

**A new 3D-aromatic organoboron species on the basis of CB₆ unit:
two states of carbon hypercoordination and structural isomerism
of non-classical forms**

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**Table of contents: Tables S1 and S2, Figure S5, atomic coordinates of optimized structures
8 and 11 calculated by B3LYP/6-311+G(df,2p) and wb97XD/6-311+G(df,2p) methods:**

page **S2**: Tables **S1, S2**

page **S3**: Figure **S5**

pages **S4-S5**: Structure **8a**

pages **S6-S7**: Structure **8b**

pages **S8-S9**: Structure **9**

pages **S10-S13**: Structure **11a**

pages **S14-S17**: Structure **11b**

pages **S18-S21**: Structure **11c**

pages **S22-S25**: Structure **11d**

Table S1 Energy parameters^a of the systems **8**, **9** and **11** calculated using B3LYP and wb97xD (italic) methods with 6-311+G(df,2p) basis set.

Structure	E_{tot}	ZPE	ΔE	λ	ω_l
8a , D_{6h}	-1067.379817	0.294095	1.26	0	179.1
	<i>-1067.053941</i>	<i>0.300121</i>	<i>3.04</i>	<i>0</i>	<i>179.6</i>
8b , D_{6h}	-1067.381833	0.294016	0	0	185.1
	<i>-1067.058787</i>	<i>0.299387</i>	<i>0</i>	<i>0</i>	<i>168.7</i>
9 , C_{6v}	-1067.332951	0.290588	30.67	1	<i>i</i> 942.5
	<i>-1067.013577</i>	<i>0.295923</i>	<i>28.37</i>	<i>1</i>	<i>I</i> 801.4
11a , D_{3h}	-3195.026252	0.758115	0	0	23.0
	<i>-3194.093830</i>	<i>0.774374</i>	<i>0</i>	<i>0</i>	22.5
11b , D_{3h}	-3195.001556	0.758597	15.50	0	18.9
	<i>-3194.072744</i>	<i>0.776648</i>	<i>13.23</i>	<i>0</i>	<i>11.4</i>
11c , C_{2v}	-3195.018733	0.758506	4.72	0	21.1
	<i>-3194.087169</i>	<i>0.775014</i>	<i>4.18</i>	<i>0</i>	18.1
11d , C_{2v}	-3195.010263	0.758489	10.04	0	19.2
	<i>-3194.080063</i>	<i>0.775941</i>	<i>8.64</i>	<i>0</i>	16.1

^a E_{tot} (a.u.) – total energy; ZPE (a.u.) – harmonic zero-point energy correction; ΔE (kcal·mol⁻¹) – relative energy; λ – number of negative hessian eigenvalues; ω_l (cm⁻¹) – value of the lowest harmonic vibration frequencies.

Table S2 AIM parameters (a.u.)^a for the bond critical point (BCP) corresponding to the C-B bonding in systems **8a** and **8b** calculated using B3LYP and wb97xD (italic) methods with 6-311+G(df,2p) basis set.

Structure	$\rho(r)$	$\nabla^2\rho(r)$	$V_b(r)$	$G_b(r)$	$H_b(r)$	$-G(r)/V(r)$
1a	0.144	-0.071	-0.148	0.065	-0.083	0.439
	<i>0.145</i>	<i>-0.073</i>	<i>-0.149</i>	<i>0.065</i>	<i>-0.084</i>	<i>0.436</i>
1b	0.124	-0.037	-0.113	0.052	-0.061	0.460
	<i>0.126</i>	<i>-0.045</i>	<i>-0.119</i>	<i>0.053</i>	<i>-0.064</i>	<i>0.445</i>

^a $\rho(r)$ - electron density; $\nabla^2\rho(r)$ - Laplacian of the electron density; $V_b(r)$ - potential electron energy density; $G_b(r)$ - kinetic electron energy density; $H_b(r)$ - total electron energy density.

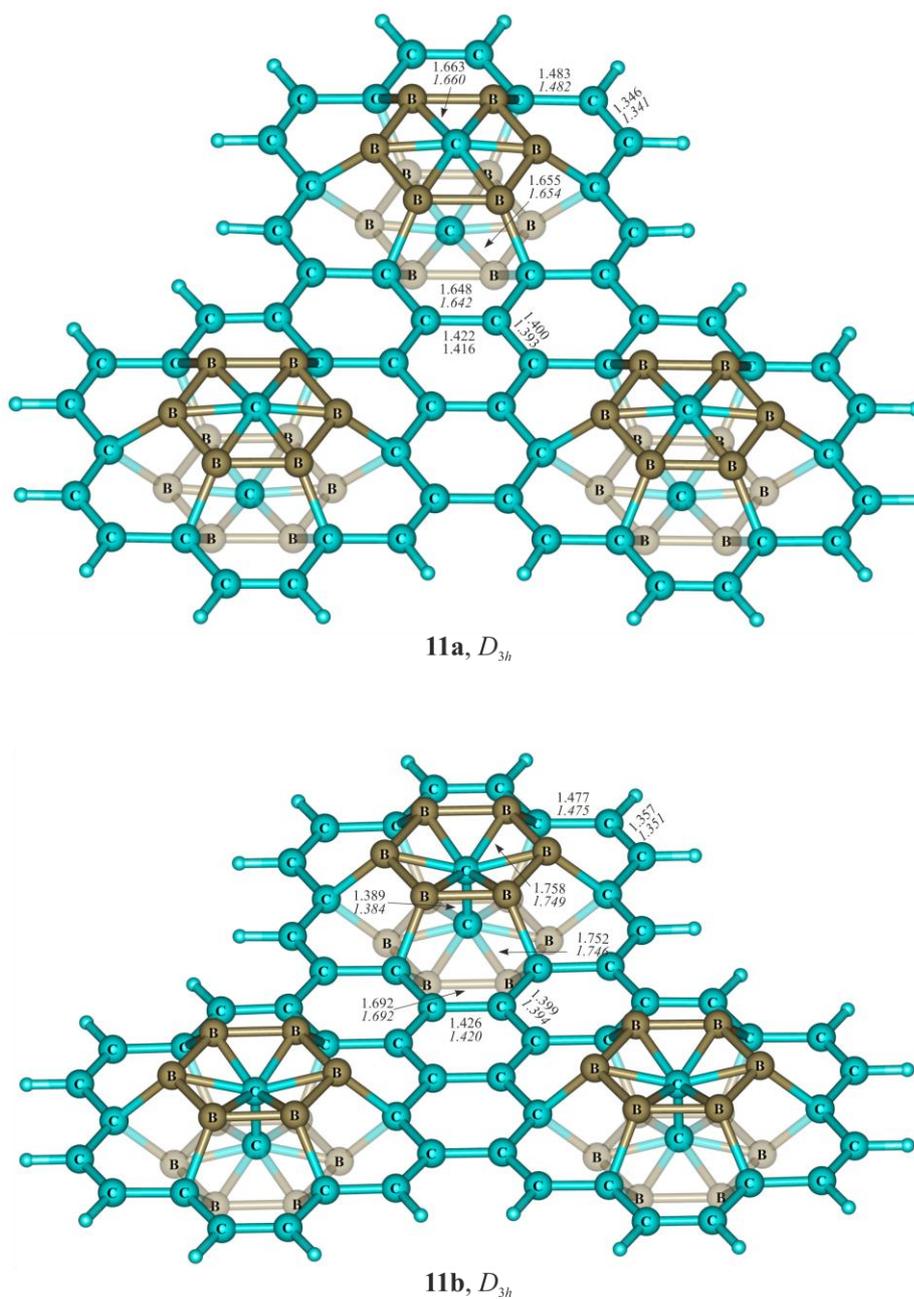


Figure S5 Geometric characteristics (bond lengths are in angstroms) of the systems **11a** and **11b** calculated using B3LYP and wb97XD (values in italic) methods with 6-311+G(df,2p) basis set.

8a [B3LYP/6-311+G(df,2p)]*D*_{6h}

C	0.00000000	0.00000000	1.24198700
C	0.00000000	0.00000000	-1.24198700
B	0.00000000	1.64440600	-1.11515800
B	1.42409800	0.82220300	-1.11515800
B	1.42409800	-0.82220300	-1.11515800
B	0.00000000	-1.64440600	-1.11515800
B	-1.42409800	-0.82220300	-1.11515800
B	-1.42409800	0.82220300	-1.11515800
B	0.00000000	1.64440600	1.11515800
B	1.42409800	0.82220300	1.11515800
B	1.42409800	-0.82220300	1.11515800
B	0.00000000	-1.64440600	1.11515800
B	-1.42409800	-0.82220300	1.11515800
B	-1.42409800	0.82220300	1.11515800
C	0.00000000	2.87129300	0.00000000
C	2.48661300	1.43564700	0.00000000
C	2.48661300	-1.43564700	0.00000000
C	0.00000000	-2.87129300	0.00000000
C	-2.48661300	-1.43564700	0.00000000
C	-2.48661300	1.43564700	0.00000000
C	1.29730600	3.59519200	0.00000000
H	1.28432400	4.67904500	0.00000000
C	2.46487400	2.92109600	0.00000000
H	3.41001000	3.45178000	0.00000000
C	-1.29730600	3.59519200	0.00000000
H	-1.28432400	4.67904500	0.00000000
C	-2.46487400	2.92109600	0.00000000
H	-3.41001000	3.45178000	0.00000000
C	-3.76218100	0.67409600	0.00000000
H	-4.69433400	1.22726500	0.00000000
C	-3.76218100	-0.67409600	0.00000000
H	-4.69433400	-1.22726500	0.00000000
C	-2.46487400	-2.92109600	0.00000000
H	-3.41001000	-3.45178000	0.00000000
C	-1.29730600	-3.59519200	0.00000000
H	-1.28432400	-4.67904500	0.00000000
C	1.29730600	-3.59519200	0.00000000
H	1.28432400	-4.67904500	0.00000000
C	2.46487400	-2.92109600	0.00000000
H	3.41001000	-3.45178000	0.00000000
C	3.76218100	-0.67409600	0.00000000
H	4.69433400	-1.22726500	0.00000000
C	3.76218100	0.67409600	0.00000000
H	4.69433400	1.22726500	0.00000000

8a [wb97XD/6-311+G(df,2p)]

 D_{6h}

C	0.00000000	0.00000000	1.246874000
C	0.00000000	0.00000000	-1.246874000
B	0.00000000	1.639353000	-1.079079000
B	1.419721000	0.819677000	-1.079079000
B	1.419721000	-0.819677000	-1.079079000
B	0.00000000	-1.639353000	-1.079079000
B	-1.419721000	-0.819677000	-1.079079000
B	-1.419721000	0.819677000	-1.079079000
B	0.00000000	1.639353000	1.079079000
B	1.419721000	0.819677000	1.079079000
B	1.419721000	-0.819677000	1.079079000
B	0.00000000	-1.639353000	1.079079000
B	-1.419721000	-0.819677000	1.079079000
B	-1.419721000	0.819677000	1.079079000
C	0.00000000	2.873346000	0.000000000
C	2.488390000	1.436673000	0.000000000
C	2.488390000	-1.436673000	0.000000000
C	0.00000000	-2.873346000	0.000000000
C	-2.488390000	-1.436673000	0.000000000
C	-2.488390000	1.436673000	0.000000000
C	1.299281000	3.593484000	0.000000000
H	1.286259000	4.677182000	0.000000000
C	2.462408000	2.921952000	0.000000000
H	3.407429000	3.452523000	0.000000000
C	-1.299281000	3.593484000	0.000000000
H	-1.286259000	4.677182000	0.000000000
C	-2.462408000	2.921952000	0.000000000
H	-3.407429000	3.452523000	0.000000000
C	-3.761689000	0.671531000	0.000000000
H	-4.693687000	1.224658000	0.000000000
C	-3.761689000	-0.671531000	0.000000000
H	-4.693687000	-1.224658000	0.000000000
C	-2.462408000	-2.921952000	0.000000000
H	-3.407429000	-3.452523000	0.000000000
C	-1.299281000	-3.593484000	0.000000000
H	-1.286259000	-4.677182000	0.000000000
C	1.299281000	-3.593484000	0.000000000
H	1.286259000	-4.677182000	0.000000000
C	2.462408000	-2.921952000	0.000000000
H	3.407429000	-3.452523000	0.000000000
C	3.761689000	-0.671531000	0.000000000
H	4.693687000	-1.224658000	0.000000000
C	3.761689000	0.671531000	0.000000000
H	4.693687000	1.224658000	0.000000000

8b [B3LYP/6-311+G(df,2p)]*D*_{6h}

C	0.000000000	0.000000000	0.693552000
C	0.000000000	0.000000000	-0.693552000
B	0.000000000	1.689041000	-1.135070000
B	1.462752000	0.844520000	-1.135070000
B	1.462752000	-0.844520000	-1.135070000
B	0.000000000	-1.689041000	-1.135070000
B	-1.462752000	-0.844520000	-1.135070000
B	-1.462752000	0.844520000	-1.135070000
B	0.000000000	1.689041000	1.135070000
B	1.462752000	0.844520000	1.135070000
B	1.462752000	-0.844520000	1.135070000
B	0.000000000	-1.689041000	1.135070000
B	-1.462752000	-0.844520000	1.135070000
B	-1.462752000	0.844520000	1.135070000
C	0.000000000	2.910937000	0.000000000
C	2.520945000	1.455468000	0.000000000
C	2.520945000	-1.455468000	0.000000000
C	0.000000000	-2.910937000	0.000000000
C	-2.520945000	-1.455468000	0.000000000
C	-2.520945000	1.455468000	0.000000000
C	1.300541000	3.612583000	0.000000000
H	1.309190000	4.697173000	0.000000000
C	2.478318000	2.932592000	0.000000000
H	3.413276000	3.482378000	0.000000000
C	-1.300541000	3.612583000	0.000000000
H	-1.309190000	4.697173000	0.000000000
C	-2.478318000	2.932592000	0.000000000
H	-3.413276000	3.482378000	0.000000000
C	-3.778859000	0.679990000	0.000000000
H	-4.722466000	1.214795000	0.000000000
C	-3.778859000	-0.679990000	0.000000000
H	-4.722466000	-1.214795000	0.000000000
C	-2.478318000	-2.932592000	0.000000000
H	-3.413276000	-3.482378000	0.000000000
C	-1.300541000	-3.612583000	0.000000000
H	-1.309190000	-4.697173000	0.000000000
C	1.300541000	-3.612583000	0.000000000
H	1.309190000	-4.697173000	0.000000000
C	2.478318000	-2.932592000	0.000000000
H	3.413276000	-3.482378000	0.000000000
C	3.778859000	-0.679990000	0.000000000
H	4.722466000	-1.214795000	0.000000000
C	3.778859000	0.679990000	0.000000000
H	4.722466000	1.214795000	0.000000000

8b [wb97XD/6-311+G(df,2p)]

 D_{6h}

C	0.00000000	0.00000000	0.69197900
C	0.00000000	0.00000000	-0.69197900
B	0.00000000	1.68808100	-1.10560200
B	1.46192100	0.84404100	-1.10560200
B	1.46192100	-0.84404100	-1.10560200
B	0.00000000	-1.68808100	-1.10560200
B	-1.46192100	-0.84404100	-1.10560200
B	-1.46192100	0.84404100	-1.10560200
B	0.00000000	1.68808100	1.10560200
B	1.46192100	0.84404100	1.10560200
B	1.46192100	-0.84404100	1.10560200
B	0.00000000	-1.68808100	1.10560200
B	-1.46192100	-0.84404100	1.10560200
B	-1.46192100	0.84404100	1.10560200
C	0.00000000	2.91250100	0.00000000
C	2.52230000	1.45625100	0.00000000
C	2.52230000	-1.45625100	0.00000000
C	0.00000000	-2.91250100	0.00000000
C	-2.52230000	-1.45625100	0.00000000
C	-2.52230000	1.45625100	0.00000000
C	1.30294600	3.60961200	0.00000000
H	1.30958300	4.69395900	0.00000000
C	2.47454300	2.93319100	0.00000000
H	3.41029600	3.48111200	0.00000000
C	-1.30294600	3.60961200	0.00000000
H	-1.30958300	4.69395900	0.00000000
C	-2.47454300	2.93319100	0.00000000
H	-3.41029600	3.48111200	0.00000000
C	-3.77748900	0.67642200	0.00000000
H	-4.71988000	1.21284700	0.00000000
C	-3.77748900	-0.67642200	0.00000000
H	-4.71988000	-1.21284700	0.00000000
C	-2.47454300	-2.93319100	0.00000000
H	-3.41029600	-3.48111200	0.00000000
C	-1.30294600	-3.60961200	0.00000000
H	-1.30958300	-4.69395900	0.00000000
C	1.30294600	-3.60961200	0.00000000
H	1.30958300	-4.69395900	0.00000000
C	2.47454300	-2.93319100	0.00000000
H	3.41029600	-3.48111200	0.00000000
C	3.77748900	-0.67642200	0.00000000
H	4.71988000	-1.21284700	0.00000000
C	3.77748900	0.67642200	0.00000000
H	4.71988000	1.21284700	0.00000000

9 [B3LYP/6-311+G(df,2p)]

 C_{6v}

B	1.138395000	-1.203509000	-1.140151000
B	-0.472888000	-1.587066000	-1.140347000
B	-1.611156000	-0.383911000	-1.140401000
B	-1.138453000	1.203417000	-1.140170000
B	0.472884000	1.587077000	-1.139813000
B	1.611183000	0.383831000	-1.139799000
B	1.154643000	-1.220354000	1.118387000
B	-0.479680000	-1.610056000	1.118822000
B	-1.634242000	-0.389438000	1.118753000
B	-1.154254000	1.220719000	1.118263000
B	0.479887000	1.609908000	1.117746000
B	1.634122000	0.389625000	1.117821000
C	1.981952000	-2.095528000	0.015157000
C	-0.823673000	-2.763771000	0.015104000
C	-2.805396000	-0.668739000	0.015203000
C	-1.982071000	2.095414000	0.015077000
C	0.823798000	2.764285000	0.014364000
C	2.805912000	0.668844000	0.014630000
C	-0.001212000	-0.001131000	1.201808000
C	0.000097000	0.000157000	-0.667179000
C	1.531522000	-3.510611000	-0.031971000
H	2.280728000	-4.293577000	-0.065990000
C	0.216532000	-3.823777000	-0.031932000
H	-0.099270000	-4.860417000	-0.065950000
C	3.419961000	-1.724364000	-0.031758000
H	4.160030000	-2.515998000	-0.065328000
C	3.806089000	-0.428876000	-0.031938000
H	4.858782000	-0.171548000	-0.065619000
C	3.203457000	2.099703000	-0.031965000
H	4.259063000	2.344855000	-0.065253000
C	2.274517000	3.081743000	-0.032062000
H	2.577904000	4.122106000	-0.065397000
C	-0.216661000	3.823977000	-0.032108000
H	0.098833000	4.860723000	-0.065736000
C	-1.531611000	3.510543000	-0.031830000
H	-2.280888000	4.293472000	-0.065294000
C	-3.420056000	1.724281000	-0.031957000
H	-4.160155000	2.515858000	-0.066017000
C	-3.805912000	0.428747000	-0.031961000
H	-4.858513000	0.171092000	-0.066003000
C	-3.203263000	-2.099560000	-0.032069000
H	-4.258882000	-2.344514000	-0.066295000
C	-2.274363000	-3.081557000	-0.032020000
H	-2.577548000	-4.121946000	-0.066236000

9 [wb97XD/6-311+G(df,2p)]

 C_{6v}

B	0.265207000	-1.633644000	-1.127513000
B	-1.281379000	-1.046098000	-1.127680000
B	-1.547015000	0.586605000	-1.127673000
B	-0.265978000	1.633504000	-1.127421000
B	1.281655000	1.046841000	-1.127566000
B	1.547495000	-0.587209000	-1.127649000
B	0.267943000	-1.649144000	1.055312000
B	-1.294971000	-1.057291000	1.056606000
B	-1.562989000	0.592703000	1.056583000
B	-0.267808000	1.649208000	1.055384000
B	1.294054000	1.056461000	1.053957000
B	1.561893000	-0.592062000	1.053941000
C	0.463004000	-2.849477000	0.027877000
C	-2.235978000	-1.825707000	0.028621000
C	-2.699361000	1.023491000	0.028790000
C	-0.463305000	2.849470000	0.027862000
C	2.236345000	1.826192000	0.026101000
C	2.699814000	-1.023836000	0.026326000
C	-0.003596000	-0.000735000	1.311471000
C	0.003983000	0.000606000	-0.636555000
C	-0.708139000	-3.763365000	-0.028074000
H	-0.526424000	-4.830866000	-0.075093000
C	-1.965494000	-3.286350000	-0.027996000
H	-2.809549000	-3.964695000	-0.075234000
C	1.863449000	-3.345416000	-0.026769000
H	2.029049000	-4.415649000	-0.071335000
C	2.905355000	-2.495116000	-0.027478000
H	3.920675000	-2.871845000	-0.072310000
C	3.829339000	-0.058774000	-0.027083000
H	4.839176000	-0.450113000	-0.070734000
C	3.613443000	1.268580000	-0.027139000
H	4.447297000	1.959659000	-0.071085000
C	1.965483000	3.286811000	-0.027745000
H	2.809321000	3.965569000	-0.072908000
C	0.707926000	3.763447000	-0.026995000
H	0.526062000	4.831031000	-0.071684000
C	-1.863634000	3.345285000	-0.027861000
H	-2.029409000	4.415388000	-0.074676000
C	-2.905228000	2.494662000	-0.027777000
H	-3.920619000	2.870959000	-0.074611000
C	-3.828922000	0.058797000	-0.028472000
H	-4.838456000	0.450364000	-0.076545000
C	-3.613013000	-1.268477000	-0.028495000
H	-4.446485000	-1.959706000	-0.076851000

11a [B3LYP/6-311+G(df,2p)] D_{3h}

C	-4.334623000	2.502596000	1.240279000
C	-4.334623000	2.502596000	-1.240279000
B	-2.683944000	2.500857000	-1.113796000
B	-3.507777000	1.073935000	-1.113796000
B	-5.156794000	1.099167000	-1.124347000
B	-5.993265000	2.514307000	-1.116935000
B	-5.174086000	3.933166000	-1.116935000
B	-3.530303000	3.916331000	-1.124347000
B	-2.683944000	2.500857000	1.113796000
B	-3.507777000	1.073935000	1.113796000
B	-5.156794000	1.099167000	1.124347000
B	-5.993265000	2.514307000	1.116935000
B	-5.174086000	3.933166000	1.116935000
B	-3.530303000	3.916331000	1.124347000
C	-1.465161000	2.518867000	0.000000000
C	-2.913983000	0.009434000	0.000000000
C	-5.776098000	0.045312000	0.000000000
C	-7.219101000	2.509844000	0.000000000
C	-5.783139000	4.997003000	0.000000000
C	-2.927290000	4.979592000	0.000000000
C	-0.699895000	1.224909000	0.000000000
C	-1.410750000	-0.006328000	0.000000000
C	-0.734927000	3.825813000	0.000000000
C	-1.460988000	4.974791000	0.000000000
H	-0.9722233000	5.939449000	0.000000000
C	-3.677807000	6.261001000	0.000000000
H	-3.114286000	7.186901000	0.000000000
C	-5.024269000	6.270983000	0.000000000
H	-5.573984000	7.205185000	0.000000000
C	-7.267239000	4.974336000	0.000000000
H	-7.798535000	5.919217000	0.000000000
C	-7.941521000	3.806445000	0.000000000
H	-9.025460000	3.794121000	0.000000000
C	-7.942965000	1.215653000	0.000000000
H	-9.026866000	1.224620000	0.000000000
C	-7.261090000	0.054574000	0.000000000
H	-7.781182000	-0.896400000	0.000000000
C	-5.038789000	-1.222142000	0.000000000
H	-5.629831000	-2.127746000	0.000000000
C	-3.680714000	-1.276441000	0.000000000
C	0.000000000	-5.005192000	-1.240279000
C	0.000000000	-5.005192000	1.240279000
B	1.626491000	-5.015498000	1.124347000
B	0.823834000	-3.574792000	1.113796000
B	-0.823834000	-3.574792000	1.113796000
B	-1.626491000	-5.015498000	1.124347000
B	-0.819178000	-6.447473000	1.116935000
B	0.819178000	-6.447473000	1.116935000
B	1.626491000	-5.015498000	-1.124347000
B	0.823834000	-3.574792000	-1.113796000
B	-0.823834000	-3.574792000	-1.113796000
B	-1.626491000	-5.015498000	-1.124347000
B	-0.819178000	-6.447473000	-1.116935000
B	0.819178000	-6.447473000	-1.116935000
C	2.848808000	-5.024904000	0.000000000
C	1.448822000	-2.528301000	0.000000000
C	-1.448822000	-2.528301000	0.000000000
C	-2.848808000	-5.024904000	0.000000000
C	-1.435962000	-7.506846000	0.000000000
C	1.435962000	-7.506846000	0.000000000
C	3.577801000	-3.752648000	0.000000000
H	4.657597000	-3.811703000	0.000000000
C	2.945787000	-2.549372000	0.000000000
C	3.583282000	-6.315575000	0.000000000
H	4.666896000	-6.290501000	0.000000000
C	2.918696000	-7.486636000	0.000000000
H	3.452881000	-8.429805000	0.000000000
C	0.674282000	-8.780781000	0.000000000
H	1.226925000	-9.713338000	0.000000000
C	-0.674282000	-8.780781000	0.000000000
H	-1.226925000	-9.713338000	0.000000000
C	-2.918696000	-7.486636000	0.000000000
H	-3.452881000	-8.429805000	0.000000000
C	-3.583282000	-6.315575000	0.000000000

H	-4.666896000	-6.290501000	0.000000000
C	-3.577801000	-3.752648000	0.000000000
H	-4.657597000	-3.811703000	0.000000000
C	-2.945787000	-2.549372000	0.000000000
C	-0.710855000	-1.218581000	0.000000000
C	0.710855000	-1.218581000	0.000000000
C	4.334623000	2.502596000	-1.240279000
C	4.334623000	2.502596000	1.240279000
B	5.993265000	2.514307000	1.116935000
B	5.174086000	3.933166000	1.116935000
B	3.530303000	3.916331000	1.124347000
B	2.683944000	2.500857000	1.113796000
B	3.507777000	1.073935000	1.113796000
B	5.156794000	1.099167000	1.124347000
B	5.993265000	2.514307000	-1.116935000
B	5.174086000	3.933166000	-1.116935000
B	3.530303000	3.916331000	-1.124347000
B	2.683944000	2.500857000	-1.113796000
B	3.507777000	1.073935000	-1.113796000
B	5.156794000	1.099167000	-1.124347000
C	7.219101000	2.509844000	0.000000000
C	5.783139000	4.997003000	0.000000000
C	2.927290000	4.979592000	0.000000000
C	1.465161000	2.518867000	0.000000000
C	2.913983000	0.009434000	0.000000000
C	5.776098000	0.045312000	0.000000000
C	7.941521000	3.806445000	0.000000000
H	9.025460000	3.794121000	0.000000000
C	7.267239000	4.974336000	0.000000000
H	7.798535000	5.919217000	0.000000000
C	7.942965000	1.215653000	0.000000000
H	9.026866000	1.224620000	0.000000000
C	7.261090000	0.054574000	0.000000000
H	7.781182000	-0.896400000	0.000000000
C	5.038789000	-1.222142000	0.000000000
H	5.629831000	-2.127746000	0.000000000
C	3.680714000	-1.276441000	0.000000000
C	1.410750000	-0.006328000	0.000000000
C	0.699895000	1.224909000	0.000000000
C	0.734927000	3.825813000	0.000000000
C	1.460988000	4.974791000	0.000000000
H	0.972233000	5.939449000	0.000000000
C	3.677807000	6.261001000	0.000000000
H	3.114286000	7.186901000	0.000000000
C	5.024269000	6.270983000	0.000000000
H	5.573984000	7.205185000	0.000000000

11a [wb97XD/6-311+G(df,2p)]

D_{3h}

C	-4.327867000	2.498695000	1.244976000
C	-4.327867000	2.498695000	-1.244976000
B	-2.682510000	2.496935000	-1.078482000
B	-3.503665000	1.074654000	-1.078482000
B	-5.147543000	1.097900000	-1.086803000
B	-5.980056000	2.509661000	-1.081052000
B	-5.163458000	3.924050000	-1.081052000
B	-3.524580000	3.908953000	-1.086803000
B	-2.682510000	2.496935000	1.078482000
B	-3.503665000	1.074654000	1.078482000
B	-5.147543000	1.097900000	1.086803000
B	-5.980056000	2.509661000	1.081052000
B	-5.163458000	3.924050000	1.081052000
B	-3.524580000	3.908953000	1.086803000
C	-1.456682000	2.515814000	0.000000000
C	-2.907100000	0.003617000	0.000000000
C	-5.771228000	0.040954000	0.000000000
C	-7.213243000	2.505255000	0.000000000
C	-5.776236000	4.994224000	0.000000000
C	-2.921081000	4.977553000	0.000000000
C	-0.696542000	1.219497000	0.000000000
C	-1.404387000	-0.006525000	0.000000000
C	-0.735278000	3.824521000	0.000000000
C	-1.453264000	4.968029000	0.000000000
H	-0.965616000	5.933131000	0.000000000
C	-3.673862000	6.256709000	0.000000000
H	-3.110571000	7.182513000	0.000000000
C	-5.015091000	6.266282000	0.000000000
H	-5.565212000	7.199982000	0.000000000
C	-7.260147000	4.967031000	0.000000000
H	-7.791607000	5.911589000	0.000000000
C	-7.931648000	3.803957000	0.000000000
H	-9.015390000	3.791935000	0.000000000
C	-7.934305000	1.210055000	0.000000000
H	-9.017973000	1.219624000	0.000000000
C	-7.255400000	0.053303000	0.000000000
H	-7.775524000	-0.897423000	0.000000000
C	-5.029071000	-1.225451000	0.000000000
H	-5.621050000	-2.130318000	0.000000000
C	-3.679771000	-1.275491000	0.000000000
C	0.000000000	-4.997391000	-1.244976000
C	0.000000000	-4.997391000	1.244976000
B	1.622963000	-5.006853000	1.086803000
B	0.821154000	-3.571590000	1.078482000
B	-0.821154000	-3.571590000	1.078482000
B	-1.622963000	-5.006853000	1.086803000
B	-0.816598000	-6.433711000	1.081052000
B	0.816598000	-6.433711000	1.081052000
B	1.622963000	-5.006853000	-1.086803000
B	0.821154000	-3.571590000	-1.078482000
B	-0.821154000	-3.571590000	-1.078482000
B	-1.622963000	-5.006853000	-1.086803000
B	-0.816598000	-6.433711000	-1.081052000
B	0.816598000	-6.433711000	-1.081052000
C	2.850147000	-5.018507000	0.000000000
C	1.450418000	-2.519431000	0.000000000
C	-1.450418000	-2.519431000	0.000000000
C	-2.850147000	-5.018507000	0.000000000
C	-1.437007000	-7.499479000	0.000000000
C	1.437007000	-7.499479000	0.000000000
C	3.575807000	-3.742578000	0.000000000
H	4.655435000	-3.802814000	0.000000000
C	2.944494000	-2.549030000	0.000000000
C	3.581538000	-6.310012000	0.000000000
H	4.664953000	-6.285090000	0.000000000
C	2.919214000	-7.476337000	0.000000000
H	3.452762000	-8.419606000	0.000000000
C	0.671501000	-8.770987000	0.000000000
H	1.223782000	-9.703524000	0.000000000
C	-0.671501000	-8.770987000	0.000000000
H	-1.223782000	-9.703524000	0.000000000
C	-2.919214000	-7.476337000	0.000000000
H	-3.452762000	-8.419606000	0.000000000
C	-3.581538000	-6.310012000	0.000000000

H	-4.664953000	-6.285090000	0.000000000
C	-3.575807000	-3.742578000	0.000000000
H	-4.655435000	-3.802814000	0.000000000
C	-2.944494000	-2.549030000	0.000000000
C	-0.707844000	-1.212972000	0.000000000
C	0.707844000	-1.212972000	0.000000000
C	4.327867000	2.498695000	-1.244976000
C	4.327867000	2.498695000	1.244976000
B	5.980056000	2.509661000	1.081052000
B	5.163458000	3.924050000	1.081052000
B	3.524580000	3.908953000	1.086803000
B	2.682510000	2.496935000	1.078482000
B	3.503665000	1.074654000	1.078482000
B	5.147543000	1.097900000	1.086803000
B	5.980056000	2.509661000	-1.081052000
B	5.163458000	3.924050000	-1.081052000
B	3.524580000	3.908953000	-1.086803000
B	2.682510000	2.496935000	-1.078482000
B	3.503665000	1.074654000	-1.078482000
B	5.147543000	1.097900000	-1.086803000
C	7.213243000	2.505255000	0.000000000
C	5.776236000	4.994224000	0.000000000
C	2.921081000	4.977553000	0.000000000
C	1.456682000	2.515814000	0.000000000
C	2.907100000	0.003617000	0.000000000
C	5.771228000	0.040954000	0.000000000
C	7.931648000	3.803957000	0.000000000
H	9.015390000	3.791935000	0.000000000
C	7.260147000	4.967031000	0.000000000
H	7.791607000	5.911589000	0.000000000
C	7.934305000	1.210055000	0.000000000
H	9.017973000	1.219624000	0.000000000
C	7.255400000	0.053303000	0.000000000
H	7.775524000	-0.897423000	0.000000000
C	5.029071000	-1.225451000	0.000000000
H	5.621050000	-2.130318000	0.000000000
C	3.679771000	-1.275491000	0.000000000
C	1.404387000	-0.006525000	0.000000000
C	0.696542000	1.219497000	0.000000000
C	0.735278000	3.824521000	0.000000000
C	1.453264000	4.968029000	0.000000000
H	0.965616000	5.933131000	0.000000000
C	3.673862000	6.256709000	0.000000000
H	3.110571000	7.182513000	0.000000000
C	5.015091000	6.266282000	0.000000000
H	5.565212000	7.199982000	0.000000000

11b [B3LYP/6-311+G(df,2p)]*D*_{3h}

C	4.339617000	2.505479000	0.694302000
C	4.339617000	2.505479000	-0.694302000
B	6.038339000	2.512819000	-1.145344000
B	5.180129000	1.064676000	-1.151727000
B	3.493956000	1.040173000	-1.148341000
B	2.647794000	2.505768000	-1.148341000
B	3.512101000	3.953785000	-1.151727000
B	5.195334000	3.972945000	-1.145344000
B	6.038339000	2.512819000	1.145344000
B	5.180129000	1.064676000	1.151727000
B	3.493956000	1.040173000	1.148341000
B	2.647794000	2.505768000	1.148341000
B	3.512101000	3.953785000	1.151727000
B	5.195334000	3.972945000	1.145344000
C	7.250973000	2.510025000	0.000000000
C	5.805263000	0.009210000	0.000000000
C	2.907320000	-0.004156000	0.000000000
C	1.450061000	2.519891000	0.000000000
C	2.910607000	5.022900000	0.000000000
C	5.799232000	5.024515000	0.000000000
C	7.960559000	1.214681000	0.000000000
H	9.045327000	1.209375000	0.000000000
C	7.281796000	0.039656000	0.000000000
H	7.824808000	-0.899277000	0.000000000
C	7.956604000	3.809048000	0.000000000
H	9.041330000	3.816179000	0.000000000
C	7.277034000	4.986097000	0.000000000
H	7.825573000	5.921932000	0.000000000
C	5.032224000	6.286706000	0.000000000
H	5.570013000	7.228795000	0.000000000
C	3.675241000	6.286393000	0.000000000
H	3.133608000	7.226121000	0.000000000
C	1.462736000	4.994974000	0.000000000
H	0.949196000	5.947408000	0.000000000
C	0.727065000	3.820914000	0.000000000
C	0.699388000	1.227101000	0.000000000
C	1.412394000	-0.007863000	0.000000000
C	3.672541000	-1.280800000	0.000000000
C	5.057142000	-1.230721000	0.000000000
H	5.625204000	-2.151676000	0.000000000
C	-4.339617000	2.505479000	-0.694302000
C	-4.339617000	2.505479000	0.694302000
B	-2.647794000	2.505768000	1.148341000
B	-3.512101000	3.953785000	1.151727000
B	-5.195334000	3.972945000	1.145344000
B	-6.038339000	2.512819000	1.145344000
B	-5.180129000	1.064676000	1.151727000
B	-3.493956000	1.040173000	1.148341000
B	-2.647794000	2.505768000	-1.148341000
B	-3.512101000	3.953785000	-1.151727000
B	-5.195334000	3.972945000	-1.145344000
B	-6.038339000	2.512819000	-1.145344000
B	-5.180129000	1.064676000	-1.151727000
B	-3.493956000	1.040173000	-1.148341000
C	-1.450061000	2.519891000	0.000000000
C	-2.910607000	5.022900000	0.000000000
C	-5.799232000	5.024515000	0.000000000
C	-7.250973000	2.510025000	0.000000000
C	-5.805263000	0.009210000	0.000000000
C	-2.907320000	-0.004156000	0.000000000
C	-0.727065000	3.820914000	0.000000000
C	-1.462736000	4.994974000	0.000000000
H	-0.949196000	5.947408000	0.000000000
C	-0.699388000	1.227101000	0.000000000
C	-1.412394000	-0.007863000	0.000000000
C	-3.672541000	-1.280800000	0.000000000
C	-5.057142000	-1.230721000	0.000000000
H	-5.625204000	-2.151676000	0.000000000
C	-7.281796000	0.039656000	0.000000000
H	-7.824808000	-0.899277000	0.000000000
C	-7.960559000	1.214681000	0.000000000
H	-9.045327000	1.209375000	0.000000000
C	-7.956604000	3.809048000	0.000000000
H	-9.041330000	3.816179000	0.000000000

C	-7.277034000	4.986097000	0.000000000
H	-7.825573000	5.921932000	0.000000000
C	-5.032224000	6.286706000	0.000000000
H	-5.570013000	7.228795000	0.000000000
C	-3.675241000	6.286393000	0.000000000
H	-3.133608000	7.226121000	0.000000000
C	0.000000000	-5.010958000	-0.694302000
C	0.000000000	-5.010958000	0.694302000
B	-1.668028000	-5.018462000	1.151727000
B	-0.843004000	-6.485764000	1.145344000
B	0.843004000	-6.485764000	1.145344000
B	1.668028000	-5.018462000	1.151727000
B	0.846162000	-3.545941000	1.148341000
B	-0.846162000	-3.545941000	1.148341000
B	-1.668028000	-5.018462000	-1.151727000
B	-0.843004000	-6.485764000	-1.145344000
B	0.843004000	-6.485764000	-1.145344000
B	1.668028000	-5.018462000	-1.151727000
B	0.846162000	-3.545941000	-1.148341000
B	-0.846162000	-3.545941000	-1.148341000
C	-2.894656000	-5.032110000	0.000000000
C	-1.451741000	-7.534540000	0.000000000
C	1.451741000	-7.534540000	0.000000000
C	2.894656000	-5.032110000	0.000000000
C	1.457259000	-2.515735000	0.000000000
C	-1.457259000	-2.515735000	0.000000000
C	-3.606555000	-6.326049000	0.000000000
H	-4.691201000	-6.326845000	0.000000000
C	-2.928335000	-7.501387000	0.000000000
H	-3.475313000	-8.438170000	0.000000000
C	-3.594406000	-3.764253000	0.000000000
H	-4.676008000	-3.795732000	0.000000000
C	-2.945476000	-2.540114000	0.000000000
C	-0.713006000	-1.219238000	0.000000000
C	0.713006000	-1.219238000	0.000000000
C	2.945476000	-2.540114000	0.000000000
C	3.594406000	-3.764253000	0.000000000
C	3.606555000	-6.326049000	0.000000000
C	2.928335000	-7.501387000	0.000000000
H	3.475313000	-8.438170000	0.000000000
C	0.679570000	-8.795145000	0.000000000
H	1.215757000	-9.738111000	0.000000000
C	-0.679570000	-8.795145000	0.000000000
H	-1.215757000	-9.738111000	0.000000000
H	4.676008000	-3.795732000	0.000000000
H	4.691201000	-6.326845000	0.000000000

11b [wb97XD/6-311+G(df,2p)]

 D_{3h}

C	4.342597000	2.507200000	0.692199000
C	4.342597000	2.507200000	-0.692199000
B	6.041084000	2.516089000	-1.109264000
B	5.182552000	1.065262000	-1.113229000
B	3.493173000	1.039601000	-1.109541000
B	2.646907000	2.505376000	-1.109541000
B	3.513820000	3.955591000	-1.113229000
B	5.199539000	3.973688000	-1.109264000
B	6.041084000	2.516089000	1.109264000
B	5.182552000	1.065262000	1.113229000
B	3.493173000	1.039601000	1.109541000
B	2.646907000	2.505376000	1.109541000
B	3.513820000	3.955591000	1.113229000
B	5.199539000	3.973688000	1.109264000
C	7.261346000	2.511102000	0.000000000
C	5.805357000	0.009495000	0.000000000
C	2.904467000	-0.015369000	0.000000000
C	1.438924000	2.523026000	0.000000000
C	2.910902000	5.022839000	0.000000000
C	5.805351000	5.032959000	0.000000000
C	7.960977000	1.212098000	0.000000000
H	9.045334000	1.204361000	0.000000000
C	7.280889000	0.044888000	0.000000000
H	7.820512000	-0.895581000	0.000000000
C	7.958666000	3.814056000	0.000000000
H	9.043047000	3.820952000	0.000000000
C	7.282403000	4.985379000	0.000000000
H	7.830565000	5.921032000	0.000000000
C	5.030196000	6.288360000	0.000000000
H	5.565674000	7.231309000	0.000000000
C	3.679319000	6.282991000	0.000000000
H	3.134660000	7.220552000	0.000000000
C	1.456145000	4.989292000	0.000000000
H	0.949005000	5.944728000	0.000000000
C	0.733085000	3.829854000	0.000000000
C	0.697176000	1.222108000	0.000000000
C	1.406964000	-0.007282000	0.000000000
C	3.683293000	-1.280056000	0.000000000
C	5.048926000	-1.233588000	0.000000000
H	5.622788000	-2.150502000	0.000000000
C	-4.342597000	2.507200000	-0.692199000
C	-4.342597000	2.507200000	0.692199000
B	-2.646907000	2.505376000	1.109541000
B	-3.513820000	3.955591000	1.113229000
B	-5.199539000	3.973688000	1.109264000
B	-6.041084000	2.516089000	1.109264000
B	-5.182552000	1.065262000	1.113229000
B	-3.493173000	1.039601000	1.109541000
B	-2.646907000	2.505376000	-1.109541000
B	-3.513820000	3.955591000	-1.113229000
B	-5.199539000	3.973688000	-1.109264000
B	-6.041084000	2.516089000	-1.109264000
B	-5.182552000	1.065262000	-1.113229000
B	-3.493173000	1.039601000	-1.109541000
C	-1.438924000	2.523026000	0.000000000
C	-2.910902000	5.022839000	0.000000000
C	-5.805351000	5.032959000	0.000000000
C	-7.261346000	2.511102000	0.000000000
C	-5.805357000	0.009495000	0.000000000
C	-2.904467000	-0.015369000	0.000000000
C	-0.733085000	3.829854000	0.000000000
C	-1.456145000	4.989292000	0.000000000
H	-0.949005000	5.944728000	0.000000000
C	-0.697176000	1.222108000	0.000000000
C	-1.406964000	-0.007282000	0.000000000
C	-3.683293000	-1.280056000	0.000000000
C	-5.048926000	-1.233588000	0.000000000
H	-5.622788000	-2.150502000	0.000000000
C	-7.280889000	0.044888000	0.000000000
H	-7.820512000	-0.895581000	0.000000000
C	-7.960977000	1.212098000	0.000000000
H	-9.045334000	1.204361000	0.000000000
C	-7.958666000	3.814056000	0.000000000
H	-9.043047000	3.820952000	0.000000000

C	-7.282403000	4.985379000	0.000000000
H	-7.830565000	5.921032000	0.000000000
C	-5.030196000	6.288360000	0.000000000
H	-5.565674000	7.231309000	0.000000000
C	-3.679319000	6.282991000	0.000000000
H	-3.134660000	7.220552000	0.000000000
C	0.000000000	-5.014399000	-0.692199000
C	0.000000000	-5.014399000	0.692199000
B	-1.668732000	-5.020853000	1.113229000
B	-0.841546000	-6.489777000	1.109264000
B	0.841546000	-6.489777000	1.109264000
B	1.668732000	-5.020853000	1.113229000
B	0.846266000	-3.544977000	1.109541000
B	-0.846266000	-3.544977000	1.109541000
B	-1.668732000	-5.020853000	-1.113229000
B	-0.841546000	-6.489777000	-1.109264000
B	0.841546000	-6.489777000	-1.109264000
B	1.668732000	-5.020853000	-1.113229000
B	0.846266000	-3.544977000	-1.109541000
B	-0.846266000	-3.544977000	-1.109541000
C	-2.894455000	-5.032334000	0.000000000
C	-1.455994000	-7.544061000	0.000000000
C	1.455994000	-7.544061000	0.000000000
C	2.894455000	-5.032334000	0.000000000
C	1.465543000	-2.507658000	0.000000000
C	-1.465543000	-2.507658000	0.000000000
C	-3.601570000	-6.327879000	0.000000000
H	-4.685852000	-6.324971000	0.000000000
C	-2.930781000	-7.500457000	0.000000000
H	-3.479660000	-8.435670000	0.000000000
C	-3.592781000	-3.755704000	0.000000000
H	-4.673784000	-3.794226000	0.000000000
C	-2.950208000	-2.549797000	0.000000000
C	-0.709788000	-1.214826000	0.000000000
C	0.709788000	-1.214826000	0.000000000
C	2.950208000	-2.549797000	0.000000000
C	3.592781000	-3.755704000	0.000000000
C	3.601570000	-6.327879000	0.000000000
C	2.930781000	-7.500457000	0.000000000
H	3.479660000	-8.435670000	0.000000000
C	0.676263000	-8.799436000	0.000000000
H	1.212481000	-9.741984000	0.000000000
C	-0.676263000	-8.799436000	0.000000000
H	-1.212481000	-9.741984000	0.000000000
H	4.673784000	-3.794226000	0.000000000
H	4.685852000	-6.324971000	0.000000000

11c [B3LYP/6-311+G(df,2p)]

C_{2v}

C	1.238729000	0.000000000	4.998947000
C	-1.238729000	0.000000000	4.998947000
B	-1.114255000	0.824618000	3.577791000
B	-1.114255000	-0.824618000	3.577791000
B	-1.123323000	-1.628807000	5.017558000
B	-1.118849000	-0.819529000	6.447195000
B	-1.118849000	0.819529000	6.447195000
B	-1.123323000	1.628807000	5.017558000
B	1.114255000	0.824618000	3.577791000
B	1.114255000	-0.824618000	3.577791000
B	1.123323000	-1.628807000	5.017558000
B	1.118849000	-0.819529000	6.447195000
B	1.118849000	0.819529000	6.447195000
B	1.123323000	1.628807000	5.017558000
C	0.000000000	1.448142000	2.532362000
C	0.000000000	-1.448142000	2.532362000
C	0.000000000	-2.852511000	5.028105000
C	0.000000000	-1.434949000	7.507739000
C	0.000000000	1.434949000	7.507739000
C	0.000000000	2.852511000	5.028105000
C	0.000000000	0.709199000	1.226184000
C	0.000000000	-0.709199000	1.226184000
C	0.000000000	2.949065000	2.549189000
C	0.000000000	3.581699000	3.758469000
H	0.000000000	4.661241000	3.818045000
C	0.000000000	3.585243000	6.319818000
H	0.000000000	4.668795000	6.296981000
C	0.000000000	2.917760000	7.489039000
H	0.000000000	3.450236000	8.433087000
C	0.000000000	0.674375000	8.780953000
H	0.000000000	1.227199000	9.713296000
C	0.000000000	-0.674375000	8.780953000
H	0.000000000	-1.227199000	9.713296000
C	0.000000000	-2.917760000	7.489039000
H	0.000000000	-3.450236000	8.433087000
C	0.000000000	-3.585243000	6.319818000
H	0.000000000	-4.668795000	6.296981000
C	0.000000000	-3.581699000	3.758469000
H	0.000000000	-4.661241000	3.818045000
C	0.000000000	-2.949065000	2.549189000
C	-0.694404000	-4.337883000	-2.502965000
C	0.694404000	-4.337883000	-2.502965000
B	1.151618000	-3.509460000	-3.949996000
B	1.149476000	-2.647131000	-2.500685000
B	1.151051000	-3.494990000	-1.036640000
B	1.153226000	-5.179207000	-1.065430000
B	1.144459000	-6.036743000	-2.514149000
B	1.144077000	-5.192808000	-3.973777000
B	-1.151618000	-3.509460000	-3.949996000
B	-1.149476000	-2.647131000	-2.500685000
B	-1.151051000	-3.494990000	-1.036640000
B	-1.153226000	-5.179207000	-1.065430000
B	-1.144459000	-6.036743000	-2.514149000
B	-1.144077000	-5.192808000	-3.973777000
C	0.000000000	-2.907705000	-5.019123000
C	0.000000000	-1.450041000	-2.511826000
C	0.000000000	-2.909090000	0.009080000
C	0.000000000	-5.804803000	-0.008237000
C	0.000000000	-7.248126000	-2.510799000
C	0.000000000	-5.793694000	-5.024166000
C	0.000000000	-1.460936000	-4.987760000
H	0.000000000	-0.945835000	-5.939208000
C	0.000000000	-0.726617000	-3.812255000
C	0.000000000	-3.669610000	-6.285299000
H	0.000000000	-3.125280000	-7.223464000
C	0.000000000	-5.025510000	-6.287319000
H	0.000000000	-5.563309000	-7.229429000
C	0.000000000	-7.273663000	-4.987285000
H	0.000000000	-7.820324000	-5.924258000
C	0.000000000	-7.953925000	-3.812007000
H	0.000000000	-9.038678000	-3.819024000
C	0.000000000	-7.958384000	-1.215970000
H	0.000000000	-9.043239000	-1.211671000
C	0.000000000	-7.280440000	-0.040140000

H	0.00000000	-7.824541000	0.898280000
C	0.00000000	-5.055499000	1.231617000
H	0.00000000	-5.622793000	2.153377000
C	0.00000000	-3.674294000	1.279665000
C	0.00000000	-1.413716000	0.017260000
C	0.00000000	-0.699045000	-1.217758000
C	-0.694404000	4.337883000	-2.502965000
C	0.694404000	4.337883000	-2.502965000
B	1.144077000	5.192808000	-3.973777000
B	1.144459000	6.036743000	-2.514149000
B	1.153226000	5.179207000	-1.065430000
B	1.151051000	3.494990000	-1.036640000
B	1.149476000	2.647131000	-2.500685000
B	1.151618000	3.509460000	-3.949996000
B	-1.144077000	5.192808000	-3.973777000
B	-1.144459000	6.036743000	-2.514149000
B	-1.153226000	5.179207000	-1.065430000
B	-1.151051000	3.494990000	-1.036640000
B	-1.149476000	2.647131000	-2.500685000
B	-1.151618000	3.509460000	-3.949996000
C	0.00000000	5.793694000	-5.024166000
C	0.00000000	7.248126000	-2.510799000
C	0.00000000	5.804803000	-0.008237000
C	0.00000000	2.909090000	0.009080000
C	0.00000000	1.450041000	-2.511826000
C	0.00000000	2.907705000	-5.019123000
C	0.00000000	7.273663000	-4.987285000
H	0.00000000	7.820324000	-5.924258000
C	0.00000000	7.953925000	-3.812007000
H	0.00000000	9.038678000	-3.819024000
C	0.00000000	5.025510000	-6.287319000
H	0.00000000	5.563309000	-7.229429000
C	0.00000000	3.669610000	-6.285299000
H	0.00000000	3.125280000	-7.223464000
C	0.00000000	1.460936000	-4.987760000
H	0.00000000	0.945835000	-5.939208000
C	0.00000000	0.726617000	-3.812255000
C	0.00000000	0.699045000	-1.217758000
C	0.00000000	1.413716000	0.017260000
C	0.00000000	3.674294000	1.279665000
C	0.00000000	5.055499000	1.231617000
H	0.00000000	5.622793000	2.153377000
C	0.00000000	7.280440000	-0.040140000
H	0.00000000	7.824541000	0.898280000
C	0.00000000	7.958384000	-1.215970000
H	0.00000000	9.043239000	-1.211671000

11c [wb97XD/6-311+G(df,2p)]

C_{2v}

C	1.244009000	0.000000000	4.997319000
C	-1.244009000	0.000000000	4.997319000
B	-1.079067000	0.821662000	3.576713000
B	-1.079067000	-0.821662000	3.576713000
B	-1.087100000	-1.624152000	5.011797000
B	-1.082281000	-0.816650000	6.437728000
B	-1.082281000	0.816650000	6.437728000
B	-1.087100000	1.624152000	5.011797000
B	1.079067000	0.821662000	3.576713000
B	1.079067000	-0.821662000	3.576713000
B	1.087100000	-1.624152000	5.011797000
B	1.082281000	-0.816650000	6.437728000
B	1.082281000	0.816650000	6.437728000
B	1.087100000	1.624152000	5.011797000
C	0.000000000	1.451343000	2.524911000
C	0.000000000	-1.451343000	2.524911000
C	0.000000000	-2.851462000	5.024265000
C	0.000000000	-1.436494000	7.503573000
C	0.000000000	1.436494000	7.503573000
C	0.000000000	2.851462000	5.024265000
C	0.000000000	0.706337000	1.220720000
C	0.000000000	-0.706337000	1.220720000
C	0.000000000	2.948321000	2.554070000
C	0.000000000	3.578446000	3.750061000
H	0.000000000	4.658009000	3.811515000
C	0.000000000	3.582305000	6.316193000
H	0.000000000	4.665704000	6.292014000
C	0.000000000	2.918726000	7.481514000
H	0.000000000	3.451318000	8.425294000
C	0.000000000	0.671575000	8.774842000
H	0.000000000	1.224141000	9.707182000
C	0.000000000	-0.671575000	8.774842000
H	0.000000000	-1.224141000	9.707182000
C	0.000000000	-2.918726000	7.481514000
H	0.000000000	-3.451318000	8.425294000
C	0.000000000	-3.582305000	6.316193000
H	0.000000000	-4.665704000	6.292014000
C	0.000000000	-3.578446000	3.750061000
H	0.000000000	-4.658009000	3.811515000
C	0.000000000	-2.948321000	2.554070000
C	-0.692474000	-4.341891000	-2.502118000
C	0.692474000	-4.341891000	-2.502118000
B	1.113351000	-3.513648000	-3.949790000
B	1.109582000	-2.646476000	-2.499741000
B	1.110966000	-3.492466000	-1.034484000
B	1.114706000	-5.180801000	-1.062178000
B	1.108923000	-6.040418000	-2.512335000
B	1.108799000	-5.199424000	-3.969852000
B	-1.113351000	-3.513648000	-3.949790000
B	-1.109582000	-2.646476000	-2.499741000
B	-1.110966000	-3.492466000	-1.034484000
B	-1.114706000	-5.180801000	-1.062178000
B	-1.108923000	-6.040418000	-2.512335000
B	-1.108799000	-5.199424000	-3.969852000
C	0.000000000	-2.910035000	-5.017273000
C	0.000000000	-1.438502000	-2.516393000
C	0.000000000	-2.904162000	0.019698000
C	0.000000000	-5.803065000	-0.004103000
C	0.000000000	-7.260540000	-2.505601000
C	0.000000000	-5.804145000	-5.028927000
C	0.000000000	-1.455566000	-4.982969000
H	0.000000000	-0.947726000	-5.938078000
C	0.000000000	-0.732884000	-3.823026000
C	0.000000000	-3.677670000	-6.278185000
H	0.000000000	-3.132187000	-7.215317000
C	0.000000000	-5.028554000	-6.284353000
H	0.000000000	-5.563695000	-7.227536000
C	0.000000000	-7.281985000	-4.980587000
H	0.000000000	-7.830371000	-5.916165000
C	0.000000000	-7.958066000	-3.809394000
H	0.000000000	-9.042483000	-3.816232000
C	0.000000000	-7.959124000	-1.206362000
H	0.000000000	-9.043527000	-1.197787000
C	0.000000000	-7.278169000	-0.039261000

H	0.00000000	-7.817657000	0.901378000
C	0.00000000	-5.045304000	1.237852000
H	0.00000000	-5.616691000	2.156619000
C	0.00000000	-3.680086000	1.281455000
C	0.00000000	-1.407030000	0.015525000
C	0.00000000	-0.696676000	-1.214906000
C	-0.692474000	4.341891000	-2.502118000
C	0.692474000	4.341891000	-2.502118000
B	1.108799000	5.199424000	-3.969852000
B	1.108923000	6.040418000	-2.512335000
B	1.114706000	5.180801000	-1.062178000
B	1.110966000	3.492466000	-1.034484000
B	1.109582000	2.646476000	-2.499741000
B	1.113351000	3.513648000	-3.949790000
B	-1.108799000	5.199424000	-3.969852000
B	-1.108923000	6.040418000	-2.512335000
B	-1.114706000	5.180801000	-1.062178000
B	-1.110966000	3.492466000	-1.034484000
B	-1.109582000	2.646476000	-2.499741000
B	-1.113351000	3.513648000	-3.949790000
C	0.00000000	5.804145000	-5.028927000
C	0.00000000	7.260540000	-2.505601000
C	0.00000000	5.803065000	-0.004103000
C	0.00000000	2.904162000	0.019698000
C	0.00000000	1.438502000	-2.516393000
C	0.00000000	2.910035000	-5.017273000
C	0.00000000	7.281985000	-4.980587000
H	0.00000000	7.830371000	-5.916165000
C	0.00000000	7.958066000	-3.809394000
H	0.00000000	9.042483000	-3.816232000
C	0.00000000	5.028554000	-6.284353000
H	0.00000000	5.563695000	-7.227536000
C	0.00000000	3.677670000	-6.278185000
H	0.00000000	3.132187000	-7.215317000
C	0.00000000	1.455566000	-4.982969000
H	0.00000000	0.947726000	-5.938078000
C	0.00000000	0.732884000	-3.823026000
C	0.00000000	0.696676000	-1.214906000
C	0.00000000	1.407030000	0.015525000
C	0.00000000	3.680086000	1.281455000
C	0.00000000	5.045304000	1.237852000
H	0.00000000	5.616691000	2.156619000
C	0.00000000	7.278169000	-0.039261000
H	0.00000000	7.817657000	0.901378000
C	0.00000000	7.959124000	-1.206362000
H	0.00000000	9.043527000	-1.197787000

11d [B3LYP/6-311+G(df,2p)]

C_{2v}

C	0.694803000	0.000000000	5.007069000
C	-0.694803000	0.000000000	5.007069000
B	-1.150714000	0.845872000	3.541596000
B	-1.150714000	-0.845872000	3.541596000
B	-1.152522000	-1.665551000	5.014234000
B	-1.143258000	-0.842911000	6.483490000
B	-1.143258000	0.842911000	6.483490000
B	-1.152522000	1.665551000	5.014234000
B	1.150714000	0.845872000	3.541596000
B	1.150714000	-0.845872000	3.541596000
B	1.152522000	-1.665551000	5.014234000
B	1.143258000	-0.842911000	6.483490000
B	1.143258000	0.842911000	6.483490000
B	1.152522000	1.665551000	5.014234000
C	0.000000000	1.455930000	2.509955000
C	0.000000000	-1.455930000	2.509955000
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C	0.000000000	-0.714194000	1.209601000
C	0.000000000	2.938839000	2.537816000
C	0.000000000	3.589457000	3.756867000
H	0.000000000	4.671347000	3.785596000
C	0.000000000	3.606716000	6.319903000
H	0.000000000	4.691489000	6.318734000
C	0.000000000	2.929931000	7.495641000
H	0.000000000	3.477016000	8.432500000
C	0.000000000	0.678849000	8.792235000
H	0.000000000	1.216132000	9.734694000
C	0.000000000	-0.678849000	8.792235000
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C	0.000000000	-3.606716000	6.319903000
H	0.000000000	-4.691489000	6.318734000
C	0.000000000	-3.589457000	3.756867000
H	0.000000000	-4.671347000	3.785596000
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C	-1.240110000	-4.331870000	-2.501784000
C	1.240110000	-4.331870000	-2.501784000
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B	1.113909000	-2.684290000	-2.505169000
B	1.114575000	-3.507028000	-1.076660000
B	1.124092000	-5.156486000	-1.097067000
B	1.118137000	-5.994849000	-2.510511000
B	1.117945000	-5.177161000	-3.930860000
B	-1.124106000	-3.533146000	-3.919147000
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C	0.000000000	-5.787647000	-4.994058000
C	0.000000000	-1.463477000	-4.981591000
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H	0.000000000	-3.123204000	-7.189896000
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H	0.00000000	-5.62854500	2.12779700
C	0.00000000	-3.67539600	1.27579400
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C	-1.24011000	4.33187000	-2.50178400
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11d [wb97XD/6-311+G(df,2p)]

C_{2v}

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B	-1.108430000	0.841295000	6.484403000
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B	1.078916000	-3.504240000	-1.079147000
B	1.087122000	-5.148276000	-1.100926000
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