 = 1.2906174914E+00 + 7.4783651463E-01

GBL_I = 2.0383611895E+00

GBL_II = 2.0675512833E+00

GBL_III = 2.0383953187E+00 = 1.2905588564E+00 + 7.4783646227E-01

GBL_IV = 2.0675865320E+00 = 1.2905589059E+00 + 7.7702762612E-01

CP# 21 Coords = -2.42949471298157E+00 -1.25115998303443E+00 -1.04434053957810E+00

Type = (3,-1) BCP C8 H11

Rho = 2.7759410917E-01

GradRho = 3.9447611844E-15 -1.5135115383E-13 -1.9714611887E-13

HessRho_EigVals = -6.8898414382E-01 -6.8484619401E-01 3.8876460492E-01

HessRho_EigVec1 = 8.7083494250E-01 3.7614682899E-01 -3.1648075133E-01

HessRho_EigVec2 = -4.9019501268E-01 7.1269575174E-01 -5.0177048039E-01

HessRho_EigVec3 = 3.6815111903E-02 5.9209655335E-01 8.0502566360E-01

DelSqRho = -9.8506573292E-01

Bond Ellipticity = 6.0421593131E-03

V = -3.3247351186E-01

G = 4.3103539316E-02

K = 2.8936997255E-01

L = 2.4626643323E-01

Vnuc = 1.0497651004E+01

Ven = -2.9140860788E+00

Vrep = 2.5816125670E+00

DelSqV = -1.7259793737E+00

DelSqVen = 1.0340876280E+01

DelSqVrep = -1.2066855654E+01

DelSqG = 1.5856919044E+00

DelSqK = 1.4028746928E-01

Stress_EigVals = -2.1116120331E-01 -2.1087033334E-01 8.9558024786E-02

Stress_EigVec1 = -3.8341506614E-01 7.5235412839E-01 -5.3568288432E-01

Stress_EigVec2 = 9.2291002925E-01 2.9008375086E-01 -2.5315705679E-01

Stress_EigVec3 = 3.5070856455E-02 5.9145133611E-01 8.0557765116E-01

-DivStress = 4.7694718454E-03 1.2090730544E-01 1.6763542214E-01

$$\text{BPL} = 2.0406027031\text{E}+00 = 1.2905385633\text{E}+00 + 7.5006413981\text{E}-01$$

$$\text{GBL\_I} = 2.0404658164\text{E}+00$$

$$\text{GBL\_II} = 2.0695579979\text{E}+00$$

$$\text{GBL\_III} = 2.0405073805\text{E}+00 = 1.2904432802\text{E}+00 + 7.5006410030\text{E}-01$$

$$\text{GBL\_IV} = 2.0696010425\text{E}+00 = 1.2904432899\text{E}+00 + 7.7915775254\text{E}-01$$

Number of NACPs = 11

Number of NNACPs = 0

Number of BCPs = 10

Number of RCPs = 0

Number of CCPs = 0

$$\text{NumNACP} + \text{NumNNACP} - \text{NumBCP} + \text{NumRCP} - \text{NumCCP} = 1$$

Poincare-Hopf Relationship is Satisfied

Bond Path Angles and Corresponding Geometric Bond Angles:

BPA = A-B-C Bond Path Angle

GBA_I = A-B-C Geometric Bond Angle in Terms of Nuclear Attractors

GBA_II = A-B-C Geometric Bond Angle in Terms of Nuclei

GBA_III = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nuclear Attractor B

GBA_IV = A-B-C Geometric Bond Angle in Terms of A|B and C|B BCPs and Nucleus B

Atom A	Atom B	Atom C	BPA	GBA_I	GBA_II	GBA_III	GBA_IV

H3	C1	H2	108.33310337	106.59049110	106.57590633	107.08506077	107.08510171
C4	C1	H2	109.41603336	109.48919834	109.49265494	109.46294318	109.46294339
C4	C1	H3	109.41603970	109.48920748	109.49266410	109.46295173	109.46295193
H5	C4	C1	111.12308368	111.63637774	111.64360029	111.55568148	111.55568265
H6	C4	C1	109.52225972	110.67163066	110.67996078	110.30632236	110.30632585
H6	C4	H5	108.90677034	107.97717602	107.96859578	108.25564833	108.25564469
H7	C4	C1	109.52225407	110.67162255	110.67995264	110.30631461	110.30631810
H7	C4	H5	108.90677049	107.97717680	107.96859658	108.25564879	108.25564515

H7	C4	H6	108.82071022	107.76338270	107.75536521	108.05646254	108.05646136
C8	C1	H2	109.41418798	109.49298156	109.49645958	109.46618596	109.46618591
C8	C1	H3	109.41419610	109.49299361	109.49647165	109.46619704	109.46619699
C8	C1	C4	110.80557125	112.13051747	112.13049753	111.78191296	111.78187513
H9	C8	C1	109.52450302	110.67584952	110.68419526	110.31000893	110.31001241
H10	C8	C1	111.12075527	111.63182015	111.63902420	111.55186090	111.55186207
H10	C8	H9	108.90694504	107.97722999	107.96865465	108.25558893	108.25558530
H11	C8	C1	109.52449639	110.67583972	110.68418542	110.30999964	110.31000311
H11	C8	H9	108.81815421	107.75920078	107.75115893	108.05288426	108.05288307
H11	C8	H10	108.90694463	107.97722995	107.96865461	108.25558864	108.25558502

Total time for electron density critical point search, analysis and connectivity = 4 sec (NProc = 1)

Virial-Based Atomic Energy Components:

$$E_e(A) = E(A) - W(A) = -T(A)$$

= Contribution of Atom A to Electronic Energy of Molecule.

Not additive to give molecular E_e unless molecular electronic virial theorem is satisfied.

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$V_{en}(A) = V_{en}(A, Mol)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$$V_{enO}(A) = V_{en}(A, A)$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$$V_{ee}(A) = V_{ee}(A, Mol)$$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A) - W(A)$ = Contribution of Atom A to the Nuclear Repulsion Energy of Molecule Minus the Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule.

Calculation of $V_{nn}(A) - W(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

See "2EDM Note" and "DFT Note".

Atom A	$E_e(A)$	$T(A)$	$V_{en}(A)$	$V_{enO}(A)$	$V_{ee}(A)$	$V_{nn}(A) - W(A)$

C1	-3.7673949711E+01	3.7673949711E+01	-1.2715602963E+02	-8.9221170619E+01
H2	-6.4885293891E-01	6.4885293891E-01	-8.7391490022E+00	-1.3378226426E+00
H3	-6.4885294396E-01	6.4885294396E-01	-8.7391573537E+00	-1.3378233098E+00
C4	-3.7680549022E+01	3.7680549022E+01	-1.2287210387E+02	-8.9280225120E+01
H5	-6.3588475021E-01	6.3588475021E-01	-7.9549167088E+00	-1.3200649848E+00
H6	-6.3743237540E-01	6.3743237540E-01	-8.3114248157E+00	-1.3228754186E+00
H7	-6.3743311660E-01	6.3743311660E-01	-8.3114083154E+00	-1.3228745652E+00
C8	-3.7680282413E+01	3.7680282413E+01	-1.2287082938E+02	-8.9280120015E+01
H9	-6.3732141783E-01	6.3732141783E-01	-8.3100817437E+00	-1.3227197613E+00
H10	-6.3578889639E-01	6.3578889639E-01	-7.9538642881E+00	-1.3199293905E+00
H11	-6.3732140009E-01	6.3732140009E-01	-8.3100713699E+00	-1.3227188995E+00
Total	-1.1815366899E+02	1.1815366899E+02	-4.3952903648E+02	-2.7838834473E+02

More Virial-Based Atomic Energy Components:

$$E(A) = E_e(A) + W(A)$$

$= T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A)$ = Contribution of Atom A to Total Energy E of Molecule

Not additive to give molecular E unless molecular virial theorem is satisfied.

$$E_e(A) = E(A) - W(A) = \text{Contribution of Atom A to Electronic Energy of Molecule}$$

Not additive to give molecular E_e unless molecular virial theorem is satisfied.

$W(A)$ = Contribution of Atom A to Nuclear Virial of Energy-Gradient-Based Forces on Nuclei of Molecule

$V_{nn}(A)$ = Contribution of Atom A to Nuclear Repulsion Energy of Molecule

Calculation of $V_{nn}(A)$ assumes satisfaction of the atomic virial theorem:

$$2T(A) + V_{en}(A) + V_{ee}(A) + V_{nn}(A) - W(A) = 0$$

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E(A)$	$E_e(A)$	$W(A)$	$V_{nn}(A)$	$V_{eeC}(A)$	$V_{eeX}(A)$

C1	-3.7673949711E+01
H2	-6.4885293891E-01
H3	-6.4885294396E-01
C4	-3.7680549022E+01
H5	-6.3588475021E-01
H6	-6.3743237540E-01
H7	-6.3743311660E-01
C8	-3.7680282413E+01
H9	-6.3732141783E-01
H10	-6.3578889639E-01
H11	-6.3732140009E-01

Total	-1.1815366899E+02

IQA Atomic Energy Components:

$E\_IQA(A)$ = Contribution of Atom A to Total Energy E of Molecule, Using IQA Additive Atomic Energy Definition

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$V_{ne}(A,Mol)/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Molecule

$V_{en}(A,Mol)/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Molecule

$V_{ee}(A) = V_{ee}(A,Mol) = (1/2)[V_{ee}(A,Mol) + V_{ee}(Mol,A)]$

= Half of Two-Electron Interaction Energy Between Atom A and Molecule

$V_{nn}(A,Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A)$ = Coulomb Part of $V_{ee}(A)$

$V_{eeX}(A)$ = Exchange-Correlation Part of $V_{ee}(A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA(A)$	$T(A)$	$V_{ne}(A,Mol)/2$	$V_{en}(A,Mol)/2$	$V_{ee}(A)$	$V_{nn}(A,Mol)/2$
$V_{eeC}(A)$	$V_{eeX}(A)$					

C1 1.9735669010E+01	3.7673949711E+01 -6.3950920871E+01 -6.3578014813E+01
H2 3.6641933786E+00	6.4885293891E-01 -4.2341867560E+00 -4.3695745011E+00
H3 3.6641932594E+00	6.4885294396E-01 -4.2341866307E+00 -4.3695786769E+00
C4 1.7399255924E+01	3.7680549022E+01 -6.1640959111E+01 -6.1436051933E+01
H5 3.3428715799E+00	6.3588475021E-01 -3.9095710266E+00 -3.9774583544E+00
H6 3.4948799082E+00	6.3743237540E-01 -4.0617284209E+00 -4.1557124078E+00
H7 3.4948799652E+00	6.3743311660E-01 -4.0617284846E+00 -4.1557041577E+00
C8 1.7398042823E+01	3.7680282413E+01 -6.1639552797E+01 -6.1435414691E+01
H9 3.4945431258E+00	6.3732141783E-01 -4.0613783963E+00 -4.1550408718E+00
H10 3.3426300463E+00	6.3578889639E-01 -3.9093208004E+00 -3.9769321440E+00
H11 3.4945431815E+00	6.3732140009E-01 -4.0613784537E+00 -4.1550356849E+00
Total 8.2525702202E+01	1.1815366899E+02 -2.1976491175E+02 -2.1976451824E+02

IQA Intraatomic ("Self") Energy Components:

$$E\_IQA\_Intra(A) = T(A) + Vne(A,A) + Vee(A,A)$$

= Intraatomic ("Self") Contribution to $E\_IQA(A)$

$T(A)$ = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

$$Vne(A,A) = (1/2)[Vne(A,A) + Ven(A,A)]$$

= Attraction Energy Between Electron Density Distribution of Atom A and Nucleus of Atom A

$Vee(A,A)$ = Two-electron Interaction Energy of Atom A With Itself

$VeeC(A,A)$ = Coulomb Part of $Vee(A,A)$

$VeeX(A,A)$ = Exchange-Correlation Part of $Vee(A,A)$

See "2EDM Note" and "DFT Note".

Atom A	$E\_IQA\_Intra(A)$	$T(A)$	$Vne(A,A)$	$Vee(A,A)$	$VeeC(A,A)$	$VeeX(A,A)$
C1	3.7673949711E+01	-8.9221170619E+01				
H2	6.4885293891E-01	-1.3378226426E+00				
H3	6.4885294396E-01	-1.3378233098E+00				
C4	3.7680549022E+01	-8.9280225120E+01				
H5	6.3588475021E-01	-1.3200649848E+00				
H6	6.3743237540E-01	-1.3228754186E+00				
H7	6.3743311660E-01	-1.3228745652E+00				
C8	3.7680282413E+01	-8.9280120015E+01				
H9	6.3732141783E-01	-1.3227197613E+00				
H10	6.3578889639E-01	-1.3199293905E+00				
H11	6.3732140009E-01	-1.3227188995E+00				
Total	1.1815366899E+02	-2.7838834473E+02				

IQA Atomic Contributions to Interatomic ("Interaction") Energy Components:

$$E\_IQA\_Inter(A) = E\_IQA\_Inter(A,A')/2$$

$$= Vne(A,A')/2 + Ven(A,A')/2 + Vee(A,A') + Vnn(A)$$

$$= \text{Interatomic ("Interaction") Contribution to } E\_IQA(A) = E\_IQA(A) - E\_IQA\_Intra(A)$$

$Vne(A,A')/2$ = Half of Attraction Energy Between Nucleus of Atom A and Electron Density Distribution of Other Atoms in Molecule

$$= (1/2)[Vne(A,Mol) - Vne(A,A)]$$

$Ven(A,A')/2$ = Half of Attraction Energy Between Electron Density Distribution of Atom A and Nuclei of Other Atoms in Molecule

$$= (1/2)[Ven(A,Mol) - Ven(A,A)]$$

$Vee(A,A')$ = Half of Two-electron Interaction Energy Between Atom A and Other Atoms in Molecule

$$= Vee(A,Mol) - Vee(A,A)$$

$V_{nn}(A) = V_{nn}(A, Mol)/2$ = Half of Repulsion Energy Between Nucleus of Atom A and Other Nuclei of Molecule

$V_{eeC}(A, A') = \text{Coulomb Part of } V_{ee}(A, A')$

$V_{eeX}(A, A') = \text{Exchange-Correlation Part of } V_{ee}(A, A')$

See "2EDM Note" and "DFT Note".

Atom A	$E_{IQA\_Inter}(A)$	$V_{ne}(A, A')/2$	$V_{en}(A, A')/2$	$V_{ee}(A, A')$	$V_{nn}(A)$	$V_{eeC}(A, A')$
$V_{eeX}(A, A')$						
C1	-1.9340335561E+01	-1.8967429503E+01		1.9735669010E+01		
H2	-3.5652754348E+00	-3.7006631798E+00		3.6641933786E+00		
H3	-3.5652749758E+00	-3.7006670219E+00		3.6641932594E+00		
C4	-1.7000846551E+01	-1.6795939373E+01		1.7399255924E+01		
H5	-3.2495385342E+00	-3.3174258620E+00		3.3428715799E+00		
H6	-3.4002907116E+00	-3.4942746986E+00		3.4948799082E+00		
H7	-3.4002912020E+00	-3.4942668751E+00		3.4948799652E+00		
C8	-1.6999492790E+01	-1.6795354683E+01		1.7398042823E+01		
H9	-3.4000185157E+00	-3.4936809912E+00		3.4945431258E+00		
H10	-3.2493561052E+00	-3.3169674488E+00		3.3426300463E+00		
H11	-3.4000190039E+00	-3.4936762352E+00		3.4945431815E+00		
Total	-8.0570739385E+01	-8.0570345872E+01		8.2525702202E+01		

Atomic Electron Populations, Localization and Delocalization Data:

$N(A)$ = Average Number of Electrons in Atom A

$LI(A)$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\%Loc(A) = 100 * LI(A) / N(A)$

= Percentage of Average Number of Electrons in Atom A that are Localized in Atom A

$DI(A, A')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

= $N(A) - LI(A)$

$\%Deloc(A, A') = 100 * (DI(A, A')/2) / N(A)$

= Percentage of Average Number of Electrons in Atom A That are Shared With Other

Atoms of Molecule

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	Li(A)	%Loc(A)	DI(A,A')/2	%Deloc(A,A')
C1	5.8380888206E+00	3.7824704697E+00	6.4789532772E+01	2.0556183509E+00	3.5210467228E+01
H2	1.0627639944E+00	5.0224491486E-01	4.7258367568E+01	5.6051907954E-01	5.2741632432E+01
H3	1.0627650652E+00	5.0224571897E-01	4.7258395615E+01	5.6051934623E-01	5.2741604385E+01
C4	5.8662708352E+00	3.8491380686E+00	6.5614735097E+01	2.0171327666E+00	3.4385264903E+01
H5	1.0481655938E+00	4.9057233654E-01	4.6802942153E+01	5.5759325726E-01	5.3197057847E+01
H6	1.0518545522E+00	4.9141310925E-01	4.6718731998E+01	5.6044144295E-01	5.3281268002E+01
H7	1.0518521394E+00	4.9141205014E-01	4.6718738474E+01	5.6044008926E-01	5.3281261526E+01
C8	5.8664515424E+00	3.8493540938E+00	6.5616396316E+01	2.0170974486E+00	3.4383603684E+01
H9	1.0517741596E+00	4.9135056551E-01	4.6716356456E+01	5.6042359409E-01	5.3283643544E+01
H10	1.0480945472E+00	4.9051370762E-01	4.6800520900E+01	5.5758083958E-01	5.3199479100E+01
H11	1.0517726590E+00	4.9134955658E-01	4.6716327181E+01	5.6042310242E-01	5.3283672819E+01
Total	2.5999853909E+01	1.5432064591E+01	5.9354428088E+01	1.0567789318E+01	4.0645571912E+01

More Atomic Electron Populations, Localization and Delocalization Data:

N(A) = Average Number of Electrons in Atom A

$$= \text{LI}(\text{A}) + \text{DI}(\text{A}, \text{A}')/2 = \text{LI}(\text{A}) + \text{DI\_Bond}(\text{A}, \text{A}')/2 + \text{DI\_NonBond}(\text{A}, \text{A}')/2$$

$\text{LI}(\text{A})$ = Electron Localization Index of Atom A = Average Number of Electrons Localized in Atom A

$\text{DI}(\text{A}, \text{A}')/2$ = Electron Delocalization Index of Atom A = Average Number of Electrons in Atom A that are Delocalized (Shared) Between Atom A and Other Atoms of Molecule

$$= \text{N}(\text{A}) - \text{LI}(\text{A}) = \text{DI\_Bond}(\text{A}, \text{A}')/2 + \text{DI\_NonBond}(\text{A}, \text{A}')/2$$

$\text{DI\_Bond}(\text{A}, \text{A}')/2$ = Bonding Contribution to $\text{DI}(\text{A}, \text{A}')/2$ = Average Number of Electrons in Atom A that are Shared With Atoms to Which Atom A is Bonded

$\text{DI\_NonBond}(\text{A}, \text{A}')/2$ = Non-Bonding Contribution to $\text{DI}(\text{A}, \text{A}')/2$ = Average Number of Electrons in Atom A

that are Shared with Atoms to Which Atom A is NOT bonded

$$= \text{DI}(\text{A}, \text{A}')/2 - \text{DI\_Bond}(\text{A}, \text{A}')/2$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	N(A)	LI(A)	DI(A,A')/2	DI_Bond(A,A')/2	DI_NonBond(A,A')/2
C1	5.8380888206E+00	3.7824704697E+00	2.0556183509E+00	1.9320575137E+00	1.2356083723E-01
H2	1.0627639944E+00	5.0224491486E-01	5.6051907954E-01	4.7605026756E-01	8.4468811984E-02
H3	1.0627650652E+00	5.0224571897E-01	5.6051934623E-01	4.7608347326E-01	8.4435872969E-02
C4	5.8662708352E+00	3.8491380686E+00	2.0171327666E+00	1.9363323490E+00	8.0800417588E-02
H5	1.0481655938E+00	4.9057233654E-01	5.5759325726E-01	4.8358282709E-01	7.4010430175E-02
H6	1.0518545522E+00	4.9141310925E-01	5.6044144295E-01	4.8139721973E-01	7.9044223218E-02
H7	1.0518521394E+00	4.9141205014E-01	5.6044008926E-01	4.8138929211E-01	7.9050797147E-02
C8	5.8664515424E+00	3.8493540938E+00	2.0170974486E+00	1.9363056162E+00	8.0791832470E-02
H9	1.0517741596E+00	4.9135056551E-01	5.6042359409E-01	4.8138289565E-01	7.9040698444E-02
H10	1.0480945472E+00	4.9051370762E-01	5.5758083958E-01	4.8356252247E-01	7.4018317118E-02

H11	1.0517726590E+00	4.9134955658E-01	5.6042310242E-01	4.8139943521E-01
7.9023667208E-02				

Total	2.5999853909E+01	1.5432064591E+01	1.0567789318E+01	9.6495434120E+00
9.1824590555E-01				

Atomic Electron Pair Contributions:

D2(A,A) = Average Number of Electron Pairs Formed in Atom A

$$= (1/2)[N(A) * N(A) - LI(A)]$$

D2(A,A') = Half of Average Number of Electron Pairs Formed

Between Atom A and Other Atoms of Molecule

$$= (1/2)[N(A) * N(A') - DI(A,A') / 2]$$

$$D2(A,Mol) = D2(A,A) + D2(A,A')$$

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	D2(A,A)	D2(A,A')	D2(A,Mol)
C1	1.5150405304E+01	5.7825704954E+01	7.2976110258E+01
H2	3.1361119647E-01	1.2970938734E+01	1.3284549930E+01
H3	3.1361193242E-01	1.2970951383E+01	1.3284563315E+01
C4	1.5281997722E+01	5.8046387718E+01	7.3328385440E+01
H5	3.0403938774E-01	1.2798030535E+01	1.3102069922E+01
H6	3.0749244487E-01	1.2840689458E+01	1.3148181902E+01
H7	3.0749043651E-01	1.2840661306E+01	1.3148151742E+01
C8	1.5282949803E+01	5.8047694477E+01	7.3330644280E+01
H9	3.0743915865E-01	1.2839737836E+01	1.3147176995E+01
H10	3.0399423613E-01	1.2797187604E+01	1.3101181840E+01
H11	3.0743808482E-01	1.2839720153E+01	1.3147158238E+01

Total	4.8180469706E+01	2.7681770416E+02	3.2499817386E+02

Diatomic Electron Pair Contributions and Delocalization Data:

$2 * D2(A,B) = 2 * D2(B,A) =$ Average Number of Electron Pairs Formed Between Atoms A and B

$$= N(A) * N(B) - DI(A,B) / 2$$

$DI(A,B) = DI(B,A) =$ Electron Delocalization Index. Average Number of Electrons Delocalized

(Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path

$$\%Deloc(A,B) = 100 * (DI(A,B)/2) / N(A)$$

= Percentage of Average Number of Electrons in Atom A That are Shared With Atom B

$$\%Deloc(B,A) = 100 * (DI(A,B)/2) / N(B)$$

= Percentage of Average Number of Electrons in Atom B That are Shared With Atom A

Note: ECP-Modeled Core Electrons are NOT Included Here

See "2EDM Note".

Atom A	Atom B	$2 * D2(A,B)$	$DI(A,B)$	$\%Deloc(A,B)$	$\%Deloc(B,A)$	
C1	H2	5.7284603271E+00	9.5210053512E-01	8.1542141990E+00	4.4793601408E+01	(Bonded)
C1	H3	5.7284333728E+00	9.5216694653E-01	8.1547829760E+00	4.4796680739E+01	(Bonded)
H2	H3	1.1082786997E+00	4.2379492109E-02	1.9938336419E+00	1.9938316330E+00	
C1	C4	3.3757847172E+01	9.7992602013E-01	8.3925240797E+00	8.3522057510E+00	(Bonded)
H2	C4	6.2125609208E+00	4.3801008483E-02	2.0607119132E+00	3.7332923857E-01	
H3	C4	6.2125694455E+00	4.3796522290E-02	2.0604987746E+00	3.7329100139E-01	
C1	H5	6.0987936233E+00	4.0980424001E-02	3.5097465335E-01	1.9548640140E+00	
H2	H5	1.1121279690E+00	3.6493684813E-03	1.7169232777E-01	1.7408358483E-01	
H3	H5	1.1121290971E+00	3.6493571286E-03	1.7169162066E-01	1.7408304328E-01	
C4	H5	5.6652404263E+00	9.6716565418E-01	8.2434452939E+00	4.6136109595E+01	(Bonded)
C1	H6	6.1201909912E+00	4.1258621737E-02	3.5335726301E-01	1.9612322659E+00	
H2	H6	1.1160549345E+00	3.6364218527E-03	1.7108322600E-01	1.7285763726E-01	
H3	H6	1.1118016112E+00	1.2145321190E-02	5.7140197714E-01	5.7732892654E-01	
C4	H6	5.6890664627E+00	9.6279443946E-01	8.2061881092E+00	4.5766519594E+01	(Bonded)
H5	H6	1.0813340047E+00	4.2367493217E-02	2.0210305255E+00	2.0139425707E+00	
C1	H7	6.1201874390E+00	4.1237553948E-02	3.5317682906E-01	1.9602353032E+00	
H2	H7	1.1117979812E+00	1.2145199993E-02	5.7139685089E-01	5.7732448972E-01	

H3	H7	1.1160536007E+00	3.6362136684E-03	1.7107325916E-01	1.7284813769E-01
C4	H7	5.6890602362E+00	9.6277858423E-01	8.2060529702E+00	4.5765870894E+01 (Bonded)
H5	H7	1.0813315115E+00	4.2367421531E-02	2.0210271059E+00	2.0139437828E+00
H6	H7	1.0848824957E+00	4.3025930674E-02	2.0452414540E+00	2.0452461455E+00
C1	C8	3.3758904403E+01	9.7992152565E-01	8.3924855870E+00	8.3519101673E+00 (Bonded)
H2	C8	6.2127555208E+00	4.3795906804E-02	2.0604718938E+00	3.7327425691E-01
H3	C8	6.2127645320E+00	4.3790447865E-02	2.0602129906E+00	3.7322773016E-01
C4	C8	3.4390419930E+01	4.7547318079E-02	4.0526016795E-01	4.0524768453E-01
H5	C8	6.1435588417E+00	1.0907645425E-02	5.2032071503E-01	9.2966296115E-02
H6	C8	6.1667702129E+00	7.7670944868E-03	3.6920952952E-01	6.6199255467E-02
H7	C8	6.1667499232E+00	7.7793646551E-03	3.6979364132E-01	6.6303834600E-02
C1	H9	6.1197181559E+00	4.1265614168E-02	3.5341714931E-01	1.9617145844E+00
H2	H9	1.1159709317E+00	3.6335507279E-03	1.7094814780E-01	1.7273436007E-01
H3	H9	1.1117182586E+00	1.2141149347E-02	5.7120570408E-01	5.7717473072E-01
C4	H9	6.1661057789E+00	7.7725976220E-03	6.6248199583E-02	3.6949936215E-01
H5	H9	1.1020129313E+00	8.4111054198E-04	4.0122979945E-02	3.9985320722E-02
H6	H9	1.1030506735E+00	6.5255282564E-03	3.1019156797E-01	3.1021527753E-01
H7	H9	1.1060472165E+00	5.2736692427E-04	2.5068491308E-02	2.5070349916E-02
C8	H9	5.6887992452E+00	9.6276579130E-01	8.2056911605E+00	4.5768655871E+01 (Bonded)
C1	H10	6.0983762565E+00	4.0985604812E-02	3.5101902413E-01	1.9552436811E+00
H2	H10	1.1120532920E+00	3.6477109594E-03	1.7161434611E-01	1.7401631223E-01
H3	H10	1.1120544061E+00	3.6477274327E-03	1.7161494822E-01	1.7401709810E-01
C4	H10	6.1429545294E+00	1.0903890812E-02	9.2937158192E-02	5.2017686960E-01
H5	H10	1.0973550302E+00	2.4432263941E-03	1.1654772913E-01	1.1655562948E-01
H6	H10	1.1020222812E+00	8.4147876771E-04	3.9999768312E-02	4.0143266176E-02
H7	H10	1.1020197809E+00	8.4142179041E-04	3.9997151638E-02	4.0140548038E-02
C8	H10	5.6650333505E+00	9.6712504493E-01	8.2428452527E+00	4.6137299708E+01 (Bonded)
H9	H10	1.0811793803E+00	4.2358762601E-02	2.0136814645E+00	2.0207510245E+00
C1	H11	6.1197224003E+00	4.1239603944E-02	3.5319438613E-01	1.9604808887E+00
H2	H11	1.1117155531E+00	1.2141118317E-02	5.7120481973E-01	5.7717407906E-01
H3	H11	1.1159704713E+00	3.6335344373E-03	1.7094720914E-01	1.7273383208E-01

C4	H11	6.1660963986E+00	7.7737522614E-03	6.6258040924E-02	3.6955477949E-01
H5	H11	1.1020113679E+00	8.4109160369E-04	4.0122076543E-02	3.9984477467E-02
H6	H11	1.1060481536E+00	5.2741136531E-04	2.5070546313E-02	2.5072498358E-02
H7	H11	1.1030467656E+00	6.5251118638E-03	3.1017248620E-01	3.1019592532E-01
C8	H11	5.6887739024E+00	9.6279887043E-01	8.2059730952E+00	4.5770293713E+01
(Bonded)					
H9	H11	1.0847179428E+00	4.3018723370E-02	2.0450551564E+00	2.0450580742E+00
H10	H11	1.0811778813E+00	4.2358614974E-02	2.0207439819E+00	2.0136773195E+00

Areas of Interatomic Surfaces:

Area_IAS(A|B),0.0004 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.0004

Area_IAS(A|B),0.001 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.001

Area_IAS(A|B),0.002 = Area of the Part of Interatomic Surface Between Atoms

A and B Whose Electron Density is Greater Than 0.002

Atom A	Atom B	Area_IAS(A B),0.0004	Area_IAS(A B),0.001	Area_IAS(A B),0.002

C1	H2	4.3745533549E+01	3.4003525926E+01	2.7145807758E+01

C1	H3	4.3745533961E+01	3.4003526106E+01	2.7145807834E+01

C1	C4	6.5533998306E+01	5.0785793404E+01	3.9973254245E+01

C1	C8	6.5531179322E+01	5.0785792041E+01	3.9973242746E+01

C1	Total	2.1855624514E+02	1.6957863748E+02	1.3423811258E+02

H2	C1	4.3745533549E+01	3.4003525926E+01	2.7145807758E+01

H2	Total	4.3745533549E+01	3.4003525926E+01	2.7145807758E+01

H3	C1	4.3745533961E+01	3.4003526106E+01	2.7145807834E+01

H3	Total	4.3745533961E+01	3.4003526106E+01	2.7145807834E+01
C4	C1	6.5533998306E+01	5.0785793404E+01	3.9973254245E+01
C4	H5	4.2154660366E+01	3.2778742108E+01	2.6308309423E+01
C4	H6	4.5672158856E+01	3.5376413967E+01	2.8050343077E+01
C4	H7	4.5672159081E+01	3.5376414175E+01	2.8050343242E+01

C4	Total	1.9903297661E+02	1.5431736365E+02	1.2238224999E+02
H5	C4	4.2154660366E+01	3.2778742108E+01	2.6308309423E+01

H5	Total	4.2154660366E+01	3.2778742108E+01	2.6308309423E+01
H6	C4	4.5672158856E+01	3.5376413967E+01	2.8050343077E+01

H6	Total	4.5672158856E+01	3.5376413967E+01	2.8050343077E+01
H7	C4	4.5672159081E+01	3.5376414175E+01	2.8050343242E+01

H7	Total	4.5672159081E+01	3.5376414175E+01	2.8050343242E+01
C8	C1	6.5531179322E+01	5.0785792041E+01	3.9973242746E+01
C8	H9	4.5693611016E+01	3.5391126584E+01	2.8058666402E+01
C8	H10	4.2156375401E+01	3.2780420008E+01	2.6308423392E+01
C8	H11	4.5693611321E+01	3.5391126836E+01	2.8058666601E+01

C8	Total	1.9907477706E+02	1.5434846547E+02	1.2239899914E+02
H9	C8	4.5693611016E+01	3.5391126584E+01	2.8058666402E+01

H9	Total	4.5693611016E+01	3.5391126584E+01	2.8058666402E+01

H10	C8	4.2156375401E+01	3.2780420008E+01	2.6308423392E+01

H10	Total	4.2156375401E+01	3.2780420008E+01	2.6308423392E+01

H11	C8	4.5693611321E+01	3.5391126836E+01	2.8058666601E+01

H11	Total	4.5693611321E+01	3.5391126836E+01	2.8058666601E+01

Total	Total	9.7119764236E+02	7.5334576231E+02	5.9814572944E+02

Some Properties of Interatomic Surfaces:

$N_{IAS}(A|B)$ = Integral of Electron Density $\rho(r)$ Over Interatomic Surface Between Atoms A and B

$G_{IAS}(A|B)$ = Integral of Lagrangian Kinetic Energy Density $G(r)$ Over Interatomic Surface Between Atoms A and B

$K_{IAS}(A|B)$ = Integral of Hamiltonian Kinetic Energy Density $K(r)$ Over Interatomic Surface Between Atoms A and B

$L_{IAS}(A|B)$ = Integral of Lagrangian Density $L(r)$ Over Interatomic Surface Between Atoms A and B

$\Delta \rho_{IAS}(A|B)$ = Integral of Laplacian of Electron Density $\Delta \rho(r)$ Over Interatomic Surface Between Atoms A and B

$V_{IAS}(A|B)$ = Integral of Virial Field $V(r)$ Over Interatomic Surface Between Atoms A and B

Atom A	Atom B	$N_{IAS}(A B)$	$G_{IAS}(A B)$	$K_{IAS}(A B)$	$L_{IAS}(A B)$	$\Delta \rho_{IAS}(A B)$	$V_{IAS}(A B)$

C1	H2	1.0002454274E+00	5.7097110311E-01	4.2103484588E-01	-1.4993625723E-01	5.9974502891E-01	-9.9200594899E-01

C1	H3	1.0002453970E+00	5.7097104792E-01	4.2103483945E-01	-1.4993620847E-01	5.9974483390E-01	-9.9200588737E-01

C1	C4	1.2100866130E+00	8.1110038129E-01	3.5653560879E-01	-4.5456477251E-01	1.8182590900E+00	-1.1676359901E+00

C1 C8 1.2098186409E+00 8.1081858253E-01 3.5632026042E-01 -4.5449832210E-01
1.8179932884E+00 -1.1671388429E+00

C1 Total 4.4203960783E+00 2.7638611149E+00 1.5549255545E+00 -1.2089355603E+00
4.8357422412E+00 -4.3187866694E+00

H2 C1 1.0002454274E+00 5.7097110311E-01 4.2103484588E-01 -1.4993625723E-01
5.9974502891E-01 -9.9200594899E-01

H2 Total 1.0002454274E+00 5.7097110311E-01 4.2103484588E-01 -1.4993625723E-01
5.9974502891E-01 -9.9200594899E-01

H3 C1 1.0002453970E+00 5.7097104792E-01 4.2103483945E-01 -1.4993620847E-01
5.9974483390E-01 -9.9200588737E-01

H3 Total 1.0002453970E+00 5.7097104792E-01 4.2103483945E-01 -1.4993620847E-01
5.9974483390E-01 -9.9200588737E-01

C4 C1 1.2100866130E+00 8.1110038129E-01 3.5653560879E-01 -4.5456477251E-01
1.8182590900E+00 -1.1676359901E+00

C4 H5 9.8805981410E-01 5.4849641329E-01 4.1902091299E-01 -1.2947550030E-01
5.1790200120E-01 -9.6751732627E-01

C4 H6 9.9849607186E-01 5.5958869653E-01 4.1643768699E-01 -1.4315100954E-01
5.7260403817E-01 -9.7602638353E-01

C4 H7 9.9849608182E-01 5.5958871370E-01 4.1643767719E-01 -1.4315103651E-01
5.7260414605E-01 -9.7602639089E-01

C4 Total 4.1951385808E+00 2.4787742048E+00 1.6084318860E+00 -8.7034231886E-01
3.4813692754E+00 -4.0872060908E+00

H5 C4 9.8805981410E-01 5.4849641329E-01 4.1902091299E-01 -1.2947550030E-01
5.1790200120E-01 -9.6751732627E-01

H5 Total 9.8805981410E-01 5.4849641329E-01 4.1902091299E-01 -1.2947550030E-01
5.1790200120E-01 -9.6751732627E-01

H6 C4 9.9849607186E-01 5.5958869653E-01 4.1643768699E-01 -1.4315100954E-01
5.7260403817E-01 -9.7602638353E-01

H6 Total 9.9849607186E-01 5.5958869653E-01 4.1643768699E-01 -1.4315100954E-01
5.7260403817E-01 -9.7602638353E-01

H7 C4 9.9849608182E-01 5.5958871370E-01 4.1643767719E-01 -1.4315103651E-01
5.7260414605E-01 -9.7602639089E-01

H7 Total 9.9849608182E-01 5.5958871370E-01 4.1643767719E-01 -1.4315103651E-01
5.7260414605E-01 -9.7602639089E-01

C8 C1 1.2098186409E+00 8.1081858253E-01 3.5632026042E-01 -4.5449832210E-01
1.8179932884E+00 -1.1671388429E+00

C8 H9 9.9832977335E-01 5.5940377037E-01 4.1627176503E-01 -1.4313200534E-01
5.7252802137E-01 -9.7567553540E-01

C8 H10 9.8792563757E-01 5.4834701627E-01 4.1887562190E-01 -1.2947139436E-01
5.1788557746E-01 -9.6722263817E-01

C8 H11 9.9832977402E-01 5.5940378411E-01 4.1627174973E-01 -1.4313203438E-01
5.7252813753E-01 -9.7567553385E-01

C8 Total 4.1944038258E+00 2.4779731533E+00 1.6077393971E+00 -8.7023375618E-01
3.4809350248E+00 -4.0857125503E+00

H9 C8 9.9832977335E-01 5.5940377037E-01 4.1627176503E-01 -1.4313200534E-01
5.7252802137E-01 -9.7567553540E-01

H9 Total 9.9832977335E-01 5.5940377037E-01 4.1627176503E-01 -1.4313200534E-01
5.7252802137E-01 -9.7567553540E-01

H10 C8 9.8792563757E-01 5.4834701627E-01 4.1887562190E-01 -1.2947139436E-01
5.1788557746E-01 -9.6722263817E-01

H10 Total 9.8792563757E-01 5.4834701627E-01 4.1887562190E-01 -1.2947139436E-01
5.1788557746E-01 -9.6722263817E-01

H11 C8 9.9832977402E-01 5.5940378411E-01 4.1627174973E-01 -1.4313203438E-01
 5.7252813753E-01 -9.7567553385E-01

H11 Total 9.9832977402E-01 5.5940378411E-01 4.1627174973E-01 -1.4313203438E-01
 5.7252813753E-01 -9.7567553385E-01

Total Total 2.0780066462E+01 1.2197379018E+01 8.1164819367E+00 -4.0808970815E+00
 1.6323588326E+01 -2.0313860955E+01

IsoDensity Surface Data:

IDS = IsoDensity Surface = Isosurface of the Electron Density Distribution

Area_IDS(A) = Surface Area of Atom A's Part of IDS

ESP = Total Electrostatic Potential

ESP_Int_IDS(A) = Surface Integral of ESP Over Atom A's Part of IDS

ESP_Max_IDS(A) = Maximum Value of ESP on Atom A's Part of IDS

ESP_Min_IDS(A) = Minimum Value of ESP on Atom A's Part of IDS

ESP_Avg_IDS(A) = Average Value of ESP on Atom A's Part of IDS

ESP_MAD_IDS(A) = Mean Absolute Deviation of ESP on Atom A's Part of IDS

ESP_Var_IDS(A) = Variance of ESP on Atom A's Part of IDS

|ESP|_Int_IDS(A) = Surface Integral of |ESP| Over Atom A's Part of IDS

ESP*ESP_Int_IDS(A) = Surface Integral of ESP*ESP Over Atom A's Part of IDS

Area_ESP+_IDS(A) = Surface Area of Positive ESP Regions of Atom A's Part of IDS

ESP+_Int_IDS(A) = Surface Integral of ESP Over Positive ESP Regions of Atom A's Part of IDS

Area_ESP-_IDS(A) = Surface Area of Negative ESP Regions of Atom A's Part of IDS

ESP-_Int_IDS(A) = Surface Integral of ESP Over Negative ESP Regions of Atom A's Part of IDS

ESP+_Min_IDS(A) = Minimum Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Avg_IDS(A) = Average Value of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_MAD_IDS(A) = Mean Absolute Deviation of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP+_Var_IDS(A) = Variance of ESP on Positive ESP Regions of Atom A's Part of IDS

ESP*ESP+_Int_IDS(A) = Surface Integral of ESP*ESP Over Positive Regions of Atom A's Part of IDS

ESP- _Min_IDS(A) = Minimum Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP- _Avg_IDS(A) = Average Value of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP- _MAD_IDS(A) = Mean Absolute Deviation of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP- _Var_IDS(A) = Variance of ESP on Negative ESP Regions of Atom A's Part of IDS

ESP-*ESP- _Int_IDS(A) = Surface Integral of ESP*ESP Over Negative Regions of Atom A's Part of IDS

0.0004 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	6.9815792670E+00				

H2	4.8740035105E+01				

H3	4.8866487028E+01				

C4	1.6160020210E+01				

H5	5.2249465034E+01				

H6	4.7831690357E+01				

H7	4.7879736285E+01				

C8	1.6573897804E+01				

H9	4.7730248542E+01				

H10	5.2373190615E+01				

H11	4.7684697982E+01				

Total	4.3307104823E+02				

0.001 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
	ESP_MAD_IDS(A)	ESP_Var_IDS(A)			

C1	8.6650557785E+00	1.9407954157E-04	5.1596194561E-03	-4.1999221584E-03	2.2397956404E-05
O5	2.0293922068E-03	6.2734107804E-06			

H2 4.1495945718E+01 1.5223145849E-01 9.7685380949E-03 -3.9647097891E-03 3.6685863127E-03 2.7015573873E-03 1.0882112587E-05

H3 4.1688400280E+01 1.5267150979E-01 9.7645081999E-03 -3.9379070869E-03 3.6622060038E-03 2.6955537869E-03 1.0844279293E-05

C4 1.6982172028E+01 -4.7690561659E-02 4.9879824526E-03 -5.0746010456E-03 -2.8082722034E-03 1.9748616697E-03 5.3847163951E-06

H5 4.3544258168E+01 1.2966388717E-01 1.1172363155E-02 -4.3233054770E-03 2.9777493663E-03 3.6151139663E-03 1.8221255548E-05

H6 4.1049134397E+01 1.2795805692E-01 1.0986618906E-02 -4.8149265313E-03 3.1171925743E-03 4.0357338826E-03 2.1352340275E-05

H7 4.0887809108E+01 1.2777239981E-01 1.0991563412E-02 -4.7475440373E-03 3.1249509965E-03 4.0357265087E-03 2.1339469525E-05

C8 1.7128142098E+01 -4.7883589975E-02 5.1015790501E-03 -5.0731485236E-03 -2.7956091034E-03 1.9914460141E-03 5.4797970502E-06

H9 4.0973855478E+01 1.2801035331E-01 1.0980426781E-02 -4.8366671301E-03 3.1241959492E-03 4.0436580577E-03 2.1416860312E-05

H10 4.3689701095E+01 1.2891268330E-01 1.1165207257E-02 -4.3683947389E-03 2.9506423727E-03 3.6248512358E-03 1.8350033520E-05

H11 4.0869154924E+01 1.2894518465E-01 1.0986768996E-02 -4.7928786105E-03 3.1550734262E-03 4.0288116137E-03 2.1285075092E-05

Total 3.7697362907E+02 9.8078546135E-01 1.1172363155E-02 -5.0746010456E-03 2.6017349377E-03 1.9735956255E-05

0.001 IsoDensity Surface:

Atom A	ESP _Int_IDS(A)	ESP*ESP_Int_IDS(A)	Area_ESP+_IDS(A)	ESP+_Int_IDS(A)	Area_ESP-_IDS(A)	ESP-_Int_IDS(A)
C1	1.7614066853E-02	5.4363801319E-05	4.9859398421E+00	8.9040731975E-03	3.6791159364E+00	-8.7099936559E-03
H2	1.7217496567E-01	1.0100377982E-03	3.5713857184E+01	1.6220321208E-01	5.7820885338E+00	-9.9717535878E-03
H3	1.7264650849E-01	1.0111951757E-03	3.5907846185E+01	1.6265900914E-01	5.7805540948E+00	-9.9874993475E-03
C4	5.5087581880E-02	2.2537225881E-04	3.0228399138E+00	3.6985101107E-03	1.3959332114E+01	-5.1389071770E-02

H5	1.8288656370E-01 1.2130518706E+01	1.1795376135E-03 -2.6611338268E-02	3.1413739462E+01	1.5627522543E-01
H6	1.9105357980E-01 1.2552253542E+01	1.2753649905E-03 -3.1547761437E-02	2.8496880855E+01	1.5950581836E-01
H7	1.9038317182E-01 1.2527283406E+01	1.2718066445E-03 -3.1305386003E-02	2.8360525702E+01	1.5907778582E-01
C8	5.5711702479E-02 1.3935015848E+01	2.2772254258E-04 -5.1797646227E-02	3.1931262501E+00	3.9140562519E-03
H9	1.9110063430E-01 1.2782534907E+01	1.2774607665E-03 -3.1545140495E-02	2.8191320571E+01	1.5955549380E-01
H10	1.8365306888E-01 1.2331798702E+01	1.1820827053E-03 -2.7370192792E-02	3.1357902393E+01	1.5628287609E-01
H11	1.9091772194E-01 1.2490733286E+01	1.2767345570E-03 -3.0986268645E-02	2.8378421638E+01	1.5993145329E-01

Total	1.6032295658E+00 1.1795122908E+02	9.9916788539E-03 -3.1122205223E-01	2.5902240000E+02	1.2920075136E+00

0.001 IsoDensity Surface:

Atom A	ESP+_Min_IDS(A) ESP+*ESP+_Int_IDS(A)	ESP+_Avg_IDS(A)	ESP+_MAD_IDS(A)	ESP+_Var_IDS(A)

C1	1.4357415466E-04 2.6652732449E-05	1.7858364681E-03	1.2823316105E-03	2.1563665345E-06
H2	5.9062497046E-05 9.8537586363E-04	4.5417444340E-03	2.2613820458E-03	6.9634127364E-06
H3	1.0875371379E-05 9.8664589296E-04	4.5299015792E-03	2.2591616340E-03	6.9571588699E-06
C4	2.0726222351E-05 8.9036718748E-06	1.2235216605E-03	8.6924572716E-04	1.4484606422E-06
H5	2.3254183885E-05 1.1013901185E-03	4.9747412473E-03	2.7865753048E-03	1.0312726665E-05
H6	1.5938104516E-05 1.1734675164E-03	5.5973079710E-03	2.7105122442E-03	9.8489490571E-06
H7	2.5097252134E-05 1.1708812574E-03	5.6091268366E-03	2.7039014077E-03	9.8232939245E-06

C8	3.9308817953E-06	1.2257756022E-03	8.2263331128E-04	1.4100843241E-06
9.3003319293E-06				
H9	2.0908440916E-06	5.6597381951E-03	2.6788835033E-03	9.6614159485E-06
1.1754103967E-03				
H10	3.4890969030E-05	4.9838434387E-03	2.7817034377E-03	1.0261822834E-05
1.1006786254E-03				
H11	2.4227134219E-05	5.6356711918E-03	2.6848628079E-03	9.7167272529E-06
1.1770664669E-03				

Total	2.0908440916E-06	4.9880146026E-03	9.5405668771E-06	8.9157728741E-03

0.001 IsoDensity Surface:

Atom A	ESP-_Max_IDS(A)	ESP-_Avg_IDS(A)	ESP-_MAD_IDS(A)	ESP-_Var_IDS(A)	ESP-*ESP-_Int_IDS(A)

C1	-9.3936023364E-05	-2.3674148373E-03	1.2339464171E-03	1.9273381917E-06	
2.7711068870E-05					
H2	-2.0041964875E-05	-1.7245937224E-03	9.7939361354E-04	1.2910059894E-06	
2.4661934567E-05					
H3	-2.2342682322E-06	-1.7277754318E-03	9.6780208180E-04	1.2616656819E-06	
2.4549282722E-05					
C4	-2.2921218970E-05	-3.6813417254E-03	1.1413886717E-03	1.9548107731E-06	
2.1646858694E-04					
H5	-4.8080437659E-08	-2.1937510599E-03	1.1117926961E-03	1.6296783348E-06	
7.8147495056E-05					
H6	-1.8647694139E-08	-2.5133145480E-03	1.1604964188E-03	1.8011129477E-06	
1.0189747415E-04					
H7	-2.0949308797E-05	-2.4989764333E-03	1.1651772200E-03	1.8115631753E-06	
1.0092538716E-04					
C8	-3.2664186294E-05	-3.7170855628E-03	1.0988093333E-03	1.8576173834E-06	
2.1842221065E-04					
H9	-2.4579369667E-05	-2.4678313593E-03	1.1952519296E-03	1.8933867975E-06	
1.0205036978E-04					
H10	-3.7093153521E-05	-2.2194809899E-03	1.1263422752E-03	1.6750563163E-06	
8.1404079899E-05					
H11	-4.4984222323E-05	-2.4807405567E-03	1.1727934033E-03	1.8252888976E-06	
9.9668090118E-05					

Total	-1.8647694139E-08	-2.6385655721E-03	2.1595890913E-06	1.0759059799E-03

0.002 IsoDensity Surface:

Atom A	Area_IDS(A)	ESP_Int_IDS(A)	ESP_Max_IDS(A)	ESP_Min_IDS(A)	ESP_Avg_IDS(A)
ESP_MAD_IDS(A)	ESP_Var_IDS(A)				

C1	1.0248201074E+01
H2	3.6059555292E+01
H3	3.6180182128E+01
C4	1.7928211337E+01
H5	3.7068500293E+01
H6	3.5741834623E+01
H7	3.5440337019E+01
C8	1.7526722378E+01
H9	3.5681522082E+01
H10	3.6845786795E+01
H11	3.5771824980E+01

Total	3.3449267800E+02

Atomic Surface Area and Volume Data:

$\text{Area}(A) = \text{Area\_IAS}(A|\text{Total}) + \text{Area\_IDS}(A)$

$\text{Vol}(A)$ = Volume Bounded by Interatomic Surfaces (IASs) of Atom A and by an
Isosurface of the Electron Density Distribution (IsoDensity Surface)

$N(\text{Vol}(A))$ = Average Number of Electrons in $\text{Vol}(A)$

$N(\text{Vol}(A))/\text{Vol}(A)$ = Average Electron Density in $\text{Vol}(A)$

$\%N(\text{Vol}(A)) = 100 * N(\text{Vol}(A)) / N(A)$

= Percentage of Atom A's Electron Population in $\text{Vol}(A)$

IASs and 0.0004 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	2.2553782441E+02	5.9563834281E+01	5.8367852320E+00	9.7992100449E-02	9.9977670970E+01
H2	9.2485568654E+01	7.0205387286E+01	1.0523692774E+00	1.4989864996E-02	9.9021916677E+01
H3	9.2612020989E+01	7.0167081079E+01	1.0523556029E+00	1.4997853504E-02	9.9020530234E+01
C4	2.1519299682E+02	7.2823989253E+01	5.8630189139E+00	8.0509444401E-02	9.9944565781E+01
H5	9.4404125400E+01	7.1174070095E+01	1.0369311960E+00	1.4568946172E-02	9.8928184815E+01
H6	9.3503849213E+01	7.0482817670E+01	1.0414600690E+00	1.4776084490E-02	9.9011794618E+01
H7	9.3551895366E+01	7.0484860843E+01	1.0414578967E+00	1.4775625350E-02	9.9011815215E+01
C8	2.1564867486E+02	7.2794073616E+01	5.8631838372E+00	8.0544796383E-02	9.9944298434E+01
H9	9.3423859558E+01	7.0462631388E+01	1.0413672724E+00	1.4779000612E-02	9.9010539753E+01
H10	9.4529566016E+01	7.1115896296E+01	1.0368326146E+00	1.4579477566E-02	9.8925485078E+01
H11	9.3378309303E+01	7.0484462246E+01	1.0413729310E+00	1.4774503455E-02	9.9011219030E+01
Total	1.4042686906E+03	7.6975910405E+02	2.5907134843E+01	3.3656159059E-02	9.9643386204E+01

IASs and 0.001 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))
C1	1.7824369326E+02	5.5846050019E+01	5.8343072705E+00	1.0447126106E-01	9.9935226232E+01

H2	7.5499471644E+01	5.1999728045E+01	1.0405858559E+00	2.0011371118E-02
9.7913164258E+01				
H3	7.5691926386E+01	5.2022884800E+01	1.0406106751E+00	2.0002940612E-02
9.7915400965E+01				
C4	1.7129953568E+02	6.5137886508E+01	5.8579635000E+00	8.9931740405E-02
9.9858388139E+01				
H5	7.6323000276E+01	5.1962499093E+01	1.0244961037E+00	1.9716066809E-02
9.7741817664E+01				
H6	7.6425548364E+01	5.2202721285E+01	1.0296118228E+00	1.9723336206E-02
9.7885379737E+01				
H7	7.6264223283E+01	5.2184921568E+01	1.0295923416E+00	1.9729690314E-02
9.7883752187E+01				
C8	1.7147660757E+02	6.5147531863E+01	5.8581654376E+00	8.9921525346E-02
9.9858754395E+01				
H9	7.6364982062E+01	5.2169262495E+01	1.0294907917E+00	1.9733665811E-02
9.7881354310E+01				
H10	7.6470121103E+01	5.2007233527E+01	1.0244631768E+00	1.9698474757E-02
9.7745301684E+01				
H11	7.6260281760E+01	5.2176174511E+01	1.0295004558E+00	1.9731236823E-02
9.7882412809E+01				

Total	1.1303193914E+03	6.0285689371E+02	2.5798787432E+01	4.2794214847E-02
9.9226663049E+01				

IASs and 0.002 IsoDensity Surface:

Atom A	Area(A)	Vol(A)	N(Vol(A))	N(Vol(A))/Vol(A)	%N(Vol(A))

C1	1.4448631365E+02	5.2378076401E+01	5.8292474528E+00	1.1129174367E-01	
9.9848557155E+01					
H2	6.3205363050E+01	3.9199253373E+01	1.0222396895E+00	2.6078039799E-02	
9.6186895162E+01					
H3	6.3325989962E+01	3.9188869748E+01	1.0222193253E+00	2.6084429887E-02	
9.6184882114E+01					
C4	1.4031046133E+02	5.9019709558E+01	5.8491192475E+00	9.9104507482E-02	
9.9707623663E+01					
H5	6.3376809716E+01	3.8919392555E+01	1.0057472101E+00	2.5841801326E-02	
9.5953083736E+01					

H6	6.3792177700E+01	3.9500931639E+01	1.0114036975E+00	2.5604552994E-02
9.6154330015E+01				
H7	6.3490680261E+01	3.9497529803E+01	1.0114020155E+00	2.5606715675E-02
9.6154390671E+01				
C8	1.3992572152E+02	5.8993075216E+01	5.8492512986E+00	9.9151489852E-02
9.9706803272E+01				
H9	6.3740188484E+01	3.9453391286E+01	1.0112200042E+00	2.5630749886E-02
9.6144214513E+01				
H10	6.3154210187E+01	3.8878593359E+01	1.0055932965E+00	2.5864960885E-02
9.5944903012E+01				
H11	6.3830491581E+01	3.9474993436E+01	1.0112613756E+00	2.5617771850E-02
9.6148285187E+01				

Total	9.3263840744E+02	4.8450381637E+02	2.5628704613E+01	5.2896806479E-02
9.8572494687E+01				

Bond Contributions to Atomic Net Charges:

$q(A|B)$ = Contribution of Bond Between Atom A and Atom B to $q(A)$

$q(A)^*$ = Sum of $q(A|B)$ Over all B

$q(A)$ = Net Charge of Atom A

Atom A	Atom B	$q(A B)$	$q(A)^*$	$q(A)$

C1	H2	6.2777908143E-02		
C1	H3	6.2778978743E-02		
C1	C4	1.8198774471E-02		
C1	C8	1.8148561371E-02		
C1		1.6190422273E-01	1.6191117940E-01	
H2	C1	-6.2770951471E-02		
H2		-6.2770951471E-02	-6.2763994800E-02	
H3	C1	-6.2772022071E-02		
H3		-6.2772022071E-02	-6.2765065400E-02	
C4	C1	-1.8191817800E-02		
C4	H5	4.8179507343E-02		

C4	H6	5.1868465643E-02
C4	H7	5.1866052843E-02
C4		1.3372220803E-01 1.3372916470E-01
H5	C4	-4.8172550671E-02
H5		-4.8172550671E-02 -4.8165594000E-02
H6	C4	-5.1861508971E-02
H6		-5.1861508971E-02 -5.1854552300E-02
H7	C4	-5.1859096171E-02
H7		-5.1859096171E-02 -5.1852139500E-02
C8	C1	-1.8141604700E-02
C8	H9	5.1788072943E-02
C8	H10	4.8108460243E-02
C8	H11	5.1786572243E-02
C8		1.3354150073E-01 1.3354845740E-01
H9	C8	-5.1781116271E-02
H9		-5.1781116271E-02 -5.1774159600E-02
H10	C8	-4.8101503571E-02
H10		-4.8101503571E-02 -4.8094546900E-02
H11	C8	-5.1779615571E-02
H11		-5.1779615571E-02 -5.1772658900E-02

Atomic Dipole Moments:

Mu_Intra(A) = Intraatomic Dipole Moment Contribution of Atom A

Mu_Bond(A) = Bonding Dipole Moment Contribution of Atom A

Mu(A) = Mu_Intra(A) + Mu_Bond(A)

= Total Dipole Moment Contribution of Atom A

Atom A	Mu_Intra_X(A)	Mu_Bond_X(A)	Mu_X(A)

C1	3.5615708229E-04	-6.7541578709E-05	2.8861550358E-04

H2	8.3276341662E-06	-4.4989692467E-06	3.8286649195E-06

H3	9.8403898302E-06	-4.5007393418E-06	5.3396504884E-06
C4	1.1355222871E-02	-7.6455750790E-02	-6.5100527919E-02
H5	-1.1040736455E-01	-3.1036376155E-02	-1.4144374071E-01
H6	-1.2283831334E-02	-1.4811062695E-03	-1.3764937603E-02
H7	-1.2289802369E-02	-1.4810310282E-03	-1.3770833397E-02
C8	-1.1301125773E-02	7.6338552045E-02	6.5037426272E-02
H9	1.2288862831E-02	1.4852314923E-03	1.3774094323E-02
H10	1.1039950060E-01	3.0986614674E-02	1.4138611527E-01
H11	1.2288882212E-02	1.4851831675E-03	1.3774065380E-02

Total	4.2466959429E-04	-2.3522415158E-04	1.8944544271E-04

Atom A	Mu_Intra_Y(A)	Mu_Bond_Y(A)	Mu_Y(A)

C1	3.8236573019E-03	-6.6884114257E-02	-6.3060456955E-02
H2	-8.3665577014E-02	-2.9647373870E-02	-1.1331295088E-01
H3	-8.3665295870E-02	-2.9647895622E-02	-1.1331319149E-01
C4	-1.7357158871E-02	5.7863122185E-02	4.0505963314E-02
H5	-6.9466675329E-02	-2.0923070004E-02	-9.0389745333E-02
H6	8.1915689809E-02	2.3918035286E-02	1.0583372510E-01
H7	8.1917563715E-02	2.3916921432E-02	1.0583448515E-01
C8	-1.7202707993E-02	5.7751323908E-02	4.0548615915E-02
H9	8.1903596180E-02	2.3882929904E-02	1.0578652608E-01
H10	-6.9483430861E-02	-2.0899995770E-02	-9.0383426631E-02
H11	8.1903699661E-02	2.3882232710E-02	1.0578593237E-01

Total	-9.3766392711E-03	4.3212115902E-02	3.3835476630E-02

Atom A	Mu_Intra_Z(A)	Mu_Bond_Z(A)	Mu_Z(A)

C1	2.1286635774E-04	1.0929724775E-06	2.1395933022E-04
H2	-1.0158882522E-01	-3.9156239892E-02	-1.4074506511E-01

H3	1.0158821515E-01	3.9156894541E-02	1.4074510969E-01
C4	-1.2241867411E-04	-2.5146554138E-06	-1.2493332952E-04
H5	1.7937051153E-06	2.0116908251E-09	1.7957168061E-06
H6	-1.0422709851E-01	-3.2533791109E-02	-1.3676088962E-01
H7	1.0422439922E-01	3.2532279536E-02	1.3675667876E-01
C8	7.8110340555E-05	-1.5603803823E-06	7.6549960173E-05
H9	-1.0423031721E-01	-3.2483408521E-02	-1.3671372573E-01
H10	-8.8623352787E-07	6.3555548814E-10	-8.8559797238E-07
H11	1.0423065218E-01	3.2482471827E-02	1.3671312401E-01

Total	1.6649110577E-04	-4.7730336420E-06	1.6171807213E-04

Atom A	Mu_Intra(A)	Mu_Bond(A)	Mu(A)

C1	3.8461038878E-03	6.6884148369E-02	6.3061480389E-02
H2	1.3160630021E-01	4.9113927964E-02	1.8069033789E-01
H3	1.3160565066E-01	4.9114764838E-02	1.8069052354E-01
C4	2.0741914975E-02	9.5883380959E-02	7.6673511773E-02
H5	1.3044311071E-01	3.7430355372E-02	1.6785898203E-01
H6	1.3313286902E-01	4.0406851543E-02	1.7347562308E-01
H7	1.3313245991E-01	4.0404972411E-02	1.7347323506E-01
C8	2.0582874125E-02	9.5722463110E-02	7.6642435560E-02
H9	1.3312841260E-01	4.0345657543E-02	1.7341037333E-01
H10	1.3044537898E-01	3.7376197133E-02	1.6780702429E-01
H11	1.3312874031E-01	4.0344488896E-02	1.7340953446E-01

Total	9.3877274978E-03	4.3212756379E-02	3.3836393441E-02

Bond Contributions to Atomic Dipole Moments:

Mu_Bond(A|B) = Contribution of Bond Between Atom A and Atom B to Mu_Bond(A)

Mu_Bond(A) = Sum of Mu_Bond(A|B) Over All B

= Total Bonding Dipole Moment Contribution of Atom A

Atom A	Atom B	Mu_Bond_X(A B)	Mu_Bond_X(A)

C1	H2	-5.8406813995E-06	
C1	H3	-5.8428541940E-06	
C1	C4	-2.1636578705E-02	
C1	C8	2.1580720662E-02	
C1		-6.7541578709E-05	
H2	C1	-4.4989692467E-06	
H2		-4.4989692467E-06	
H3	C1	-4.5007393418E-06	
H3		-4.5007393418E-06	
C4	C1	-2.1970435861E-02	
C4	H5	-5.1126604636E-02	
C4	H6	-1.6793985598E-03	
C4	H7	-1.6793117322E-03	
C4		-7.6455750790E-02	
H5	C4	-3.1036376155E-02	
H5		-3.1036376155E-02	
H6	C4	-1.4811062695E-03	
H6		-1.4811062695E-03	
H7	C4	-1.4810310282E-03	
H7		-1.4810310282E-03	
C8	C1	2.1914918510E-02	
C8	H9	1.6865615082E-03	
C8	H10	5.1050566021E-02	
C8	H11	1.6865060058E-03	
C8		7.6338552045E-02	
H9	C8	1.4852314923E-03	
H9		1.4852314923E-03	
H10	C8	3.0986614674E-02	

H10		3.0986614674E-02
H11	C8	1.4851831675E-03
H11		1.4851831675E-03

Atom A	Atom B	Mu_Bond_Y(A B)	Mu_Bond_Y(A)

C1	H2	-4.8076778459E-02	
C1	H3	-4.8077623057E-02	
C1	C4	1.4656179566E-02	
C1	C8	1.4614107693E-02	
C1		-6.6884114257E-02	
H2	C1	-2.9647373870E-02	
H2		-2.9647373870E-02	
H3	C1	-2.9647895622E-02	
H3		-2.9647895622E-02	
C4	C1	1.4689391863E-02	
C4	H5	-3.5372314181E-02	
C4	H6	3.9273936467E-02	
C4	H7	3.9272108036E-02	
C4		5.7863122185E-02	
H5	C4	-2.0923070004E-02	
H5		-2.0923070004E-02	
H6	C4	2.3918035286E-02	
H6		2.3918035286E-02	
H7	C4	2.3916921432E-02	
H7		2.3916921432E-02	
C8	C1	1.4647676341E-02	
C8	H9	3.9220238481E-02	
C8	H10	-3.5335685481E-02	
C8	H11	3.9219094567E-02	
C8		5.7751323908E-02	
H9	C8	2.3882929904E-02	

H9		2.3882929904E-02
H10	C8	-2.0899995770E-02
H10		-2.0899995770E-02
H11	C8	2.3882232710E-02
H11		2.3882232710E-02

Atom A	Atom B	Mu_Bond_Z(A B)	Mu_Bond_Z(A)

C1	H2	-6.5073076931E-02	
C1	H3	6.5074169726E-02	
C1	C4	8.3642232354E-11	
C1	C8	9.3695488573E-11	
C1		1.0929724775E-06	
H2	C1	-3.9156239892E-02	
H2		-3.9156239892E-02	
H3	C1	3.9156894541E-02	
H3		3.9156894541E-02	
C4	C1	-8.3610259238E-11	
C4	H5	3.2877644712E-09	
C4	H6	-5.4161431761E-02	
C4	H7	5.4158913902E-02	
C4		-2.5146554138E-06	
H5	C4	2.0116908251E-09	
H5		2.0116908251E-09	
H6	C4	-3.2533791109E-02	
H6		-3.2533791109E-02	
H7	C4	3.2532279536E-02	
H7		3.2532279536E-02	
C8	C1	-9.3659573399E-11	
C8	H9	-5.4084377893E-02	
C8	H10	8.0760640205E-10	
C8	H11	5.4082816799E-02	

C8		-1.5603803823E-06
H9	C8	-3.2483408521E-02
H9		-3.2483408521E-02
H10	C8	6.3555548814E-10
H10		6.3555548814E-10
H11	C8	3.2482471827E-02
H11		3.2482471827E-02

Atom A	Atom B	Mu_Bond(A B)	Mu_Bond(A)

C1	H2	8.0906625207E-02	
C1	H3	8.0908006023E-02	
C1	C4	2.6133219043E-02	
C1	C8	2.6063377524E-02	
C1		6.6884148369E-02	
H2	C1	4.9113927964E-02	
H2		4.9113927964E-02	
H3	C1	4.9114764838E-02	
H3		4.9114764838E-02	
C4	C1	2.6428739759E-02	
C4	H5	6.2170172206E-02	
C4	H6	6.6923263187E-02	
C4	H7	6.6920150273E-02	
C4		9.5883380959E-02	
H5	C4	3.7430355372E-02	
H5		3.7430355372E-02	
H6	C4	4.0406851543E-02	
H6		4.0406851543E-02	
H7	C4	4.0404972411E-02	
H7		4.0404972411E-02	
C8	C1	2.6359402032E-02	
C8	H9	6.6829570763E-02	

C8	H10	6.2086801814E-02
C8	H11	6.6827634659E-02
C8		9.5722463110E-02
H9	C8	4.0345657543E-02
H9		4.0345657543E-02
H10	C8	3.7376197133E-02
H10		3.7376197133E-02
H11	C8	4.0344488896E-02
H11		4.0344488896E-02

Atomic Traceless Quadrupole Moment Tensors:

Q(A) = Traceless Form of Quadrupole Moment Tensor of Atom A's Electronic Charge

Density Distribution, Using the Nucleus of Atom A as Origin

$$Q_{XX}(A) = -[3\langle \text{Rho} * x * x \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{XY}(A) = -3\langle \text{Rho} * x * y \rangle(A)$$

$$Q_{XZ}(A) = -3\langle \text{Rho} * x * z \rangle(A)$$

$$Q_{YY}(A) = -[3\langle \text{Rho} * y * y \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

$$Q_{YZ}(A) = -3\langle \text{Rho} * y * z \rangle(A)$$

$$Q_{ZZ}(A) = -[3\langle \text{Rho} * z * z \rangle(A) - \langle \text{Rho} * r * r \rangle(A)]$$

Atom A	Q_XX(A)	Q_XY(A)	Q_XZ(A)	Q_YY(A)	Q_YZ(A)	Q_ZZ(A)
C1	5.1533324100E-02	5.5690219139E-04	-5.1744635386E-06	-4.2830743165E-03	1.2700831812E-03	-4.7250249783E-02
H2	-1.9777226122E-01	3.0282862323E-05	6.1438446916E-05	-1.1895390789E-02	3.3527508139E-01	2.0966765201E-01
H3	-1.9777351190E-01	3.4440370873E-05	-6.0545347330E-05	-1.1893314793E-02	-3.3527675948E-01	2.0966682669E-01
C4	6.2573609226E-02	3.0551411593E-02	3.3075329561E-04	-1.9303870871E-02	-2.0051927038E-04	-4.3269738355E-02
H5	2.4948207912E-01	3.3408330809E-01	-3.8560995818E-06	1.3642826108E-02	1.2410775745E-06	-2.6312490522E-01

H6 -1.9996132163E-01 -1.6991307525E-02 -8.5859955681E-03 -2.2491327181E-02 -3.4681446910E-01 2.2245264881E-01

H7 -1.9994079671E-01 -1.7006341255E-02 8.6057513379E-03 -2.2503056292E-02 3.4680867760E-01 2.2244385300E-01

C8 6.2349197539E-02 -3.1275497268E-02 6.3058937161E-04 -1.7499021933E-02 -6.3779276041E-04 -4.4850175605E-02

H9 -1.9999002522E-01 1.7072915332E-02 8.4922503632E-03 -2.2445951853E-02 -3.4684043553E-01 2.2243597707E-01

H10 2.4933781584E-01 -3.3416209014E-01 -2.0880529126E-06 1.3786649185E-02 -6.9292984427E-07 -2.6312446502E-01

H11 -1.9998864923E-01 1.7070326422E-02 -8.4904592459E-03 -2.2446091130E-02 3.4683339889E-01 2.2243474036E-01

Eigenvalues and Eigenvectors of Atomic Traceless Quadrupole Moment Tensors:

$Q\_EigVal\_n(A)$ = nth Eigenvalue of $Q(A)$

$Q\_EigVal\_n\_X(A)$ = X Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Y(A)$ = Y Component of the nth Eigenvector of $Q(A)$

$Q\_EigVal\_n\_Z(A)$ = Z Component of the nth Eigenvector of $Q(A)$

Atom A	n	$Q\_EigVal\_n(A)$	$Q\_EigVec\_n\_X(A)$	$Q\_EigVec\_n\_Y(A)$	$Q\_EigVec\_n\_Z(A)$
C1	1	-4.7287764639E-02	2.1871788816E-04	-2.9523554228E-02	9.9956406093E-01
C1	2	-4.2511159094E-03	-9.9755222695E-03	9.9951428535E-01	2.9524266812E-02
C1	3	5.1538880548E-02	9.9995021932E-01	9.9776310349E-03	7.5901218990E-05
H2	1	-2.5421715077E-01	2.0277454863E-04	8.1047417912E-01	-5.8577432844E-01
H2	2	-1.9777226592E-01	9.999997404E-01	-2.2522619350E-04	3.4543215861E-05
H2	3	4.5198941669E-01	1.0393533773E-04	5.8577432024E-01	8.1047420375E-01
H3	1	-2.5421766237E-01	1.3381484407E-04	8.1047261298E-01	5.8577651515E-01
H3	2	-1.9777351826E-01	9.999998537E-01	-1.7087882493E-04	7.9855807061E-06
H3	3	4.5199118063E-01	-1.0656889704E-04	-5.8577650551E-01	8.1047262399E-01
C4	1	-4.3276552708E-02	-8.7599060286E-03	1.9526427716E-02	9.9977096511E-01
C4	2	-2.9440843401E-02	-3.1497256956E-01	9.4886191610E-01	-2.1291890314E-02
C4	3	7.2717396110E-02	9.4906034817E-01	3.1508694481E-01	2.1616521071E-03

H5	1	-2.6312490549E-01	4.8968866717E-05	-6.3593969018E-05	9.9999999678E-01
H5	2	-2.2272090132E-01	-5.7756390231E-01	8.1634547363E-01	8.0197298769E-05
H5	3	4.8584580681E-01	8.1634547610E-01	5.7756390438E-01	-3.2459317839E-06
H6	1	-2.7269851993E-01	2.5064906300E-01	7.9087574439E-01	5.5829257934E-01
H6	2	-1.9509775421E-01	-9.6806890345E-01	2.0226456570E-01	1.4809336120E-01
H6	3	4.6779627413E-01	4.2006411891E-03	-5.7758514731E-01	8.1631963851E-01
H7	1	-2.7271368614E-01	2.5082909070E-01	7.9083911145E-01	-5.5826361788E-01
H7	2	-1.9506729038E-01	-9.6802232134E-01	2.0241850127E-01	-1.4818750192E-01
H7	3	4.6778097652E-01	-4.1895874992E-03	5.7758137966E-01	8.1632236109E-01
C8	1	-4.4865175177E-02	1.3751530280E-03	2.4870264680E-02	9.9968974131E-01
C8	2	-2.8281181955E-02	3.2626638266E-01	9.4497421583E-01	-2.3957858201E-02
C8	3	7.3146357132E-02	9.4527686764E-01	-3.2619810140E-01	6.8148471386E-03
H9	1	-2.7270619080E-01	2.5087402393E-01	-7.9082422386E-01	-5.5826451712E-01
H9	2	-1.9511966067E-01	9.6800980266E-01	2.0233593614E-01	1.4838190894E-01
H9	3	4.6782585147E-01	-4.3870342860E-03	-5.7763069162E-01	8.1628643136E-01
H10	1	-2.6312446510E-01	2.6775696665E-05	3.4813888299E-05	9.9999999904E-01
H10	2	-2.2274750551E-01	5.7775057634E-01	8.1621337260E-01	-4.3885235404E-05
H10	3	4.8587197061E-01	8.1621337334E-01	-5.7775057696E-01	-1.7409376495E-06
H11	1	-2.7269883461E-01	2.5085417305E-01	-7.9082975913E-01	5.5826559623E-01
H11	2	-1.9511951036E-01	9.6801494737E-01	2.0232012425E-01	-1.4836990593E-01
H11	3	4.6781834497E-01	4.3869721728E-03	5.7762865181E-01	8.1628787513E-01

Atomic Radial Moments:

$$R-2(A) = \langle \text{Rho} / (r^*r) \rangle (A)$$

$$R-1(A) = \langle \text{Rho} / r \rangle (A)$$

$$R0(A) = \langle \text{Rho} \rangle (A) = N(A)$$

$$R+1(A) = \langle \text{Rho} * r \rangle (A)$$

$$R+2(A) = \langle \text{Rho} * r^*r \rangle (A)$$

Atom A	R-2(A)	R-1(A)	R0(A)	R+1(A)	R+2(A)

C1	1.3741095838E+02 8.3270437398E+00	1.4870195103E+01	5.8380888206E+00	5.7351402409E+00
H2	3.0030036011E+00 1.7656403536E+00	1.3378226426E+00	1.0627639948E+00	1.1947302406E+00
H3	3.0030040582E+00 1.7656421124E+00	1.3378233098E+00	1.0627650654E+00	1.1947319303E+00
C4	1.3744026300E+02 8.7113133421E+00	1.4880037520E+01	5.8662708353E+00	5.8441116095E+00
H5	2.9689988328E+00 1.7600626448E+00	1.3200649848E+00	1.0481655940E+00	1.1817533474E+00
H6	2.9708706256E+00 1.7638012075E+00	1.3228754186E+00	1.0518545523E+00	1.1863807268E+00
H7	2.9708703871E+00 1.7637847996E+00	1.3228745652E+00	1.0518521395E+00	1.1863743430E+00
C8	1.3744000234E+02 8.7121679866E+00	1.4880020003E+01	5.8664515426E+00	5.8445635617E+00
H9	2.9704318853E+00 1.7638380184E+00	1.3227197613E+00	1.0517741596E+00	1.1863462841E+00
H10	2.9686207848E+00 1.7600986333E+00	1.3199293905E+00	1.0480945469E+00	1.1817226854E+00
H11	2.9704312310E+00 1.7638299474E+00	1.3227188995E+00	1.0517726589E+00	1.1863430249E+00

Atomic Radial Distortion Moments:

$$\text{Dot} = x^*(d\rho/dx) + y^*(d\rho/dy) + z^*(d\rho/dz)$$

$$\text{GR-2(A)} = \langle \text{Dot}/(r^*r) \rangle (A)$$

$$\text{GR-1(A)} = \langle \text{Dot}/r \rangle (A)$$

$$\text{GR0(A)} = \langle \text{Dot} \rangle (A)$$

$$\text{GR+1(A)} = \langle \text{Dot} * r \rangle (A)$$

$$\text{GR+2(A)} = \langle \text{Dot} * r^*r \rangle (A)$$

Atom A	GR-2(A)	GR-1(A)	GR0(A)	GR+1(A)	GR+2(A)
C1	-1.3560993194E+02 2.2098581587E+01	-2.6687799584E+01	-1.2133511960E+01	-1.2985900498E+01	-

H2	-2.3261616181E+00	-1.9235442125E+00	-2.2639327298E+00	-3.4784132817E+00	-
	6.6666551398E+00				
H3	-2.3261623626E+00	-1.9235457284E+00	-2.2639353462E+00	-3.4784160319E+00	-
	6.6666482285E+00				
C4	-1.3573428343E+02	-2.6913674645E+01	-1.2642614249E+01	-1.4271805582E+01	-
	2.5684468162E+01				
H5	-2.2982541429E+00	-1.9038563787E+00	-2.2545421047E+00	-3.5029214314E+00	-
	6.8217245200E+00				
H6	-2.2963501168E+00	-1.8976090306E+00	-2.2343621176E+00	-3.4392968318E+00	-
	6.6170075490E+00				
H7	-2.2963490925E+00	-1.8976063194E+00	-2.2343553341E+00	-3.4392804169E+00	-
	6.6169689617E+00				
C8	-1.3573438335E+02	-2.6913878673E+01	-1.2642988912E+01	-1.4272445002E+01	-
	2.5685617817E+01				
H9	-2.2960573848E+00	-1.8974321892E+00	-2.2342541255E+00	-3.4393048461E+00	-
	6.6173685578E+00				
H10	-2.2979971037E+00	-1.9036937505E+00	-2.2544289394E+00	-3.5028893889E+00	-
	6.8219713708E+00				
H11	-2.2960564272E+00	-1.8974300941E+00	-2.2342489733E+00	-3.4392912171E+00	-
	6.6173321667E+00				

Atomic Electronic Spin Populations:

$N_{\alpha}(A)$ = Average number of Alpha electrons in Atom A

$N_{\beta}(A)$ = Average number of Beta electrons in Atom A

$N_{\text{total}}(A) = N_{\alpha}(A) + N_{\beta}(A)$

$N_{\text{spin}}(A) = N_{\alpha}(A) - N_{\beta}(A)$

Atom A	$N_{\alpha}(A)$	$N_{\beta}(A)$	$N_{\text{total}}(A)$	$N_{\text{spin}}(A)$

C1	2.9190444103E+00	2.9190444103E+00	5.8380888206E+00	0.0000000000E+00
H2	5.3138199738E-01	5.3138199738E-01	1.0627639948E+00	0.0000000000E+00
H3	5.3138253270E-01	5.3138253270E-01	1.0627650654E+00	0.0000000000E+00
C4	2.9331354177E+00	2.9331354177E+00	5.8662708353E+00	0.0000000000E+00
H5	5.2408279701E-01	5.2408279701E-01	1.0481655940E+00	0.0000000000E+00
H6	5.2592727616E-01	5.2592727616E-01	1.0518545523E+00	0.0000000000E+00

H7	5.2592606975E-01	5.2592606975E-01	1.0518521395E+00	0.0000000000E+00
C8	2.9332257713E+00	2.9332257713E+00	5.8664515426E+00	0.0000000000E+00
H9	5.2588707982E-01	5.2588707982E-01	1.0517741596E+00	0.0000000000E+00
H10	5.2404727343E-01	5.2404727343E-01	1.0480945469E+00	0.0000000000E+00
H11	5.2588632944E-01	5.2588632944E-01	1.0517726589E+00	0.0000000000E+00

Total	1.2999926955E+01	1.2999926955E+01	2.5999853910E+01	0.0000000000E+00

2EDM Note:

For post-HF, natural orbital "wavefunctions" the Muller approximation of the two-electron density matrix (2EDM) in terms of natural orbitals of the one-electron density matrix (1EDM) is used to calculate 2EDM-dependent properties (i.e., Vee contributions and electronic localization and delocalization properties). For HF single-determinant wavefunctions the expression used for the 2EDM is exact.

DFT Note:

VeeX represents the exchange-correlation functional for the wavefunction's underlying model. For Hartree-Fock wavefunctions, VeeX is the two-electron Hartree-Fock exchange functional. For wavefunctions of supported DFT models (currently LSDA and B3LYP), VeeX is the actual exchange-correlation functional of the corresponding DFT model and atomic contributions VeeX(A) to VeeX are explicitly calculated and unambiguous. However, since VeeX is at least partly just a one-electron functional for DFT models, the partitioning of VeeX(A) into interatomic (VeeX(A,B) and VeeX(A,A')) and intraatomic (VeeX(A,A)) contributions is ambiguous. Currently, interatomic contributions VeeX(A,B) and VeeX(A,A') are calculated using the Hartree-Fock exchange functional while the intratomic contribution VeeX(A,A) is calculated as VeeX(A) - VeeX(A,A'). For wavefunctions of non-supported DFT models, VeeX is (incorrectly) assumed

to be the Hartree-Fock exchange functional and the atomic energies $E_{\text{IQA}}(A)$ will not be correct and will not sum to the correct molecular energy.

Total time for AIMSum = 0 sec (NProc = 1)