

Cooperativity effects of H-bonding and charge transfer in an L-nitroarginine crystal with $Z' > 1$

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Experimental

X-ray diffraction data for the single crystals of L-nitroarginine were collected using a Bruker SMART APEX2 CCD diffractometer. The obtained images were integrated.¹ The precise unit cell dimensions and errors were determined. The absorption correction was applied semiempirically using the SADABS program.² Crystals of L-nitroarginine ($C_6H_{13}N_5O_4$, $M = 219.21$) are triclinic, space group $P1$, at 100(2) K: $a = 5.08470(10)$, $b = 7.39400(10)$, $c = 12.1779(2)$ Å, $\alpha = 81.4901(8)^\circ$, $\beta = 88.4779(8)^\circ$, $\gamma = 83.0205(9)^\circ$, $V = 449.430(13)$ Å³, $Z = 2$, $d_{\text{calc}} = 1.620$ g cm⁻³, $\mu(\text{MoK}\alpha) = 1.36$ cm⁻¹, $F(000) = 232$. Intensities of 50180 reflections were measured and 10264 independent reflections ($R_{\text{int}} = 0.0362$) were used in a further refinement. Initially, spherical atom refinements were undertaken with SHELXTL PLUS 5.0³ using the full-matrix least-squares method. All non-hydrogen atoms were allowed to have an anisotropic thermal motion. The refinement converged to $wR_2 = 0.0577$ and GOF = 1.001 for all independent reflections [$R_1 = 0.0278$ was calculated against F for 9633 observed reflections with $I > 2\sigma(I)$].

The experimental charge density in the crystal was obtained by the multipole refinement based on the Hansen-Coppens formalism⁴ using the XD program package.⁵ Before the refinement, the C–H bond distances were fixed to the ideal value of 1.08 Å to cope with the well-known shortening of the C–H bond length in X-ray diffraction experiments.⁶ N–H bond distances were fixed to those obtained from neutron diffraction experiments on analogous systems (data taken from the Cambridge Structural Database⁷). The refinement was carried out with electroneutrality constraints. The multipole expansion was truncated to hexadecapole for hydrogen atoms involved into H-bonds and octopole for all other atoms. The multipole occupancies of all atoms were refined without any local symmetry constraints. The refinement was carried out against F and converged to $R = 0.0211$, $wR = 0.0196$ and GOF = 0.8574 for 10483 merged reflections with $I > 3\sigma(I)$. All bonded pairs of atoms satisfy the Hirshfeld rigid-bond criteria.⁸ The average value of difference of the mean square displacement amplitudes along the bond was 1.8×10^{-4} Å². The residual electron density was no more than 0.2 eÅ⁻³. The κ and κ' values, as well as the multipole populations, are summarized below. The final residual Fourier maps for L-nitroarginine were flat and featureless. Analysis of deformation electron density and topology of the $\rho(r)$ function was carried out using the WINXPRO program package.⁹

References

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Table S1 Bond lengths in nitroguanidine fragment in **A** and **B** molecules.

Bond	Length, Å	
	A	B
O(3)-N(4)	1.2666(6)	1.2459(7)
N(4)-N(3)	1.3225(6)	1.3336(7)
N(3)-C(6)	1.3807(7)	1.3787(7)
C(6)-N(5)	1.3300(7)	1.3256(7)

Table S2 Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
O(1A)	6.110	1.000	0.000	0.977	-0.11000
O(2A)	6.101	1.000	0.000	0.977	-0.10060
O(3A)	6.127	0.999	0.000	0.971	-0.12730
O(4A)	6.073	1.001	0.000	1.002	-0.07270
O(1B)	6.053	1.000	0.000	0.977	-0.05280
O(2B)	6.048	1.000	0.000	0.977	-0.04780
O(3B)	6.095	0.999	0.000	0.971	-0.09500
O(4B)	6.018	1.001	0.000	1.002	-0.01800
N(1A)	5.035	1.004	0.000	0.962	-0.03460
N(2A)	5.080	1.002	0.000	0.950	-0.07970
N(3A)	5.069	1.000	0.000	0.986	-0.06920
N(4A)	5.023	0.998	0.000	0.916	-0.02330
N(5A)	5.157	1.003	0.000	0.967	-0.15700
N(1B)	5.056	1.004	0.000	0.962	-0.05610
N(2B)	5.046	1.002	0.000	0.950	-0.04610
N(3B)	5.062	1.000	0.000	0.986	-0.06230
N(4B)	5.027	0.998	0.000	0.916	-0.02750
N(5B)	5.032	1.003	0.000	0.967	-0.03170
C(1A)	4.214	0.999	0.000	0.938	-0.21420
C(2A)	4.124	1.006	0.000	0.971	-0.12390
C(3A)	4.106	1.007	0.000	0.953	-0.10550
C(4A)	4.088	1.007	0.000	0.953	-0.08830
C(5A)	4.086	1.006	0.000	0.980	-0.08580
C(6A)	4.142	1.004	0.000	0.975	-0.14190
C(1B)	4.137	0.999	0.000	0.938	-0.13690
C(2B)	4.218	1.006	0.000	0.971	-0.21750
C(3B)	4.127	1.007	0.000	0.953	-0.12710
C(4B)	4.121	1.007	0.000	0.953	-0.12140
C(5B)	4.108	1.006	0.000	0.980	-0.10830
C(6B)	4.153	1.004	0.000	0.975	-0.15320
H(1NC)	0.844	1.200	0.000	1.200	+0.15610
H(1NB)	0.858	1.200	0.000	1.200	+0.14230
H(1NA)	0.881	1.200	0.000	1.200	+0.11860
H(2NA)	0.858	1.200	0.000	1.200	+0.14220
H(5NB)	0.804	1.200	0.000	1.200	+0.19570
H(5NA)	0.942	1.200	0.000	1.200	+0.05820
H(1NE)	0.929	1.200	0.000	1.200	+0.07140
H(1ND)	0.907	1.200	0.000	1.200	+0.09340
H(1NF)	0.906	1.200	0.000	1.200	+0.09380
H(2ND)	0.860	1.200	0.000	1.200	+0.14050
H(5NE)	0.825	1.200	0.000	1.200	+0.17490
H(5ND)	0.926	1.200	0.000	1.200	+0.07390
H(2A)	0.941	1.200	0.000	1.200	+0.05940
H(2D)	0.896	1.200	0.000	1.200	+0.10430
H(3B)	0.943	1.200	0.000	1.200	+0.05720
H(3A)	0.867	1.200	0.000	1.200	+0.13310
H(3E)	0.888	1.200	0.000	1.200	+0.11230
H(3D)	0.891	1.200	0.000	1.200	+0.10920
H(4B)	0.868	1.200	0.000	1.200	+0.13200
H(4A)	0.861	1.200	0.000	1.200	+0.13900
H(4E)	0.927	1.200	0.000	1.200	+0.07310
H(4D)	0.935	1.200	0.000	1.200	+0.06540
H(5B)	0.873	1.200	0.000	1.200	+0.12750
H(5A)	0.898	1.200	0.000	1.200	+0.10150
H(5E)	0.946	1.200	0.000	1.200	+0.05400
H(5D)	0.894	1.200	0.000	1.200	+0.10640

Table S3 Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
O(1A)	-0.024(15)	-0.063(14)	-0.014(15)	0.977
O(2A)	-0.046(15)	-0.094(14)	-0.095(15)	0.977
O(3A)	0.006(16)	0.018(15)	-0.207(15)	0.971
O(4A)	-0.017(14)	0.051(14)	-0.073(15)	1.002
O(1B)	-0.061(15)	0.001(14)	-0.146(15)	0.977
O(2B)	0.030(15)	0.078(15)	-0.076(16)	0.977
O(3B)	0.029(17)	0.034(16)	0.013(17)	0.971
O(4B)	0.020(17)	-0.078(15)	-0.145(15)	1.002
N(1A)	0.008(18)	-0.009(18)	0.082(18)	0.962
N(2A)	0.030(18)	-0.001(19)	-0.063(19)	0.950
N(3A)	0.028(17)	-0.049(17)	-0.107(17)	0.986
N(4A)	0.033(19)	0.075(18)	-0.042(18)	0.916
N(5A)	0.025(18)	0.106(18)	0.036(18)	0.967
N(1B)	0.044(18)	-0.068(17)	0.070(18)	0.962
N(2B)	-0.022(18)	-0.073(19)	0.073(18)	0.950
N(3B)	-0.017(17)	-0.197(17)	-0.215(18)	0.986
N(4B)	0.008(20)	-0.032(19)	-0.083(19)	0.916
N(5B)	0.045(18)	-0.026(18)	-0.013(18)	0.967
C(1A)	0.058(23)	-0.017(23)	-0.015(21)	0.938
C(2A)	-0.075(22)	-0.053(22)	0.041(22)	0.971
C(3A)	0.032(24)	0.016(23)	0.192(22)	0.953
C(4A)	-0.022(23)	-0.056(24)	-0.036(22)	0.953
C(5A)	0.050(22)	0.071(22)	0.100(22)	0.980
C(6A)	-0.012(22)	0.068(22)	-0.008(21)	0.975
C(1B)	0.071(23)	0.106(22)	0.106(21)	0.938
C(2B)	0.110(22)	-0.084(22)	-0.001(23)	0.971
C(3B)	0.021(24)	-0.025(23)	-0.006(23)	0.953
C(4B)	0.028(23)	0.126(23)	-0.002(23)	0.953
C(5B)	0.102(22)	0.032(21)	-0.110(22)	0.980
C(6B)	-0.021(22)	0.073(22)	-0.033(22)	0.975
H(1NC)	0.000	0.000	0.147(18)	1.200
H(1NB)	0.000	0.000	0.084(20)	1.200
H(1NA)	0.000	0.000	0.120(18)	1.200
H(2NA)	0.000	0.000	0.201(19)	1.200
H(5NB)	0.000	0.000	0.227(20)	1.200
H(5NA)	0.000	0.000	0.212(20)	1.200
H(1NE)	0.000	0.000	0.226(20)	1.200
H(1ND)	0.000	0.000	0.155(21)	1.200
H(1NF)	0.000	0.000	0.140(21)	1.200
H(2ND)	0.000	0.000	0.203(20)	1.200
H(5NE)	0.000	0.000	0.237(21)	1.200
H(5ND)	0.000	0.000	0.275(22)	1.200
H(2A)	0.000	0.000	0.150(19)	1.200
H(2D)	0.000	0.000	0.117(19)	1.200
H(3B)	0.000	0.000	0.082(19)	1.200
H(3A)	0.000	0.000	0.145(20)	1.200
H(3E)	0.000	0.000	0.076(18)	1.200
H(3D)	0.000	0.000	0.139(19)	1.200
H(4B)	0.000	0.000	0.131(19)	1.200
H(4A)	0.000	0.000	0.125(19)	1.200
H(4E)	0.000	0.000	0.122(19)	1.200
H(4D)	0.000	0.000	0.184(20)	1.200
H(5B)	0.000	0.000	0.113(18)	1.200
H(5A)	0.000	0.000	0.095(21)	1.200
H(5E)	0.000	0.000	0.162(20)	1.200
H(5D)	0.000	0.000	0.161(20)	1.200

Table S4 Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
O(1A)	-0.013(11)	0.040(10)	0.014(10)	-0.101(10)	0.010(10)	0.977
O(2A)	-0.046(10)	-0.015(10)	-0.025(10)	-0.053(10)	0.057(10)	0.977
O(3A)	-0.140(11)	-0.005(11)	0.004(10)	-0.052(11)	0.004(11)	0.971
O(4A)	-0.140(11)	0.008(11)	0.019(9)	-0.073(10)	-0.007(10)	1.002
O(1B)	-0.051(10)	0.000(10)	-0.038(10)	-0.097(10)	0.013(10)	0.977
O(2B)	-0.041(10)	0.004(10)	-0.036(10)	-0.064(10)	0.025(10)	0.977
O(3B)	-0.092(12)	0.022(13)	0.006(11)	-0.048(12)	-0.040(13)	0.971
O(4B)	-0.133(12)	0.024(12)	-0.011(10)	-0.101(12)	-0.010(12)	1.002
N(1A)	0.012(12)	-0.017(11)	0.008(11)	-0.006(12)	-0.032(12)	0.962
N(2A)	-0.002(13)	-0.029(12)	-0.008(12)	-0.017(12)	-0.019(12)	0.950

H(5ND)	-0.019(51)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(2A)	-0.043(41)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(2D)	0.043(42)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(3B)	0.082(41)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(3A)	-0.038(45)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(3E)	0.022(40)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(3D)	-0.011(44)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(4B)	0.113(40)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(4A)	0.057(42)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(4E)	-0.016(41)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(4D)	0.041(48)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5B)	-0.094(41)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5A)	0.071(46)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5E)	-0.058(42)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5D)	0.049(42)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200

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O(1A)	C(1A)	Z	O(1A)	O(2A)	Y
O(2A)	C(1A)	Z	O(2A)	H(1NF)	Y
O(3A)	N(4A)	Z	O(3A)	H(5NB)	Y
O(4A)	N(4A)	Z	O(4A)	O(3A)	Y
O(1B)	C(1B)	Z	O(1B)	O(2B)	Y
O(2B)	C(1B)	Z	O(2B)	O(1B)	Y
O(3B)	N(4B)	Z	O(3B)	H(5NE)	Y
O(4B)	N(4B)	Z	O(4B)	O(3B)	Y
N(1A)	H(1NC)	Z	N(1A)	H(1NA)	Y
N(2A)	H(2NA)	Z	N(2A)	C(6A)	Y
N(3A)	N(4A)	Z	N(3A)	C(6A)	Y
N(4A)	O(4A)	Z	N(4A)	O(3A)	Y
N(5A)	H(5NA)	Z	N(5A)	H(5NB)	Y
N(1B)	H(1NF)	Z	N(1B)	H(1NE)	Y
N(2B)	H(2ND)	Z	N(2B)	C(6B)	Y
N(3B)	N(4B)	Z	N(3B)	C(6B)	Y
N(4B)	O(3B)	Z	N(4B)	O(4B)	Y
N(5B)	H(5ND)	Z	N(5B)	H(5NE)	Y
C(1A)	O(1A)	Z	C(1A)	O(2A)	Y
C(2A)	H(2A)	Z	C(2A)	N(1A)	Y
C(3A)	H(3B)	Z	C(3A)	H(3A)	Y
C(4A)	H(4A)	Z	C(4A)	H(4B)	Y
C(5A)	H(5B)	Z	C(5A)	H(5A)	Y
C(6A)	N(2A)	Z	C(6A)	N(5A)	Y
C(1B)	O(1B)	Z	C(1B)	O(2B)	Y
C(2B)	H(2D)	Z	C(2B)	N(1B)	Y
C(3B)	H(3D)	Z	C(3B)	H(3E)	Y
C(4B)	H(4D)	Z	C(4B)	H(4E)	Y
C(5B)	H(5E)	Z	C(5B)	H(5D)	Y
C(6B)	N(5B)	Z	C(6B)	N(2B)	Y
H(1NC)	N(1A)	Z	H(1NC)	H(1NB)	Y
H(1NB)	N(1A)	Z	H(1NB)	H(1NC)	Y
H(1NA)	N(1A)	Z	H(1NA)	H(1NB)	Y
H(2NA)	N(2A)	Z	H(2NA)	C(6A)	Y
H(5NB)	N(5A)	Z	H(5NB)	H(5NA)	Y
H(5NA)	N(5A)	Z	H(5NA)	H(5NB)	Y
H(1NE)	N(1B)	Z	H(1NE)	H(1ND)	Y
H(1ND)	N(1B)	Z	H(1ND)	H(1NF)	Y
H(1NF)	N(1B)	Z	H(1NF)	H(1ND)	Y
H(2ND)	N(2B)	Z	H(2ND)	C(6B)	Y
H(5NE)	N(5B)	Z	H(5NE)	O(3B)	Y
H(5ND)	N(5B)	Z	H(5ND)	H(5NE)	Y
H(2A)	C(2A)	Z	H(2A)	N(1A)	Y
H(2D)	C(2B)	Z	H(2D)	N(1B)	Y
H(3B)	C(3A)	Z	H(3B)	H(3A)	Y
H(3A)	C(3A)	Z	H(3A)	H(3B)	Y
H(3E)	C(3B)	Z	H(3E)	H(3D)	Y
H(3D)	C(3B)	Z	H(3D)	H(3E)	Y
H(4B)	C(4A)	Z	H(4B)	H(4A)	Y
H(4A)	C(4A)	Z	H(4A)	H(4B)	Y
H(4E)	C(4B)	Z	H(4E)	H(4D)	Y
H(4D)	C(4B)	Z	H(4D)	H(4E)	Y
H(5B)	C(5A)	Z	H(5B)	H(5A)	Y
H(5A)	C(5A)	Z	H(5A)	H(5B)	Y
H(5E)	C(5B)	Z	H(5E)	H(5D)	Y
H(5D)	C(5B)	Z	H(5D)	H(5E)	Y

Differences of Mean-Squares Displacement Amplitudes (DMSDA)
(1.E4 Å²) along interatomic vectors (*bonds)

ATOM-->	ATOM	/	DIST	DMSDA	ATOM	/	DIST	DMSDA	ATOM	/	DIST	DMSDA
O(1A)	C(1A)	*	1.2541	2								
O(2A)	C(1A)	*	1.2609	2								
O(3A)	N(4A)	*	1.2640	-1								
O(4A)	N(4A)	*	1.2512	-1								
O(1B)	C(1B)	*	1.2464	1								
O(2B)	C(1B)	*	1.2648	5								
O(3B)	N(4B)	*	1.2460	-2								
O(4B)	N(4B)	*	1.2452	1								
N(1A)	C(2A)		1.4959	-1								
N(2A)	C(5A)	*	1.4594	2	C(6A)	*	1.3263	2				
N(3A)	N(4A)	*	1.3209	0	C(6A)	*	1.3806	0				
N(5A)	C(6A)	*	1.3297	-3								
N(1B)	C(2B)		1.4935	0								
N(2B)	C(5B)	*	1.4613	5	C(6B)	*	1.3314	1				
N(3B)	N(4B)	*	1.3314	0	C(6B)	*	1.3772	0				
N(5B)	C(6B)	*	1.3259	0								
C(1A)	C(2A)	*	1.5374	2								
C(2A)	C(3A)	*	1.5327	1								
C(3A)	C(4A)		1.5410	-4								
C(4A)	C(5A)	*	1.5227	0								
C(1B)	C(2B)	*	1.5327	2								
C(2B)	C(3B)	*	1.5355	2								
C(3B)	C(4B)	*	1.5279	3								
C(4B)	C(5B)	*	1.5198	3								

data_FFT

_refine_diff_density_max 0.195
_refine_diff_density_min -0.203
_refine_diff_density_rms 0.043

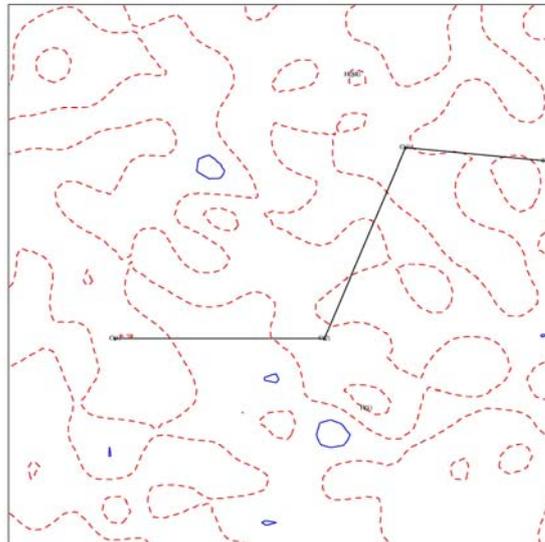


Figure S1 The residual electron density map in the area of C1 C2 C3. Contours are drawn with 0.05 eÅ⁻³ step, the negative and zero contours are dashed.

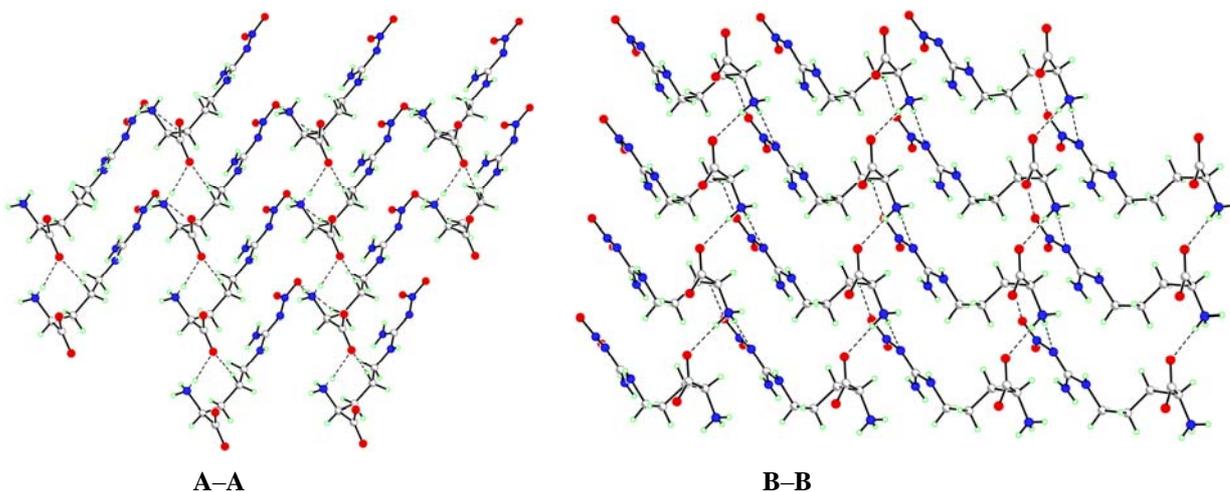


Figure S2 Corrugated **A-A** and **B-B** layers in the crystal of L-nitroarginine.

Coordinates and Uiso or Uequiv

loop_	_atom_site_label	_atom_site_fract_x	_atom_site_fract_y	_atom_site_fract_z	_atom_site_occupancy	_atom_site_symmetry_multiplicity	_atom_site_U_iso_or_equiv
O(1A)	0.361347	0.050715	0.480597	1	1	0.011	
O(2A)	0.751497	0.111833	0.402722	1	1	0.010	
O(3A)	-0.754599	0.814415	-0.080818	1	1	0.014	
O(4A)	-0.931201	0.927337	0.062423	1	1	0.012	
O(1B)	0.772267	0.594709	0.354434	1	1	0.011	
O(2B)	0.355441	0.574678	0.416969	1	1	0.010	
O(3B)	0.367507	1.263393	0.922223	1	1	0.021	
O(4B)	0.080125	1.404204	0.801912	1	1	0.020	
N(1A)	0.19964	-0.082721	0.301447	1	1	0.008	
N(2A)	-0.188089	0.551125	0.131386	1	1	0.009	
N(3A)	-0.556254	0.749959	0.089371	1	1	0.009	
N(4A)	-0.746795	0.830596	0.020896	1	1	0.009	
N(5A)	-0.311966	0.601186	-0.052575	1	1	0.012	
N(1B)	0.976945	0.352778	0.528561	1	1	0.009	
N(2B)	0.660881	0.97749	0.681641	1	1	0.010	
N(3B)	0.367262	1.192545	0.746186	1	1	0.010	
N(4B)	0.27493	1.287266	0.826755	1	1	0.011	
N(5B)	0.750752	1.05125	0.853147	1	1	0.012	
C(1A)	0.522326	0.06368	0.400799	1	1	0.007	
C(2A)	0.441999	0.015004	0.288902	1	1	0.007	
C(3A)	0.402174	0.18293	0.198131	1	1	0.009	
C(4A)	0.171252	0.329261	0.219441	1	1	0.010	
C(5A)	0.033176	0.414369	0.111337	1	1	0.009	
C(6A)	-0.351656	0.634027	0.051386	1	1	0.008	
C(1B)	0.604827	0.545078	0.425611	1	1	0.008	
C(2B)	0.703704	0.448662	0.53973	1	1	0.008	
C(3B)	0.692879	0.590595	0.620399	1	1	0.009	
C(4B)	0.89915	0.725165	0.594012	1	1	0.009	
C(5B)	0.907358	0.853538	0.68015	1	1	0.010	
C(6B)	0.596232	1.072693	0.765036	1	1	0.008	
H(1NC)	0.1469	-0.10566	0.22694	1	1	0.013	
H(1NB)	0.24022	-0.20893	0.34268	1	1	0.017	
H(1NA)	0.05883	-0.00993	0.34028	1	1	0.015	
H(2NA)	-0.22291	0.57982	0.20825	1	1	0.017	
H(5NB)	-0.4581	0.6638	-0.10951	1	1	0.016	
H(5NA)	-0.15213	0.51758	-0.07201	1	1	0.022	
H(1NE)	1.07418	0.30923	0.59973	1	1	0.021	
H(1ND)	1.10004	0.42938	0.48001	1	1	0.022	
H(1NF)	0.95716	0.24855	0.48771	1	1	0.029	
H(2ND)	0.5513	1.01326	0.61341	1	1	0.021	
H(5NE)	0.67566	1.11788	0.91945	1	1	0.024	
H(5ND)	0.91439	0.95977	0.85649	1	1	0.029	
H(2A)	0.60145	-0.08295	0.26485	1	1	0.011	

H(2D)	0.58153	0.34383	0.56821	1	1	0.015
H(3B)	0.37351	0.13502	0.12038	1	1	0.014
H(3A)	0.58389	0.24978	0.18816	1	1	0.022
H(3E)	0.72113	0.51804	0.70326	1	1	0.012
H(3D)	0.5005	0.66889	0.61322	1	1	0.015
H(4B)	0.02804	0.26752	0.27331	1	1	0.011
H(4A)	0.24654	0.43472	0.25953	1	1	0.017
H(4E)	0.86825	0.80274	0.51156	1	1	0.014
H(4D)	1.0947	0.64734	0.59352	1	1	0.024
H(5B)	0.1787	0.47737	0.05489	1	1	0.013
H(5A)	-0.04637	0.3118	0.07325	1	1	0.025
H(5E)	0.93383	0.77932	0.76259	1	1	0.017
H(5D)	1.07677	0.93125	0.6596	1	1	0.018

Uij values	U11	U22	U33	U12	U13	U23
O(1A)	0.008412	0.017262	0.007387	-0.001544	0.000539	-0.003263
O(2A)	0.007858	0.012757	0.011004	-0.002562	-0.000739	-0.003813
O(3A)	0.012712	0.018341	0.009039	0.003992	-0.003781	-0.003763
O(4A)	0.009997	0.013578	0.011673	0.003186	-0.001911	-0.003635
O(1B)	0.009493	0.015369	0.007237	-0.000454	0.000633	0.000047
O(2B)	0.007237	0.011359	0.011763	-0.000244	-0.001808	0.000352
O(3B)	0.023354	0.028298	0.010497	0.011573	-0.002732	-0.009325
O(4B)	0.020753	0.020154	0.017128	0.01259	-0.000803	-0.004431
N(1A)	0.008378	0.008484	0.008153	-0.000954	-0.000878	-0.001566
N(2A)	0.009735	0.009815	0.007291	0.002227	-0.001251	-0.001159
N(3A)	0.008868	0.01073	0.007862	0.001972	-0.001656	-0.00207
N(4A)	0.008002	0.009584	0.008405	0.000645	-0.00179	-0.001884
N(5A)	0.01205	0.01465	0.007778	0.003444	-0.00113	-0.002722
N(1B)	0.008902	0.008434	0.009157	0.000875	-0.000776	-0.001216
N(2B)	0.010002	0.011492	0.008201	0.002661	-0.00188	-0.004018
N(3B)	0.009914	0.010592	0.008101	0.002694	-0.000857	-0.00228
N(4B)	0.011628	0.01092	0.009224	0.002835	0.000641	-0.002547
N(5B)	0.012091	0.013906	0.009536	0.003227	-0.003803	-0.004868
C(1A)	0.006623	0.008627	0.00687	-0.000136	-0.000729	-0.001666
C(2A)	0.007088	0.007825	0.006662	0.000139	-0.000603	-0.001246
C(3A)	0.009069	0.009155	0.007616	0.000343	0.000338	-0.00007
C(4A)	0.010911	0.009276	0.007945	0.001913	-0.000906	-0.001176
C(5A)	0.008961	0.008713	0.00785	0.000846	-0.000528	-0.001066
C(6A)	0.008623	0.008338	0.007009	0.000618	-0.000836	-0.001182
C(1B)	0.007542	0.008227	0.006927	-0.000348	-0.000679	-0.001366
C(2B)	0.007736	0.008071	0.007229	-0.000593	-0.00051	-0.001022
C(3B)	0.008107	0.011637	0.008042	-0.001056	0.000526	-0.003156
C(4B)	0.008973	0.009973	0.009736	-0.000509	0.000883	-0.003993
C(5B)	0.008848	0.010233	0.011194	0.000674	-0.001165	-0.004468
C(6B)	0.00852	0.00849	0.00699	0.000873	-0.00087	-0.002083

Bond lengths

O(1A)	C(1A)	1.2541
O(2A)	C(1A)	1.2609
O(3A)	N(4A)	1.2640
O(4A)	N(4A)	1.2511
O(1B)	C(1B)	1.2463
O(2B)	C(1B)	1.2648
O(3B)	N(4B)	1.2460
O(4B)	N(4B)	1.2452
N(1A)	H(1NC)	0.9967
N(1A)	H(1NB)	0.9927
N(1A)	H(1NA)	0.9947
N(2A)	C(5A)	1.4593
N(2A)	C(6A)	1.3262
N(2A)	H(2NA)	0.9966
N(3A)	N(4A)	1.3209
N(3A)	C(6A)	1.3806
N(5A)	C(6A)	1.3296
N(5A)	H(5NB)	1.0468
N(5A)	H(5NA)	1.0048
N(1B)	H(1NE)	1.0003
N(1B)	H(1ND)	1.0146
N(1B)	H(1NF)	0.9932
N(2B)	C(5B)	1.4613
N(2B)	C(6B)	1.3313
N(2B)	H(2ND)	0.9972
N(3B)	N(4B)	1.3313
N(3B)	C(6B)	1.3772
N(5B)	C(6B)	1.3258
N(5B)	H(5NE)	1.0469
N(5B)	H(5ND)	1.0041
C(1A)	C(2A)	1.5374
C(2A)	C(3A)	1.5326

C(2A)	H(2A)	1.0840
C(3A)	H(3B)	1.0781
C(3A)	H(3A)	1.0954
C(4A)	C(5A)	1.5226
C(4A)	H(4B)	1.0657
C(4A)	H(4A)	1.0899
C(5A)	H(5B)	1.0950
C(5A)	H(5A)	1.0688
C(1B)	C(2B)	1.5326
C(2B)	C(3B)	1.5354
C(2B)	H(2D)	1.0644
C(3B)	C(4B)	1.5278
C(3B)	H(3E)	1.0749
C(3B)	H(3D)	1.0731
C(4B)	C(5B)	1.5197
C(4B)	H(4E)	1.0853
C(4B)	H(4D)	1.0869
C(5B)	H(5E)	1.0739
C(5B)	H(5D)	1.0959

Bond angles

H(1NC)	N(1A)	H(1NB)	102.98
H(1NC)	N(1A)	H(1NA)	113.88
H(1NB)	N(1A)	H(1NA)	110.76
C(5A)	N(2A)	C(6A)	122.21
C(5A)	N(2A)	H(2NA)	119.22
C(6A)	N(2A)	H(2NA)	118.51
N(4A)	N(3A)	C(6A)	119.68
O(3A)	N(4A)	O(4A)	119.31
O(3A)	N(4A)	N(3A)	124.65
O(4A)	N(4A)	N(3A)	116.02
C(6A)	N(5A)	H(5NB)	115.90
C(6A)	N(5A)	H(5NA)	120.11
H(5NB)	N(5A)	H(5NA)	123.95
H(1NE)	N(1B)	H(1ND)	105.33
H(1NE)	N(1B)	H(1NF)	111.18
H(1ND)	N(1B)	H(1NF)	104.47
C(5B)	N(2B)	C(6B)	122.22
C(5B)	N(2B)	H(2ND)	120.45
C(6B)	N(2B)	H(2ND)	116.25
N(4B)	N(3B)	C(6B)	118.31
O(3B)	N(4B)	O(4B)	120.07
O(3B)	N(4B)	N(3B)	124.46
O(4B)	N(4B)	N(3B)	115.44
C(6B)	N(5B)	H(5NE)	115.97
C(6B)	N(5B)	H(5ND)	118.74
H(5NE)	N(5B)	H(5ND)	124.62
O(1A)	C(1A)	O(2A)	126.19
O(1A)	C(1A)	C(2A)	118.77
O(2A)	C(1A)	C(2A)	115.02
C(1A)	C(2A)	C(3A)	112.90
C(1A)	C(2A)	H(2A)	106.18
C(3A)	C(2A)	H(2A)	109.59
C(2A)	C(3A)	H(3B)	108.20
C(2A)	C(3A)	H(3A)	109.42
H(3B)	C(3A)	H(3A)	106.17
C(5A)	C(4A)	H(4B)	107.69
C(5A)	C(4A)	H(4A)	110.71
H(4B)	C(4A)	H(4A)	108.30
N(2A)	C(5A)	C(4A)	110.90
N(2A)	C(5A)	H(5B)	110.61
N(2A)	C(5A)	H(5A)	107.02
C(4A)	C(5A)	H(5B)	108.44
C(4A)	C(5A)	H(5A)	110.81
H(5B)	C(5A)	H(5A)	109.01
N(2A)	C(6A)	N(3A)	112.84
N(2A)	C(6A)	N(5A)	120.65
N(3A)	C(6A)	N(5A)	126.49
O(1B)	C(1B)	O(2B)	127.01
O(1B)	C(1B)	C(2B)	118.20
O(2B)	C(1B)	C(2B)	114.65
C(1B)	C(2B)	C(3B)	109.39
C(1B)	C(2B)	H(2D)	108.37
C(3B)	C(2B)	H(2D)	111.09
C(2B)	C(3B)	C(4B)	113.10
C(2B)	C(3B)	H(3E)	108.48
C(2B)	C(3B)	H(3D)	107.37
C(4B)	C(3B)	H(3E)	109.84
C(4B)	C(3B)	H(3D)	107.78

H(3E)	C(3B)	H(3D)	110.21
C(3B)	C(4B)	C(5B)	113.21
C(3B)	C(4B)	H(4E)	110.50
C(3B)	C(4B)	H(4D)	108.86
C(5B)	C(4B)	H(4E)	110.88
C(5B)	C(4B)	H(4D)	106.22
H(4E)	C(4B)	H(4D)	106.82
N(2B)	C(5B)	C(4B)	111.29
N(2B)	C(5B)	H(5E)	106.79
N(2B)	C(5B)	H(5D)	110.95
C(4B)	C(5B)	H(5E)	111.99
C(4B)	C(5B)	H(5D)	107.42
H(5E)	C(5B)	H(5D)	108.36
N(2B)	C(6B)	N(3B)	113.06
N(2B)	C(6B)	N(5B)	120.39
N(3B)	C(6B)	N(5B)	126.50

==== INTEGRATED PROPERTY WITHIN ATOMIC BASIN ====

num	atom	nTheta	nPhi	RHO	CPU time (sec)
1	O(1A)	48	64	8.884784	1147.58
2	O(2A)	48	64	8.769823	1145.05
3	O(3A)	48	64	8.256421	1080.72
4	O(4A)	48	64	8.273031	1183.92
5	O(1B)	48	64	8.742317	1226.16
6	O(2B)	48	64	8.728776	1164.62
7	O(3B)	48	64	8.331635	1190.31
8	O(4B)	48	64	8.197630	1249.97
9	N(1A)	48	64	7.955899	1204.94
10	N(2A)	48	64	8.030193	1144.19
11	N(3A)	48	64	7.431194	1182.81
12	N(4A)	48	64	6.565368	1107.17
13	N(5A)	48	64	8.144688	1160.30
14	N(1B)	48	64	8.141068	1260.31
15	N(2B)	48	64	7.963539	1266.52
16	N(3B)	48	64	7.358539	1244.92
17	N(4B)	48	64	6.531746	1178.06
18	N(5B)	48	64	8.128194	1131.17
19	C(1A)	48	64	4.693256	1116.33
20	C(2A)	48	64	5.930924	1258.22
21	C(3A)	48	64	5.959822	1164.88
22	C(4A)	48	64	6.134255	1134.83
23	C(5A)	48	64	5.758685	1139.77
24	C(6A)	48	64	5.009822	1076.41
25	C(1B)	48	64	4.585177	1207.64
26	C(2B)	48	64	5.995978	1200.27
27	C(3B)	48	64	5.997486	1066.11
28	C(4B)	48	64	6.128838	1170.53
29	C(5B)	48	64	5.949305	1253.81
30	C(6B)	48	64	5.012505	1064.48
31	H(1NC)	48	64	0.579687	964.89
32	H(1NB)	48	64	0.665985	1017.84
33	H(1NA)	48	64	0.654582	985.33
34	H(2NA)	48	64	0.611545	954.58
35	H(5NB)	48	64	0.523111	956.03
36	H(5NA)	48	64	0.665691	939.03
37	H(1NE)	48	64	0.619237	956.84
38	H(1ND)	48	64	0.665808	1048.17
39	H(1NF)	48	64	0.636900	986.75
40	H(2ND)	48	64	0.564781	979.78
41	H(5NE)	48	64	0.555571	994.17
42	H(5ND)	48	64	0.633214	970.14
43	H(2A)	48	64	0.946610	1104.42
44	H(2D)	48	64	1.049544	1051.42
45	H(3B)	48	64	0.964734	1070.80
46	H(3A)	48	64	0.874748	1101.41
47	H(3E)	48	64	0.921597	981.12
48	H(3D)	48	64	0.886018	989.38
49	H(4B)	48	64	0.854270	1035.52
50	H(4A)	48	64	0.821246	992.48
51	H(4E)	48	64	0.934066	1001.77
52	H(4D)	48	64	0.998730	1076.17
53	H(5B)	48	64	0.863955	1068.20
54	H(5A)	48	64	1.058453	1121.92
55	H(5E)	48	64	0.928384	1060.50
56	H(5D)	48	64	0.870542	1105.70

num	atom	nTheta	nPhi	VOLUME	CPU time (sec)
1	O(1A)	48	64	15.362741	1.11
2	O(2A)	48	64	14.317536	1.20
3	O(3A)	48	64	14.162779	1.28
4	O(4A)	48	64	15.621755	1.33
5	O(1B)	48	64	14.776104	1.41
6	O(2B)	48	64	13.359752	1.41
7	O(3B)	48	64	14.840831	1.45
8	O(4B)	48	64	15.570889	1.39
9	N(1A)	48	64	13.910970	1.36
10	N(2A)	48	64	13.237642	1.31
11	N(3A)	48	64	13.767548	1.44
12	N(4A)	48	64	6.808079	1.34
13	N(5A)	48	64	15.168689	1.47
14	N(1B)	48	64	12.784090	1.50
15	N(2B)	48	64	13.260024	1.47
16	N(3B)	48	64	13.183619	1.56
17	N(4B)	48	64	7.118390	1.48
18	N(5B)	48	64	14.945992	1.61
19	C(1A)	48	64	5.623672	1.55
20	C(2A)	48	64	7.027929	1.56
21	C(3A)	48	64	8.752673	1.59
22	C(4A)	48	64	9.181413	1.67
23	C(5A)	48	64	7.199319	1.69
24	C(6A)	48	64	6.199084	1.59
25	C(1B)	48	64	5.071452	1.67
26	C(2B)	48	64	6.871939	1.70
27	C(3B)	48	64	9.045311	1.73
28	C(4B)	48	64	8.525482	1.75
29	C(5B)	48	64	8.782042	1.80
30	C(6B)	48	64	6.231764	1.77
31	H(1NC)	48	64	2.953375	1.58
32	H(1NB)	48	64	3.044198	1.67
33	H(1NA)	48	64	2.928138	1.69
34	H(2NA)	48	64	2.860457	1.61
35	H(5NB)	48	64	3.480183	1.72
36	H(5NA)	48	64	3.170153	1.80
37	H(1NE)	48	64	3.089486	1.73
38	H(1ND)	48	64	2.685290	1.80
39	H(1NF)	48	64	2.853688	1.83
40	H(2ND)	48	64	2.298687	1.75
41	H(5NE)	48	64	3.323672	1.84
42	H(5ND)	48	64	2.634092	1.88
43	H(2A)	48	64	5.809613	2.02
44	H(2D)	48	64	5.710038	1.97
45	H(3B)	48	64	5.732999	1.91
46	H(3A)	48	64	5.710218	2.08
47	H(3E)	48	64	5.987736	2.00
48	H(3D)	48	64	6.098348	2.02
49	H(4B)	48	64	4.792710	2.05
50	H(4A)	48	64	5.370317	2.16
51	H(4E)	48	64	5.170549	2.08
52	H(4D)	48	64	5.440189	2.22
53	H(5B)	48	64	4.932377	2.16
54	H(5A)	48	64	7.409855	2.20
55	H(5E)	48	64	5.125007	2.14
56	H(5D)	48	64	6.102789	2.31

==== INTEGRATED PROPERTY WITHIN ATOMIC BASIN ====

num	atom	nTheta	nPhi	d2RHO	CPU time (sec)
1	O(1A)	48	64	-0.007474	2301.19
2	O(2A)	48	64	0.010860	2271.78
3	O(3A)	48	64	0.007903	2115.80
4	O(4A)	48	64	-0.007746	2309.73
5	O(1B)	48	64	-0.006290	2386.09
6	O(2B)	48	64	-0.014404	2245.61
7	O(3B)	48	64	-0.006819	2320.34
8	O(4B)	48	64	-0.016939	2403.41
9	N(1A)	48	64	-0.077507	2332.67
10	N(2A)	48	64	-0.034148	2205.62

11	N(3A)	48	64	0.000681	2333.69
12	N(4A)	48	64	0.001491	2125.39
13	N(5A)	48	64	-0.010757	2238.11
14	N(1B)	48	64	-0.333170	2331.50
15	N(2B)	48	64	-0.113057	2292.42
16	N(3B)	48	64	-0.005275	2275.05
17	N(4B)	48	64	-0.014494	2236.06
18	N(5B)	48	64	-0.008879	2186.36
19	C(1A)	48	64	-0.032172	2174.05
20	C(2A)	48	64	-0.036391	2439.33
21	C(3A)	48	64	-0.070813	2254.02
22	C(4A)	48	64	-0.085480	2207.25
23	C(5A)	48	64	-0.051579	2193.16
24	C(6A)	48	64	-0.014129	2087.56
25	C(1B)	48	64	-0.026150	2344.27
26	C(2B)	48	64	-0.027140	2329.61
27	C(3B)	48	64	-0.048246	2088.36
28	C(4B)	48	64	-0.034980	2261.41
29	C(5B)	48	64	-0.022094	2432.25
30	C(6B)	48	64	0.021236	2057.70