

DFT survey of monoboron and diboron corroles: regio- and stereochemical preferences for a constrained, low-symmetry macrocycle

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Supporting information

Part A: Summaries of optimised structures, bond lengths and angles

Table 1	BF ₂ (H ₂ cor)
Table 2	BHPh(H ₂ cor)
Table 3	BF ₂ (H(N-21-Me)cor)
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Table 5	PhBOB(cor)
Table 6	[B ₂ (corrole)] ⁺ , B ₂ (corrole) and [B ₂ (corrole)] ⁻
Table 7	Molecular orbitals for [B ₂ (corrole)] ⁺

Part B: Optimised Cartesian coordinates (Å) for calculated structures (all OLYP/TZ2P no core)

BF₂(H₂cor) dipyrromethene(A) (out of plane)
BF₂(H₂cor) bipyrrrole (out of plane)
BF₂(H₂cor) dipyrromethene(B) (out of plane)
BF₂(H₂cor) dipyrromethene(A) (in plane)
BF₂(H₂cor) bipyrrrole (in plane)
BF₂(H₂cor) dipyrromethene(B) (in plane)

BHPh(H₂cor) dipyrromethene(A) (out of plane)
BHPh(H₂cor) bipyrrrole (out of plane)
BHPh(H₂cor) dipyrromethene(B) (out of plane)
BHPh(H₂cor) dipyrromethene(B) (in plane)

BF₂(H(N-21-Me)cor) dipyrromethene(A) (out of plane)
BF₂(H(N-21-Me)cor) dipyrromethene(B) (out of plane)

BPhH(H(N-21-Me)cor) dipyrromethene(A) (out of plane)
BPhH(H(N-21-Me)cor) dipyrromethene(B) (out of plane)

PhBOB(cor) *cisoid* dipyrromethene
PhBOB(cor) *cisoid* dipyrromethene/bipyrrrole (BPh in dipyr-B)
PhBOB(cor) *cisoid* dipyrromethene/bipyrrrole (BPh in bipyrrrole)
PhBOB(cor) *transoid* dipyrromethene
PhBOB(cor) *transoid* dipyrromethene/bipyrrrole (BPh in dipyr-B)
PhBOB(cor) *transoid* dipyrromethene/bipyrrrole (BPh in bipyrrrole)

[B₂(corrole)]⁺ dipyrromethene/dipyrromethene
[B₂(corrole)]⁺ dipyrromethene/bipyrrrole

B₂(corrole) dipyrromethene/dipyrromethene

[B₂(corrole)][−] dipyrromethene

BF₂(H₂corrole)

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue). Lowest energy isomer in bold. The phenyl groups were omitted

Energy / eV	Optimized geometry			File
+0.32				bipyrrole (out of plane)
0.00				dipyrromethene(A) (out of plane)
+0.46				dipyrromethene(B) (out of plane)
+0.72				dipyrromethene(A) (in plane)

BHPh(H₂corrole)

Table 2: Optimized geometries and relative energies. All OLYP/TZ2P and all-electron (no core) basis set.

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue). Lowest energy isomer in bold. The phenyl groups were omitted

Energy / eV	Optimized geometry			File
+0.10				bipyrrrole (out of plane) Note: starting geometry with H and Ph either in plane and out of plane , both optimized to out of plane as shown.
0.00				dipyrromethene(A) (out of plane) Note: starting geometry with H and Ph either in plane and out of plane , both optimized to out of plane as shown.
+1.13				dipyrromethene(B) (in plane)
+0.46				dipyrromethene(B) (out of plane)

BF₂(H(N-21-Me)corrole)

Table 3: Optimized geometries and relative energies. All OLYP/TZ2P and no core basis set.

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue). The phenyl groups were omitted

Energy / eV	Optimized geometry			File
+0.40				dipyrrromethene(B) (out of plane)
0.00				dipyrrromethene(A) (out of plane)

Table 4: Optimized geometries and relative energies. All OLYP/TZ2P and no core basis set.

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue).
The phenyl groups were omitted

Energy / eV	Optimized geometry			File
+0.41				dipyrromethene(B) (out of plane)
0.00				dipyrromethene(A) (out of plane)

BOBPh(corrole)

Table 5: Optimized geometries and relative energies. All OLYP/TZ2P and no core basis set.

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue). The phenyl groups were omitted

Energy / eV	Optimized geometry			File
0.00				<i>cisoid</i> dipyrromethene/ dipyrromethene
+0.49				<i>cisoid</i> dipyrromethene/ bipyrrole (BPh in bipyrrole)
+0.86				<i>cisoid</i> dipyrromethene/ bipyrrole (BPh in dipyr-B)
+1.94				<i>transoid</i> dipyrromethene/ bipyrrole (BPh in bipyrrole)

+1.80				<i>transoid</i> dipyrrromethene/ dipyrromethene
+2.38				<i>transoid</i> dipyrrromethene/ bipyrrole (BPh in dipyr-B)

$[\text{B}_2(\text{corrole})]^+$, $\text{B}_2(\text{corrole})$, $[\text{B}_2(\text{corrole})]^-$

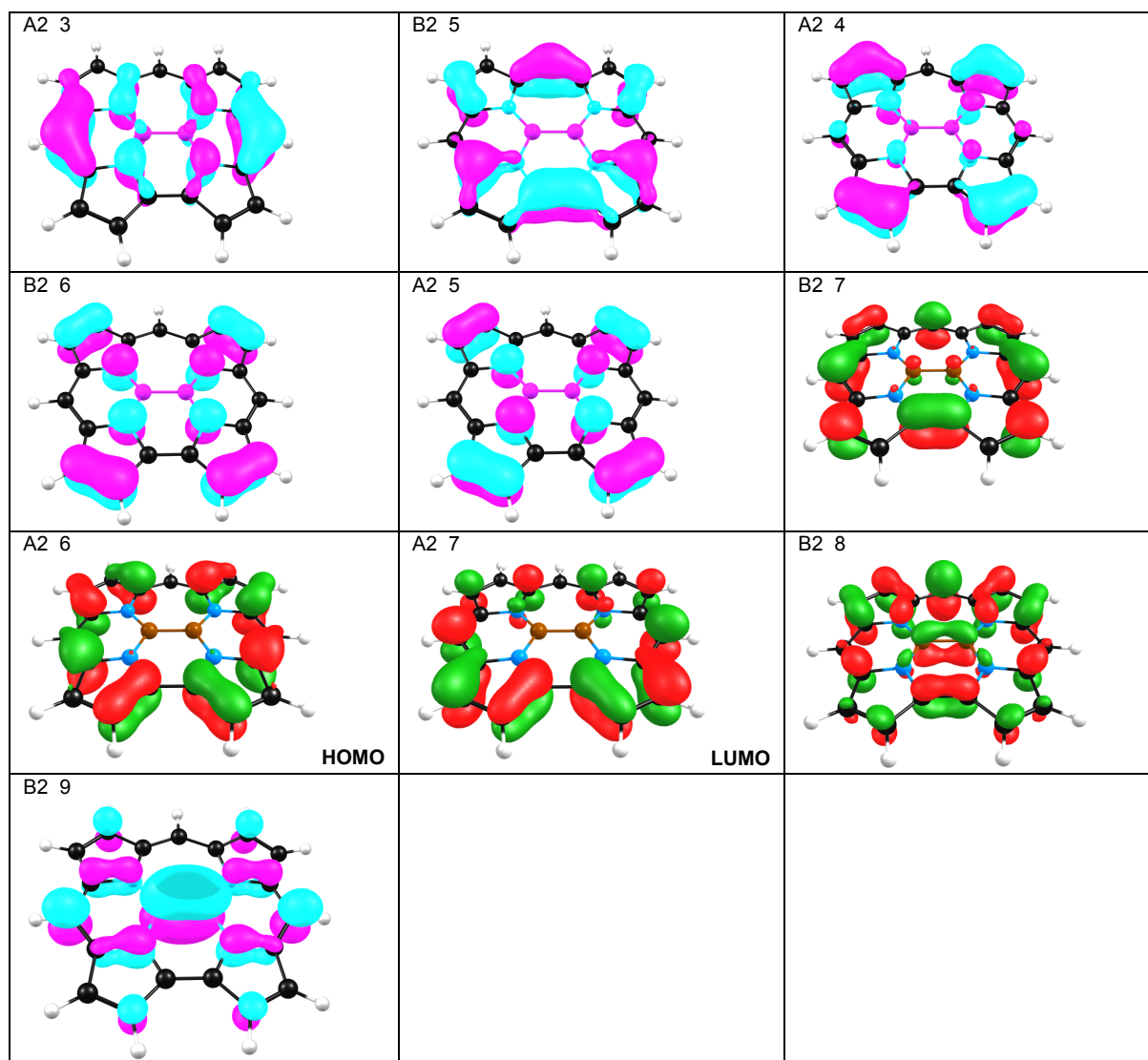
Table 6: Optimized geometries and relative energies. All OLYP/TZ2P and all-electron (no core) basis set.

Highlights of optimized distances (Å, in black) and angles (deg, in red) and dihedral angles (Å, in blue). Lowest energy isomer in bold. The phenyl groups were omitted

Energy / eV	Optimized geometry			File
0.00				$[\text{B}_2(\text{corrole})]^+$ dipyrromethene/ dipyrromethene
+0.74				$[\text{B}_2(\text{corrole})]^+$ dipyrromethene/ bipyrrole
			spin density 	$\text{B}_2(\text{corrole})$ dipyrromethene/ dipyrromethene
				$[\text{B}_2(\text{corrole})]^-$ dipyrromethene/ dipyrromethene

Molecular Orbitals [B₂(corrole)]⁺

Irrep	no.	(spin)	Occup	E (au)	E (eV)	
A2	3	A	1.00	-0.38420070502519E+00	-10.4546	
A2	3	B	1.00	-0.38420070502519E+00	-10.4546	
B2	5	A	1.00	-0.37549633382456E+00	-10.2178	
B2	5	B	1.00	-0.37549633382455E+00	-10.2178	
A2	4	A	1.00	-0.37426302545019E+00	-10.1842	
A2	4	B	1.00	-0.37426302545019E+00	-10.1842	
B2	6	A	1.00	-0.35795292272696E+00	-9.7404	
B2	6	B	1.00	-0.35795292272696E+00	-9.7404	
A2	5	A	1.00	-0.35375168492037E+00	-9.6261	
A2	5	B	1.00	-0.35375168492037E+00	-9.6261	
B2	7	A	1.00	-0.31104114207784E+00	-8.4639	
B2	7	B	1.00	-0.31104114207783E+00	-8.4639	
A2	6	A	1.00	-0.30858662593640E+00	-8.3971	
A2	6	B	1.00	-0.30858662593640E+00	-8.3971	HOMO
A2	7	A	0.00	-0.23456007846271E+00	-6.3827	LUMO
A2	7	B	0.00	-0.23456007846269E+00	-6.3827	
B2	8	A	0.00	-0.22298997171931E+00	-6.0679	
B2	8	B	0.00	-0.22298997171932E+00	-6.0679	
B2	9	A	0.00	-0.19629392956353E+00	-5.3414	
B2	9	B	0.00	-0.19629392956354E+00	-5.3414	



**Part B: Optimised Cartesian coordinates (Å) for calculated structures (all OLYP/TZ2P
no core)**

BF₂(H₂cor) dipyrromethene(A) (out of plane)

C	3.424029000	-0.337346000	2.553060000
C	2.743056000	0.014840000	1.340965000
H	4.497526000	-0.420358000	2.659271000
N	1.410029000	-0.056657000	1.638296000
C	3.246747000	0.238754000	0.050582000
H	4.331064000	0.243749000	-0.008989000
C	2.478451000	-0.608860000	3.521883000
N	-1.168339000	0.003057000	-1.392273000
C	-1.251490000	-0.432621000	-2.700077000
H	2.712014000	-0.778616000	-4.399453000
H	2.668431000	-0.949351000	4.531162000
H	4.439236000	-0.260601000	-2.416594000
C	-3.264070000	-0.794636000	-1.730216000
C	1.179099000	-0.430060000	2.947899000
H	-2.944982000	-1.314648000	-3.855623000
C	-2.663568000	-0.343358000	2.925336000
C	-1.280957000	-0.557421000	2.654700000
H	-4.264015000	-1.152227000	-1.522963000
N	-1.203230000	-0.614400000	1.286744000
C	1.169890000	-0.201996000	-2.893356000
C	-3.341416000	-0.232362000	1.712729000
C	-0.116685000	-0.599241000	3.457754000
H	-0.231587000	-0.750146000	4.525428000
H	-3.089430000	-0.215531000	3.911123000
H	-4.388242000	0.002741000	1.580805000
C	-2.392907000	-0.375558000	0.668692000
C	-0.075568000	-0.470124000	-3.469298000
H	-0.117208000	-0.809952000	-4.498174000
C	-2.362604000	-0.285084000	-0.757715000
C	3.364757000	-0.133636000	-2.397045000
C	2.618629000	0.222977000	-1.217506000
C	-2.576909000	-0.894196000	-2.929056000
N	1.277554000	0.252279000	-1.579622000
C	2.483114000	-0.409565000	-3.408462000
B	-0.013965000	1.070271000	-1.166142000
F	0.021235000	1.584152000	0.130201000
F	-0.193457000	2.127130000	-2.042047000
H	-0.400610000	-0.952044000	0.784177000
H	0.758044000	0.533675000	1.130241000

BF₂(H₂cor) bipyrrole (out of plane)

C	3.401631000	-0.142587000	2.544318000
C	2.781629000	-0.381174000	1.270043000
H	4.469958000	-0.077398000	2.699858000
N	1.441105000	-0.402624000	1.538624000
C	3.382189000	-0.440989000	0.000000000
H	4.466748000	-0.415381000	0.000000000
C	2.416335000	0.035049000	3.490347000
N	-1.408507000	0.090665000	-1.167047000
C	-1.344971000	-0.058255000	-2.539531000
H	2.554440000	0.269153000	-4.537097000
H	2.554440000	0.269153000	4.537097000
H	4.469958000	-0.077398000	-2.699858000
C	-3.331298000	-0.932142000	-1.815688000
C	1.145012000	-0.093102000	2.843189000
H	-2.823895000	-0.924957000	-3.967615000
C	-2.582501000	-0.644717000	2.950032000
C	-1.344971000	-0.058255000	2.539531000
H	-4.286956000	-1.437158000	-1.777842000
N	-1.408507000	0.090665000	1.167047000
C	1.145012000	-0.093102000	-2.843189000
C	-3.331298000	-0.932142000	1.815688000
C	-0.164763000	0.032269000	3.318401000
H	-0.289595000	0.084202000	4.395589000
H	-2.823895000	-0.924957000	3.967615000
H	-4.286956000	-1.437158000	1.777842000
C	-2.576428000	-0.484955000	0.712161000
C	-0.164763000	0.032269000	-3.318401000
H	-0.289595000	0.084202000	-4.395589000
C	-2.576428000	-0.484955000	-0.712161000
C	3.401631000	-0.142587000	-2.544318000
C	2.781629000	-0.381174000	-1.270043000
C	-2.582501000	-0.644717000	-2.950032000
N	1.441105000	-0.402624000	-1.538624000
C	2.416335000	0.035049000	-3.490347000
B	-0.995319000	1.131054000	0.000000000
F	0.304906000	1.551910000	0.000000000
F	-1.860893000	2.204557000	0.000000000
H	0.696852000	-0.543769000	-0.887885000
H	0.696852000	-0.543769000	0.887885000

BF₂(H₂cor) dipyrromethene(B) (out of plane)

C	-3.116496000	0.546092000	2.545940000
C	-2.616681000	0.401815000	1.219602000
H	-4.119259000	0.861614000	2.802421000
N	-1.285764000	0.009758000	1.270544000
C	-3.275085000	0.571032000	0.000000000
H	-4.321607000	0.853049000	0.000000000
C	-2.091458000	0.241511000	3.403167000
N	1.600329000	0.754258000	-1.342322000
C	1.589174000	0.171635000	-2.576604000
H	-2.104512000	0.297330000	-4.484137000
H	-2.104512000	0.297330000	4.484137000
H	-4.119259000	0.861614000	-2.802421000
C	3.688600000	0.100105000	-1.698661000
C	-0.917470000	-0.034655000	2.628228000
H	3.310134000	-0.615720000	-3.757476000
C	2.947697000	-0.159520000	2.846637000
C	1.589174000	0.171635000	2.576604000
H	4.737621000	-0.112427000	-1.547125000
N	1.600329000	0.754258000	1.342322000
C	-0.917470000	-0.034655000	-2.628228000
C	3.688600000	0.100105000	1.698661000
C	0.363774000	-0.108321000	3.206782000
H	0.390759000	-0.346670000	4.265803000
H	3.310134000	-0.615720000	3.757476000
H	4.737621000	-0.112427000	1.547125000
C	2.804366000	0.609551000	0.710272000
C	0.363774000	-0.108321000	-3.206782000
H	0.390759000	-0.346670000	-4.265803000
C	2.804366000	0.609551000	-0.710272000
C	-3.116496000	0.546092000	-2.545940000
C	-2.616681000	0.401815000	-1.219602000
C	2.947697000	-0.159520000	-2.846637000
N	-1.285764000	0.009758000	-1.270544000
C	-2.091458000	0.241511000	-3.403167000
B	-0.893818000	-0.928526000	0.000000000
F	0.419428000	-1.310669000	0.000000000
F	-1.728934000	-2.030959000	0.000000000
H	0.726924000	0.988310000	0.909454000
H	0.726924000	0.988310000	-0.909454000

BF₂(H₂cor) dipyrromethene(A) (in plane)

H	-4.253921000	-2.665727000	-0.828649000
H	4.455572000	1.435134000	-0.950532000
H	-2.506465000	-4.666729000	-0.600551000
H	3.215533000	3.777186000	-1.210320000
H	-4.290289000	2.558487000	0.202670000
H	4.565452000	-1.549548000	0.108838000
H	3.344970000	-3.925215000	0.001952000
H	-2.517935000	4.532254000	0.409365000
H	-4.144125000	-0.060902000	-0.601692000
H	0.459340000	-4.631732000	-0.243239000
H	0.399644000	4.629464000	-0.321610000
N	-1.150595000	-1.680252000	-0.507842000
N	1.438752000	1.484407000	0.258895000
N	-1.299892000	1.758119000	-0.789712000
N	1.290054000	-1.368220000	0.057393000
C	-3.182331000	-2.572616000	-0.708189000
C	3.464006000	1.671464000	-0.589313000
C	-2.280937000	-3.608551000	-0.594680000
C	2.813536000	2.896656000	-0.727620000
C	-2.473058000	-1.314305000	-0.645365000
C	2.554116000	0.741205000	-0.003078000
C	-0.971712000	-3.035657000	-0.444071000
C	1.472560000	2.752830000	-0.248131000
C	-3.058554000	-0.011619000	-0.637300000
C	0.320585000	-3.556785000	-0.228815000
C	0.282895000	3.549514000	-0.315012000
C	-2.572398000	1.327651000	-0.558212000
C	2.501768000	-0.702788000	0.073532000
C	1.454249000	-2.726838000	-0.023122000
C	-1.039708000	3.035116000	-0.379097000
C	-3.249407000	2.515831000	-0.089886000
C	3.498081000	-1.720726000	0.066778000
C	2.864092000	-2.956133000	0.021312000
C	-2.330695000	3.542741000	0.014508000
B	-0.031523000	-0.741307000	-0.265299000
H	0.637365000	1.118219000	0.758734000
F	-0.470566000	0.015222000	0.874058000
F	0.207317000	-0.060207000	-1.517979000
H	-0.608634000	1.185803000	-1.261129000

BF₂(H₂cor) bipyrrole (in plane)

H	-2.654238000	-0.107257000	-4.495367000
H	1.831452000	-0.356906000	4.731745000
H	-4.402920000	-0.470909000	-2.520499000
H	3.918752000	0.059990000	3.125114000
H	3.056549000	-1.153601000	-4.324991000
H	-2.052754000	-0.870545000	4.600493000
H	-4.030147000	-1.289401000	2.861023000
H	4.672309000	-0.790120000	-2.240205000
H	0.205214000	-0.647123000	-4.683118000
H	-4.185924000	-1.218086000	0.102023000
H	4.273910000	-0.064535000	0.381125000
N	-1.346900000	-1.301779000	-1.759928000
N	1.098574000	-0.311206000	1.539783000
N	1.556975000	-0.042541000	-1.653891000
N	-1.091850000	-1.058620000	1.474672000
C	-2.440165000	-0.513695000	-3.516051000
C	1.803658000	-0.304017000	3.651953000
C	-3.346550000	-0.703231000	-2.491604000
C	2.894702000	-0.092506000	2.808497000
C	-1.124326000	-0.832530000	-3.023413000
C	0.659601000	-0.470922000	2.825717000
C	-2.637847000	-1.153129000	-1.319317000
C	2.448231000	-0.119855000	1.440782000
C	0.169989000	-0.657922000	-3.596943000
C	-3.102385000	-1.238594000	0.018707000
C	3.198110000	-0.076179000	0.225669000
C	1.422830000	-0.487071000	-2.938219000
C	-0.743866000	-0.856401000	2.782524000
C	-2.437597000	-1.205706000	1.282916000
C	2.821931000	-0.167015000	-1.138719000
C	2.773202000	-0.772029000	-3.353269000
C	-1.948734000	-0.964914000	3.528148000
C	-2.981803000	-1.177754000	2.614919000
C	3.610926000	-0.582415000	-2.271962000
B	0.032079000	-0.688275000	0.572964000
H	-0.612911000	-1.744974000	-1.222704000
H	0.785317000	0.388030000	-1.160545000
F	0.495075000	-1.833426000	-0.137989000
F	-0.393757000	0.460946000	-0.159250000

BF₂(H₂cor) dipyrromethene(B) (in-plane)

H	2.884411000	0.020880000	-4.391379000
H	-1.803379000	1.132917000	4.647492000
H	4.457491000	0.020161000	-2.234998000
H	-3.875472000	1.149906000	2.965354000
H	-2.938983000	-0.076447000	-4.384371000
H	1.771931000	-1.156020000	4.647080000
H	3.840113000	-1.177532000	2.960118000
H	-4.506809000	-0.071191000	-2.224119000
H	-0.027363000	-0.025721000	-4.665449000
H	4.143868000	-0.198579000	0.259538000
H	-4.187068000	0.159361000	0.269305000
N	1.244622000	0.123075000	-1.537878000
N	-1.268550000	-0.412007000	1.840073000
N	-1.292017000	-0.163429000	-1.534556000
N	1.229545000	0.379127000	1.835817000
C	2.570194000	0.049841000	-3.356543000
C	-1.840407000	0.648261000	3.681713000
C	3.375454000	0.044385000	-2.246019000
C	-2.925959000	0.660321000	2.794781000
C	1.206706000	0.066901000	-2.902973000
C	-0.756145000	0.001172000	3.034663000
C	2.556036000	0.071964000	-1.055259000
C	-2.523788000	0.031810000	1.574158000
C	-0.026190000	-0.023774000	-3.582097000
C	3.069726000	-0.029771000	0.259050000
C	-3.112639000	-0.007892000	0.266443000
C	-1.257496000	-0.112570000	-2.899864000
C	0.720167000	-0.030358000	3.032907000
C	2.484358000	-0.064952000	1.568352000
C	-2.602300000	-0.113393000	-1.048845000
C	-2.622137000	-0.099967000	-3.350192000
C	1.806390000	-0.674603000	3.679648000
C	2.889856000	-0.689078000	2.790215000
C	-3.424682000	-0.092062000	-2.237719000
B	-0.022889000	-0.018860000	-0.746441000
H	0.681985000	0.935437000	1.189043000
H	-0.722636000	-0.970075000	1.193423000
F	0.179765000	-1.238109000	-0.013048000
F	-0.223895000	1.201900000	-0.015457000

BHPh(H₂cor) dipyrromethene(A) (out of plane)

N	-1.252132000	0.403613000	1.346581000
C	-2.208141000	0.653454000	2.327579000
C	-1.770074000	0.802950000	0.127213000
C	-3.396830000	1.128735000	1.696191000
C	-3.135555000	1.206069000	0.352778000
H	-4.301416000	1.422211000	2.210194000
H	-3.788816000	1.591401000	-0.417538000
N	2.613682000	0.829247000	1.734727000
C	3.733460000	0.780532000	0.943409000
C	2.793281000	0.254100000	2.957072000
C	4.733431000	0.202321000	1.773380000
C	4.157358000	-0.119801000	3.003350000
H	5.744320000	-0.022806000	1.462018000
H	4.636791000	-0.643614000	3.818449000
N	1.233011000	0.982656000	-0.579683000
C	2.467403000	1.266940000	-1.134843000
C	0.205449000	1.175765000	-1.464084000
C	2.184397000	1.705220000	-2.468984000
C	0.820968000	1.648749000	-2.669416000
H	2.927356000	2.052502000	-3.174920000
H	0.287554000	1.938773000	-3.565315000
N	0.381290000	0.051796000	3.159196000
C	-0.581544000	0.315477000	4.110445000
C	1.619598000	0.103999000	3.763194000
C	0.061812000	0.438502000	5.372429000
C	1.422787000	0.298261000	5.156843000
H	-0.428240000	0.673127000	6.308389000
H	2.214024000	0.427198000	5.882854000
C	-1.901945000	0.537442000	3.683568000
C	3.668485000	1.126585000	-0.428069000
C	-1.144024000	1.022712000	-1.124095000
B	-0.131541000	-0.603786000	1.822055000
H	0.769469000	-0.727422000	1.039274000
C	-0.710448000	-2.112221000	2.018136000
C	-1.451924000	-2.718528000	0.986782000
C	-0.430954000	-2.912406000	3.139136000
C	-1.906850000	-4.034719000	1.073844000
C	-0.881188000	-4.231494000	3.238928000
C	-1.626442000	-4.800743000	2.206948000
H	-1.683693000	-2.155434000	0.084978000
H	0.152528000	-2.508352000	3.962751000
H	-2.480810000	-4.463791000	0.254290000
H	-0.648561000	-4.814598000	4.128593000
H	-1.981039000	-5.826787000	2.281625000
H	1.103144000	0.308548000	0.176978000
H	-1.840265000	1.261846000	-1.922495000
H	4.597028000	1.249323000	-0.974328000
H	-2.677153000	0.731621000	4.417378000
H	1.799128000	1.376787000	1.521928000

BHPh(H₂cor) bipyrrrole (out of plane)

N	-0.915613000	0.823039000	2.368782000
C	-1.720050000	0.365927000	3.387821000
C	-1.626288000	1.161989000	1.242835000
C	-3.054552000	0.459375000	2.879334000
C	-2.998523000	0.941336000	1.589482000
H	-3.940542000	0.158170000	3.421614000
H	-3.830993000	1.091676000	0.915719000
N	2.945798000	-0.116157000	2.698863000
C	3.909868000	0.268316000	1.797584000
C	3.414384000	0.111604000	3.975664000
C	5.081772000	0.600495000	2.561750000
C	4.763727000	0.532226000	3.906244000
H	6.007013000	0.966568000	2.135510000
H	5.397002000	0.795709000	4.742112000
N	1.283307000	0.956212000	0.430705000
C	2.517812000	1.020712000	-0.173637000
C	0.293578000	1.505613000	-0.348650000
C	2.296077000	1.679935000	-1.424866000
C	0.953683000	1.978068000	-1.528275000
H	3.071811000	1.931777000	-2.135663000
H	0.467519000	2.508453000	-2.336048000
N	1.188773000	-0.306385000	4.192915000
C	0.106981000	-0.188978000	5.032826000
C	2.337060000	-0.003883000	4.891499000
C	0.629378000	0.070977000	6.343941000
C	2.004006000	0.213854000	6.249167000
H	0.022389000	0.244046000	7.223423000
H	2.687810000	0.482217000	7.042562000
C	-1.244329000	-0.054560000	4.634746000
C	3.714021000	0.645727000	0.448701000
C	-1.061934000	1.556816000	0.017489000
H	-1.754282000	1.912072000	-0.738002000
H	4.618809000	0.846758000	-0.117016000
H	-1.992043000	-0.178200000	5.412607000
B	1.635364000	-0.992313000	2.843616000
H	1.101761000	0.251863000	1.145789000
H	0.049242000	1.050554000	2.525352000
H	0.827503000	-0.891478000	1.960402000
C	1.961628000	-2.574032000	3.007524000
C	1.217802000	-3.401874000	3.865438000
C	2.966375000	-3.196350000	2.246352000
C	1.474775000	-4.770062000	3.977955000
C	3.232419000	-4.563249000	2.350243000
C	2.489233000	-5.359019000	3.222801000
H	0.419850000	-2.978514000	4.470745000
H	3.568472000	-2.607819000	1.557828000
H	0.883267000	-5.375761000	4.662286000
H	4.026987000	-5.005514000	1.751845000
H	2.698598000	-6.422937000	3.313759000

BHPh(H₂cor) dipyrromethene(B) (out of plane)

N	-0.948933000	0.852395000	1.933974000
C	-1.732140000	0.436801000	3.023598000
C	-1.586880000	1.942080000	1.362448000
C	-2.929818000	1.236139000	3.016428000
C	-2.829709000	2.170097000	2.024166000
H	-3.713006000	1.150674000	3.758431000
H	-3.520386000	2.969966000	1.793056000
N	2.919200000	0.150603000	2.519927000
C	3.781677000	0.056664000	1.470784000
C	3.185473000	-0.750160000	3.519104000
C	4.769459000	-0.879673000	1.891715000
C	4.400785000	-1.373751000	3.143384000
H	5.614591000	-1.203797000	1.300058000
H	4.894518000	-2.162819000	3.692774000
N	1.037282000	1.372142000	0.447141000
C	2.337453000	1.444719000	-0.073589000
C	0.322234000	2.439065000	-0.068376000
C	2.362968000	2.541789000	-1.002941000
C	1.145903000	3.166628000	-0.977036000
H	3.247793000	2.854075000	-1.542387000
H	0.850193000	4.061900000	-1.507443000
N	0.891859000	-0.580815000	3.809990000
C	-0.193416000	-0.828536000	4.584556000
C	2.061871000	-1.013321000	4.364278000
C	0.322825000	-1.447505000	5.761577000
C	1.709040000	-1.559832000	5.623597000
H	-0.257363000	-1.743245000	6.625397000
H	2.397354000	-1.944633000	6.363217000
C	-1.449797000	-0.381501000	4.136131000
C	3.516028000	0.759881000	0.280901000
C	-0.991073000	2.680522000	0.337478000
B	0.094819000	0.169341000	0.918730000
H	0.762689000	-0.694370000	1.424176000
H	-1.536801000	3.508182000	-0.100377000
H	4.337567000	0.863092000	-0.421523000
H	-2.296051000	-0.560562000	4.791366000
H	2.180142000	0.830837000	2.550014000
H	0.789699000	-0.483332000	2.797242000
C	-0.664264000	-0.544812000	-0.332745000
C	-0.034340000	-0.711118000	-1.579842000
C	-1.948966000	-1.103414000	-0.206859000
C	-0.655730000	-1.364792000	-2.645785000
C	-2.581253000	-1.760782000	-1.264777000
C	-1.939635000	-1.890007000	-2.496483000
H	0.967826000	-0.320482000	-1.737413000
H	-2.484380000	-1.025543000	0.735969000
H	-0.135374000	-1.460099000	-3.597348000
H	-3.581334000	-2.167916000	-1.125792000
H	-2.431665000	-2.392865000	-3.326755000

BHPh(H₂cor) dipyrromethene(B) (in plane)

N	-1.009149000	0.528067000	1.802163000
C	-1.653699000	0.359342000	3.019532000
C	-1.769185000	1.316816000	0.979273000
C	-2.919495000	1.045167000	2.896871000
C	-2.997637000	1.614520000	1.653783000
H	-3.654889000	1.105232000	3.688676000
H	-3.798662000	2.223521000	1.256147000
N	3.022017000	-0.970720000	2.190840000
C	3.839846000	-0.045462000	1.603984000
C	3.265825000	-1.097453000	3.538254000
C	4.876612000	0.178316000	2.562141000
C	4.514613000	-0.447222000	3.748816000
H	5.720445000	0.839278000	2.418217000
H	5.025265000	-0.367726000	4.698235000
N	0.952036000	0.930171000	0.243955000
C	2.275368000	1.165186000	-0.101182000
C	0.125904000	1.704443000	-0.527263000
C	2.238375000	2.101317000	-1.201258000
C	0.933677000	2.418431000	-1.470962000
H	3.119360000	2.492216000	-1.693622000
H	0.563311000	3.114444000	-2.211969000
N	0.898492000	-1.406803000	3.874243000
C	-0.046988000	-0.847188000	4.687895000
C	2.160320000	-1.326093000	4.414586000
C	0.602843000	-0.709048000	5.953558000
C	1.954234000	-0.981609000	5.780462000
H	0.137082000	-0.322678000	6.849899000
H	2.735127000	-0.851500000	6.516539000
C	-1.242986000	-0.226790000	4.241877000
C	3.498976000	0.748102000	0.477614000
C	-1.235745000	1.838300000	-0.210653000
B	0.337854000	-0.034089000	1.287091000
H	1.055331000	0.070264000	2.215935000
H	-1.856401000	2.478744000	-0.826533000
H	4.348241000	1.280553000	0.056841000
H	-1.939968000	-0.012384000	5.048121000
H	2.181919000	-1.285264000	1.736373000
H	0.711255000	-1.575244000	2.900691000
C	0.161946000	-1.556205000	0.672344000
C	1.007932000	-2.062226000	-0.337779000
C	-0.843374000	-2.438521000	1.122579000
C	0.877571000	-3.355231000	-0.847647000
C	-0.984583000	-3.733574000	0.620970000
C	-0.118897000	-4.203162000	-0.365988000
H	1.784473000	-1.431514000	-0.760403000
H	-1.554966000	-2.110423000	1.874489000
H	1.553466000	-3.695981000	-1.629162000
H	-1.779322000	-4.373172000	0.999181000
H	-0.224787000	-5.211602000	-0.759989000

BF₂(H(N-21-Me)cor dipyrromethene(A) (out of plane)

N	-1.589007000	-0.036247000	1.345921000
C	-2.593430000	0.422163000	2.197951000
C	-2.067033000	-0.000237000	0.045633000
C	-3.770914000	0.645570000	1.423153000
C	-3.456987000	0.372818000	0.117843000
H	-4.709700000	1.018201000	1.810923000
H	-4.093770000	0.506519000	-0.747202000
N	2.282668000	0.948503000	1.729960000
C	3.382897000	0.553900000	0.969072000
C	2.377535000	0.412396000	3.007044000
C	4.257481000	-0.115590000	1.853852000
C	3.634249000	-0.205563000	3.103205000
H	5.168936000	-0.617932000	1.560062000
H	3.980681000	-0.780863000	3.950449000
N	0.969607000	0.263043000	-0.623750000
C	2.188779000	0.508406000	-1.207620000
C	-0.037687000	0.133134000	-1.526761000
C	1.922345000	0.570482000	-2.617789000
C	0.578792000	0.343246000	-2.812779000
H	2.660583000	0.786362000	-3.379742000
H	0.052454000	0.342385000	-3.757860000
N	-0.029502000	0.167632000	3.237141000
C	-1.032797000	0.621798000	4.066415000
C	1.188552000	0.419154000	3.825585000
C	-0.431449000	1.073376000	5.271941000
C	0.943611000	0.935120000	5.124654000
H	-0.953503000	1.510788000	6.112630000
H	1.706867000	1.268119000	5.815055000
C	-2.340766000	0.681424000	3.548119000
C	3.365529000	0.602009000	-0.453504000
C	-1.388684000	-0.053507000	-1.196553000
B	-0.506477000	-0.870996000	2.149185000
F	0.539712000	-1.359804000	1.378035000
F	-1.132815000	-1.938285000	2.774535000
C	1.577175000	2.216779000	1.486665000
H	1.790247000	2.551189000	0.474494000
H	0.501304000	2.105304000	1.604336000
H	1.942164000	2.970823000	2.191080000
H	0.903427000	-0.132578000	0.304833000
H	4.311114000	0.584876000	-0.985469000
H	-2.056767000	-0.082919000	-2.051994000
H	-3.154182000	1.025995000	4.177274000

BF₂(H(N-21-Me)cor) dipyrromethene(B) (out of plane)

N	-1.436477000	-0.029870000	0.872268000
C	-2.312815000	0.026247000	1.970589000
C	-2.169835000	0.290282000	-0.261265000
C	-3.632391000	0.257889000	1.447195000
C	-3.541107000	0.452827000	0.095846000
H	-4.514129000	0.369497000	2.064724000
H	-4.334595000	0.722356000	-0.588490000
N	2.389080000	1.137702000	1.927306000
C	3.295958000	0.393484000	1.193542000
C	2.567751000	0.893302000	3.287795000
C	4.210139000	-0.154186000	2.129851000
C	3.752784000	0.139098000	3.413043000
H	5.020321000	-0.825989000	1.880327000
H	4.129509000	-0.276110000	4.337692000
N	0.627720000	0.045597000	-0.570494000
C	1.964648000	0.151515000	-0.965514000
C	-0.167760000	0.373897000	-1.651745000
C	1.963603000	0.439981000	-2.376382000
C	0.668107000	0.614179000	-2.785377000
H	2.860128000	0.596708000	-2.962570000
H	0.320170000	0.910511000	-3.766250000
N	0.258106000	0.687371000	3.291747000
C	-0.874526000	0.496731000	4.012573000
C	1.356673000	0.927022000	4.060652000
C	-0.493081000	0.739157000	5.366876000
C	0.880518000	0.995770000	5.395388000
H	-1.160146000	0.737213000	6.218635000
H	1.470110000	1.240909000	6.268002000
C	-2.069934000	0.146540000	3.352836000
C	3.139483000	0.151748000	-0.191960000
C	-1.555645000	0.443781000	-1.510089000
B	-0.128525000	-0.890557000	0.469590000
F	-0.547278000	-2.046523000	-0.165322000
F	0.673874000	-1.223769000	1.547792000
C	1.695760000	2.320214000	1.404436000
H	2.321304000	2.776086000	0.634528000
H	0.722131000	2.088756000	0.974043000
H	1.565348000	3.031684000	2.219613000
H	0.387777000	0.233309000	2.403557000
H	-2.168529000	0.676797000	-2.373065000
H	-2.958016000	0.076490000	3.973367000
H	4.049302000	-0.060367000	-0.749454000

BPhH(H(N-21-Me)cor) dipyrromethene(A) (out of plane)

N	-0.830069000	0.168681000	1.101810000
C	-1.805348000	0.415569000	2.064554000
C	-1.373629000	0.418005000	-0.141798000
C	-3.026194000	0.740679000	1.399323000
C	-2.767888000	0.730146000	0.054888000
H	-3.954352000	0.999915000	1.891288000
H	-3.448450000	0.995596000	-0.743458000
N	3.067557000	1.104496000	1.466399000
C	4.123366000	0.803769000	0.605684000
C	3.208361000	0.392443000	2.649397000
C	5.023227000	0.007235000	1.346496000
C	4.453668000	-0.249634000	2.598564000
H	5.910566000	-0.461099000	0.942372000
H	4.827274000	-0.942158000	3.340661000
N	1.615013000	0.787220000	-0.893036000
C	2.822782000	1.048136000	-1.494939000
C	0.577021000	0.756164000	-1.773477000
C	2.512026000	1.241475000	-2.886247000
C	1.158210000	1.065156000	-3.055254000
H	3.233648000	1.496218000	-3.651026000
H	0.604197000	1.150861000	-3.980562000
N	0.814182000	0.090363000	2.927795000
C	-0.160050000	0.353061000	3.864205000
C	2.047400000	0.281825000	3.500010000
C	0.481494000	0.629775000	5.101999000
C	1.850203000	0.572700000	4.875950000
H	-0.015269000	0.903838000	6.023352000
H	2.636575000	0.812428000	5.579218000
C	-1.494558000	0.434627000	3.425472000
C	4.033583000	1.033611000	-0.796171000
C	-0.759436000	0.548248000	-1.413180000
B	0.381249000	-0.689739000	1.641903000
H	1.299775000	-0.767198000	0.878573000
C	-0.056086000	-2.231991000	1.938189000
C	-0.759793000	-2.966765000	0.965830000
C	0.318421000	-2.931904000	3.098032000
C	-1.089373000	-4.311132000	1.144415000
C	-0.005137000	-4.278121000	3.289162000
C	-0.715628000	-4.976473000	2.313312000
H	-1.061555000	-2.485178000	0.038231000
H	0.877239000	-2.425296000	3.881312000
H	-1.639014000	-4.840563000	0.367946000
H	0.298283000	-4.780781000	4.206136000
H	-0.972509000	-6.023888000	2.459231000
C	2.355687000	2.390219000	1.430102000
H	2.614752000	2.908417000	0.509276000
H	1.276108000	2.258518000	1.472220000
H	2.674667000	3.000281000	2.280177000
H	1.538930000	0.348876000	0.023550000
H	-1.466250000	0.632812000	-2.233040000
H	4.950472000	1.060551000	-1.376037000
H	-2.286927000	0.618623000	4.142801000

BPhH(H(N-21-Me)cor) dipyrromethene(B) (out of plane)

N	-0.833093000	0.264075000	2.088856000
C	-1.446598000	-0.048543000	3.307134000
C	-1.790472000	0.849922000	1.279500000
C	-2.842612000	0.276707000	3.180238000
C	-3.047242000	0.851265000	1.956344000
H	-3.564375000	0.159779000	3.978172000
H	-3.965198000	1.268427000	1.564139000
N	3.216508000	0.999832000	2.537197000
C	3.876666000	0.565913000	1.399099000
C	3.639673000	0.256843000	3.638720000
C	4.906197000	-0.304875000	1.843327000
C	4.747728000	-0.507827000	3.210844000
H	5.576436000	-0.849471000	1.192062000
H	5.258673000	-1.247865000	3.811432000
N	0.863663000	0.824188000	0.305482000
C	2.077212000	1.098963000	-0.320555000
C	-0.142343000	1.425973000	-0.420804000
C	1.775178000	1.823711000	-1.527473000
C	0.425834000	2.054098000	-1.571733000
H	2.524766000	2.190318000	-2.217012000
H	-0.124551000	2.624693000	-2.308131000
N	1.367510000	0.206299000	4.178047000
C	0.428356000	-0.353201000	4.987979000
C	2.641240000	0.007414000	4.630134000
C	1.147528000	-0.811714000	6.133711000
C	2.507020000	-0.599962000	5.907032000
H	0.708015000	-1.267800000	7.010948000
H	3.317326000	-0.844379000	6.580264000
C	-0.905267000	-0.436135000	4.550916000
C	3.397503000	0.834891000	0.099613000
C	-1.464236000	1.378288000	0.026595000
B	0.419024000	-0.342271000	1.272604000
H	1.331587000	-0.626541000	1.988744000
C	0.010538000	-1.721531000	0.511179000
C	0.036892000	-1.905908000	-0.881587000
C	-0.337983000	-2.849023000	1.280977000
C	-0.282616000	-3.130850000	-1.475349000
C	-0.663031000	-4.075476000	0.701658000
C	-0.639639000	-4.223588000	-0.686705000
H	0.317132000	-1.082852000	-1.534127000
H	-0.351714000	-2.775613000	2.366062000
H	-0.251421000	-3.228703000	-2.559370000
H	-0.928651000	-4.919896000	1.335526000
H	-0.890055000	-5.178466000	-1.144893000
C	2.578251000	2.315792000	2.636229000
H	1.552052000	2.317132000	2.269117000
H	2.582547000	2.626780000	3.679938000
H	3.160175000	3.032280000	2.051596000
H	1.206566000	0.244452000	3.176105000
H	4.133660000	0.815359000	-0.700902000
H	-1.635480000	-0.774145000	5.279770000
H	-2.247403000	1.819311000	-0.579419000

PhBOB(cor) *cisoid* dipyrromethene/dipyrromethene

C	-0.709275000	0.295211000	-5.156474000
C	-0.240517000	-0.277803000	-3.919275000
H	-1.084503000	-0.281468000	-5.991914000
N	0.113063000	0.778226000	-3.107100000
C	-0.408583000	-1.657855000	-3.633901000
H	-0.623518000	-2.233930000	-4.530554000
C	-0.720581000	1.663009000	-5.028400000
N	-0.299552000	-0.364790000	0.637109000
C	-0.981934000	-1.208958000	1.504171000
H	-2.166725000	-4.802262000	-0.720611000
H	-1.084965000	2.386279000	-5.745849000
H	-1.495653000	-4.301748000	-3.255056000
C	-0.735305000	0.824140000	2.487162000
C	-0.233254000	1.963646000	-3.720579000
H	-1.704290000	-0.837556000	3.576697000
C	-0.366314000	4.075261000	-0.573954000
C	-0.017160000	3.140967000	-1.597844000
H	-0.817833000	1.648706000	3.181491000
N	0.332468000	1.954836000	-0.989495000
C	-1.209160000	-2.834088000	-0.292211000
C	-0.326715000	3.398906000	0.623973000
C	-0.208416000	3.162023000	-2.986773000
H	-0.497785000	4.087159000	-3.472577000
H	-0.687108000	5.095705000	-0.736471000
H	-0.627548000	3.779576000	1.590257000
C	0.051564000	2.040936000	0.350855000
C	-1.382703000	-2.477064000	1.047959000
H	-1.904813000	-3.147935000	1.719079000
C	-0.194006000	0.908578000	1.177939000
C	-1.267223000	-3.685914000	-2.395272000
C	-0.626272000	-2.405683000	-2.467277000
C	-1.204273000	-0.465997000	2.692483000
N	-0.546763000	-1.962190000	-1.151220000
C	-1.625205000	-3.941011000	-1.088478000
B	1.123076000	0.919566000	-1.903632000
B	0.199413000	-0.847163000	-0.635000000
O	1.262605000	-0.346318000	-1.256611000
C	2.574348000	1.506736000	-2.341577000
C	3.052839000	1.477793000	-3.661453000
C	3.454742000	1.999422000	-1.361917000
C	4.330819000	1.932999000	-3.994832000
C	4.734834000	2.455057000	-1.680518000
C	5.178011000	2.429316000	-3.004377000
H	2.422487000	1.091786000	-4.458791000
H	3.140893000	2.028240000	-0.320311000
H	4.662827000	1.900175000	-5.031048000
H	5.387425000	2.832221000	-0.895285000
H	6.172625000	2.789367000	-3.259821000

PhBOB(cor) *cisoid* dipyrromethene/bipyrrole (BPh in dipyr-B)

C	-1.009123000	0.496908000	-5.657385000
C	-0.740143000	-0.372108000	-4.557401000
H	-1.493491000	0.207473000	-6.580620000
N	-0.129469000	0.344368000	-3.546184000
C	-1.097684000	-1.709337000	-4.359875000
H	-1.579440000	-2.248724000	-5.167712000
C	-0.602202000	1.746787000	-5.280772000
N	-0.228065000	0.388740000	0.488346000
C	-0.501258000	-0.790562000	1.129484000
H	-1.600965000	-4.351413000	-0.583990000
H	-0.723869000	2.666940000	-5.837499000
H	-2.083264000	-4.255688000	-3.220439000
C	-1.150999000	0.988372000	2.435085000
C	-0.105113000	1.684561000	-3.925822000
H	-1.372588000	-1.091556000	3.162049000
C	-0.461720000	4.335113000	-1.134273000
C	-0.038305000	3.154114000	-1.814186000
H	-1.565486000	1.571286000	3.245963000
N	-0.033532000	2.176733000	-0.854538000
C	-0.593312000	-2.379886000	-0.893201000
C	-0.783015000	4.007245000	0.188947000
C	0.046698000	2.881836000	-3.192796000
H	0.001429000	3.768332000	-3.819107000
H	-0.595314000	5.304433000	-1.596333000
H	-1.174328000	4.684499000	0.937004000
C	-0.541610000	2.630352000	0.354150000
C	-0.537296000	-2.036289000	0.475776000
H	-0.794790000	-2.865931000	1.127876000
C	-0.671459000	1.487510000	1.209172000
C	-1.529050000	-3.542613000	-2.624842000
C	-0.987666000	-2.311280000	-3.102452000
C	-1.033309000	-0.406095000	2.396762000
N	-0.361511000	-1.653791000	-2.060332000
C	-1.269265000	-3.594702000	-1.283103000
B	0.748994000	-0.605295000	-2.571501000
B	0.405882000	0.807963000	-0.738595000
O	1.277477000	0.154953000	-1.486678000
C	1.967103000	-1.321120000	-3.375370000
C	2.818702000	-0.541270000	-4.178823000
C	2.310637000	-2.674283000	-3.223584000
C	3.939495000	-1.080592000	-4.810880000
C	3.429462000	-3.227488000	-3.851785000
C	4.248787000	-2.432779000	-4.653262000
H	2.611944000	0.518160000	-4.312718000
H	1.702222000	-3.322390000	-2.597483000
H	4.573659000	-0.444122000	-5.425245000
H	3.661592000	-4.281666000	-3.711624000
H	5.120561000	-2.859666000	-5.145060000

PhBOB(cor) *cisoid* dipyrromethene/bipyrrole (BPh in bipyrrole)

C	-1.210906000	3.453717000	-5.082739000
C	-1.519989000	2.327090000	-4.275007000
H	-1.700940000	3.701036000	-6.014730000
N	-0.676315000	2.354338000	-3.164358000
C	-2.453381000	1.300854000	-4.423473000
H	-3.088753000	1.279104000	-5.300093000
C	-0.224910000	4.166601000	-4.444294000
N	-0.371896000	0.892011000	0.610931000
C	-1.280490000	-0.082605000	0.880021000
H	-3.778249000	-2.239483000	-1.710357000
H	0.200684000	5.108273000	-4.764946000
H	-4.259587000	-1.032437000	-4.049263000
C	-1.204331000	1.355221000	2.660194000
C	0.105202000	3.525804000	-3.208056000
H	-2.508250000	-0.427243000	2.724191000
C	0.886979000	4.960408000	0.212864000
C	0.921175000	3.937488000	-0.800109000
H	-1.422125000	1.864257000	3.589105000
N	0.652088000	2.763501000	-0.170440000
C	-2.192169000	-0.706203000	-1.443906000
C	0.461714000	4.379742000	1.398622000
C	0.824317000	4.171436000	-2.192319000
H	1.186412000	5.148960000	-2.501024000
H	1.036580000	6.017317000	0.032384000
H	0.248813000	4.886550000	2.329906000
C	0.282953000	2.999506000	1.126871000
C	-1.933067000	-0.892838000	-0.079843000
H	-2.533189000	-1.690761000	0.350125000
C	-0.365248000	1.821989000	1.618368000
C	-3.499057000	-0.774529000	-3.324739000
C	-2.604990000	0.323561000	-3.439986000
C	-1.751877000	0.158795000	2.217718000
N	-1.779855000	0.321932000	-2.314733000
C	-3.240338000	-1.399376000	-2.129328000
B	-0.582494000	1.161293000	-2.324404000
B	0.810759000	1.200485000	-0.384735000
O	0.549855000	0.803139000	-1.721915000
C	2.243914000	0.658487000	0.146690000
C	3.436548000	1.177337000	-0.388072000
C	2.370378000	-0.352308000	1.112657000
C	4.689008000	0.724858000	0.028583000
C	3.618372000	-0.817212000	1.535000000
C	4.785735000	-0.275639000	0.997995000
H	3.394124000	1.955168000	-1.147615000
H	1.480666000	-0.795236000	1.553612000
H	5.591518000	1.155876000	-0.400952000
H	3.676248000	-1.601444000	2.287647000
H	5.760066000	-0.628198000	1.330405000

PhBOB(cor) *transoid* dipyrromethene/dipyrromethene

C	-0.057894000	2.259705000	3.479120000
C	-0.210589000	1.094042000	2.636218000
H	0.192867000	2.228336000	4.531762000
N	-0.571933000	1.606674000	1.410037000
C	0.058179000	-0.267366000	3.013988000
H	0.103523000	-0.366819000	4.097390000
C	-0.196966000	3.392133000	2.706783000
N	0.510724000	-1.267296000	-1.340697000
C	0.476345000	-2.605441000	-1.671642000
H	0.203076000	-4.884541000	2.176771000
H	-0.078786000	4.417904000	3.030895000
H	0.047738000	-3.012958000	4.051027000
C	0.370081000	-1.308058000	-3.552070000
C	-0.460572000	2.965118000	1.356533000
H	0.385689000	-3.514805000	-3.711731000
C	0.151093000	3.278486000	-2.446038000
C	-0.268260000	2.910460000	-1.123361000
H	0.262542000	-1.005043000	-4.585485000
N	-0.344296000	1.548014000	-1.120896000
C	0.400087000	-3.170889000	0.742749000
C	0.391397000	2.110227000	-3.151603000
C	-0.396897000	3.614726000	0.101151000
H	-0.306804000	4.695573000	0.084780000
H	0.305893000	4.288369000	-2.801681000
H	0.772054000	2.039899000	-4.161769000
C	0.134323000	0.997381000	-2.285833000
C	0.457025000	-3.557867000	-0.613395000
H	0.441783000	-4.612894000	-0.860568000
C	0.383563000	-0.426691000	-2.438303000
C	0.192874000	-2.838217000	2.992624000
C	0.255479000	-1.533095000	2.383920000
C	0.421111000	-2.627144000	-3.094289000
N	0.442928000	-1.825810000	1.037386000
C	0.266369000	-3.816302000	2.015849000
B	0.699561000	-0.868122000	0.022513000
O	0.965973000	0.367599000	0.354163000
B	-0.540411000	0.778796000	0.162443000
C	-1.934428000	-0.130015000	0.056975000
C	-2.601544000	-0.306248000	-1.173837000
C	-2.664453000	-0.551528000	1.189204000
C	-3.861943000	-0.896320000	-1.277389000
C	-3.921930000	-1.148661000	1.100970000
C	-4.531040000	-1.336214000	-0.138228000
H	-2.153976000	0.044011000	-2.095479000
H	-2.267291000	-0.401467000	2.184351000
H	-4.322244000	-1.000009000	-2.258090000
H	-4.429850000	-1.457874000	2.012429000
H	-5.513597000	-1.797754000	-0.211982000

PhBOB(cor) *transoid* dipyrromethene/bipyrrole (BPh in dipyr-B)

C	-0.686893000	1.640214000	4.433878000
C	-0.805849000	0.396815000	3.718231000
H	-0.619195000	1.743132000	5.508705000
N	-0.866186000	0.714410000	2.396436000
C	-0.822497000	-0.958653000	4.117832000
H	-0.789527000	-1.189942000	5.176408000
C	-0.644649000	2.647844000	3.500102000
N	0.152185000	-0.912915000	-1.416593000
C	-0.204808000	-2.242666000	-1.440198000
H	-0.386103000	-5.019460000	1.820656000
H	-0.532829000	3.705897000	3.698604000
H	-0.575220000	-3.980104000	4.274584000
C	-0.437609000	-1.266507000	-3.526666000
C	-0.705572000	2.067856000	2.174458000
H	-0.795634000	-3.430769000	-3.239438000
C	-0.718974000	3.259140000	-1.592218000
C	-0.391933000	2.500731000	-0.422449000
H	-0.685915000	-1.133526000	-4.571033000
N	0.034901000	1.297622000	-0.935949000
C	-0.610327000	-2.905402000	1.099816000
C	-0.598691000	2.443828000	-2.727814000
C	-0.595207000	2.804613000	0.958297000
H	-0.727006000	3.871801000	1.125613000
H	-1.090342000	4.275683000	-1.589862000
H	-0.848611000	2.731561000	-3.740188000
C	-0.165570000	1.168915000	-2.298961000
C	-0.420583000	-3.081959000	-0.302100000
H	-0.489894000	-4.131525000	-0.581361000
C	-0.088719000	-0.249373000	-2.610020000
C	-0.637791000	-3.447686000	3.334700000
C	-0.798812000	-2.023384000	3.190686000
C	-0.489145000	-2.480299000	-2.822623000
N	-0.842718000	-1.769551000	1.852605000
C	-0.541754000	-3.978387000	2.072811000
B	-0.911219000	-0.351986000	1.325516000
O	0.579367000	-0.239707000	0.892853000
B	0.346948000	0.027749000	-0.356851000
C	-2.405366000	-0.193935000	0.569290000
C	-2.857176000	-0.295386000	-0.756901000
C	-3.438726000	-0.064178000	1.530373000
C	-4.211019000	-0.251520000	-1.105650000
C	-4.792071000	-0.031865000	1.199771000
C	-5.194649000	-0.120070000	-0.131683000
H	-2.168367000	-0.413053000	-1.577705000
H	-3.198530000	0.006082000	2.585266000
H	-4.487614000	-0.327049000	-2.155697000
H	-5.531211000	0.063902000	1.992793000
H	-6.248659000	-0.090576000	-0.400534000

PhBOB(cor) *transoid* dipyrromethene/bipyrrole (BPh in bipyrrole)

C	-0.699511000	1.747459000	4.339022000
C	-0.693873000	0.482391000	3.679084000
H	-0.817825000	1.900302000	5.403497000
N	-0.515925000	0.764993000	2.336337000
C	-0.819481000	-0.867445000	4.075090000
H	-0.933554000	-1.095617000	5.128178000
C	-0.539654000	2.731684000	3.380273000
N	-0.888325000	-0.794875000	-1.701831000
C	-0.465566000	-2.089120000	-1.586150000
H	-0.855606000	-4.897368000	1.653890000
H	-0.525200000	3.797912000	3.565476000
H	-1.056654000	-3.925752000	4.119554000
C	0.432646000	-1.129194000	-3.477658000
C	-0.447345000	2.142149000	2.073964000
H	0.726288000	-3.279477000	-3.075758000
C	0.430564000	3.273315000	-1.572306000
C	-0.331568000	2.581285000	-0.559728000
H	1.007741000	-0.968208000	-4.379463000
N	-0.828292000	1.478842000	-1.198392000
C	-0.640436000	-2.779206000	0.989834000
C	0.520500000	2.460221000	-2.695544000
C	-0.316542000	2.855106000	0.848426000
H	-0.065824000	3.896510000	1.046915000
H	0.926075000	4.226352000	-1.436110000
H	1.089959000	2.662300000	-3.592635000
C	-0.229993000	1.279610000	-2.412888000
C	-0.510409000	-2.925619000	-0.420570000
H	-0.326007000	-3.969177000	-0.672871000
C	-0.262700000	-0.136657000	-2.723719000
C	-0.910210000	-3.350961000	3.214814000
C	-0.805771000	-1.929319000	3.143984000
C	0.281003000	-2.332612000	-2.797400000
N	-0.630208000	-1.635608000	1.804127000
C	-0.797790000	-3.852868000	1.931357000
B	-0.312811000	-0.302782000	1.414260000
O	0.076544000	-0.050192000	0.196174000
B	-1.199774000	0.152904000	-0.565530000
C	-2.781752000	0.079144000	-0.125308000
C	-3.650573000	0.106701000	-1.239573000
C	-3.413669000	0.054025000	1.128552000
C	-5.038210000	0.107247000	-1.116054000
C	-4.805070000	0.048293000	1.267471000
C	-5.629873000	0.075205000	0.146959000
H	-3.237192000	0.129087000	-2.243626000
H	-2.840255000	0.039006000	2.044804000
H	-5.656728000	0.130461000	-2.011053000
H	-5.238164000	0.023883000	2.265433000
H	-6.712671000	0.071598000	0.253576000

[B₂(corrole)]⁺ dipyrromethene/dipyrromethene

C	2.541359000	0.000000000	3.213593000
C	1.302118000	0.000000000	2.503630000
H	2.630004000	0.000000000	4.291382000
N	1.658804000	0.000000000	1.152018000
C	0.000000000	0.000000000	3.041071000
H	0.000000000	0.000000000	4.127492000
C	3.586022000	0.000000000	2.310358000
N	-1.391262000	0.000000000	-1.247533000
C	-2.766142000	0.000000000	-1.440417000
H	-4.641198000	0.000000000	2.547219000
H	4.641198000	0.000000000	2.547219000
H	-2.630004000	0.000000000	4.291382000
C	-1.715096000	0.000000000	-3.464152000
C	3.039067000	0.000000000	0.995453000
H	-3.917149000	0.000000000	-3.352901000
C	2.959367000	0.000000000	-2.851043000
C	2.766142000	0.000000000	-1.440417000
H	-1.533702000	0.000000000	-4.529914000
N	1.391262000	0.000000000	-1.247533000
C	-3.039067000	0.000000000	0.995453000
C	1.715096000	0.000000000	-3.464152000
C	3.584738000	0.000000000	-0.302192000
H	4.662015000	0.000000000	-0.419460000
H	3.917149000	0.000000000	-3.352901000
H	1.533702000	0.000000000	-4.529914000
C	0.708812000	0.000000000	-2.459714000
C	-3.584738000	0.000000000	-0.302192000
H	-4.662015000	0.000000000	-0.419460000
C	-0.708812000	0.000000000	-2.459714000
C	-2.541359000	0.000000000	3.213593000
C	-1.302118000	0.000000000	2.503630000
C	-2.959367000	0.000000000	-2.851043000
N	-1.658804000	0.000000000	1.152018000
C	-3.586022000	0.000000000	2.310358000
B	-0.798690000	0.000000000	0.038159000
B	0.798690000	0.000000000	0.038159000

[B₂(corrole)]⁺ dipyrromethene/bipyrrole

C	0.000000000	-2.572616000	-3.363906000
C	0.000000000	-1.222598000	-2.924109000
H	0.000000000	-2.891521000	-4.397035000
N	0.000000000	-1.234365000	-1.529174000
C	0.000000000	0.000000000	-3.601754000
H	0.000000000	0.000000000	-4.685405000
C	0.000000000	-3.376944000	-2.249201000
N	0.000000000	1.109628000	1.665411000
C	0.000000000	2.475157000	1.507196000
H	0.000000000	4.458408000	-2.239111000
H	0.000000000	-4.458408000	-2.239111000
H	0.000000000	2.891521000	-4.397035000
C	0.000000000	1.918557000	3.740916000
C	0.000000000	-2.570220000	-1.068848000
H	0.000000000	4.036383000	3.103174000
C	0.000000000	-2.988135000	2.837155000
C	0.000000000	-2.475157000	1.507196000
H	0.000000000	2.002497000	4.818758000
N	0.000000000	-1.109628000	1.665411000
C	0.000000000	2.570220000	-1.068848000
C	0.000000000	-1.918557000	3.740916000
C	0.000000000	-3.087290000	0.241662000
H	0.000000000	-4.172736000	0.266481000
H	0.000000000	-4.036383000	3.103174000
H	0.000000000	-2.002497000	4.818758000
C	0.000000000	-0.720330000	2.993510000
C	0.000000000	3.087290000	0.241662000
H	0.000000000	4.172736000	0.266481000
C	0.000000000	0.720330000	2.993510000
C	0.000000000	2.572616000	-3.363906000
C	0.000000000	1.222598000	-2.924109000
C	0.000000000	2.988135000	2.837155000
N	0.000000000	1.234365000	-1.529174000
C	0.000000000	3.376944000	-2.249201000
B	0.000000000	0.000000000	0.791291000
B	0.000000000	0.000000000	-0.804566000

B₂(corrole) dipyrromethene/dipyrromethene

C	-2.536782000	3.216857000	0.000000000
C	-2.135862000	1.849839000	0.000000000
H	-3.566825000	3.549016000	0.000000000
N	-0.729010000	1.885859000	0.000000000
C	-2.958323000	0.708425000	0.000000000
H	-4.015617000	0.962096000	0.000000000
C	-1.418332000	4.030448000	0.000000000
N	0.893499000	-1.656632000	0.000000000
C	0.760487000	-3.043738000	0.000000000
H	-3.571195000	-3.920185000	0.000000000
H	-1.407685000	5.112157000	0.000000000
H	-4.788313000	-1.548586000	0.000000000
C	2.968486000	-2.471307000	0.000000000
C	-0.257432000	3.197827000	0.000000000
H	2.337808000	-4.606542000	0.000000000
C	3.458893000	2.234502000	0.000000000
C	2.057641000	2.369209000	0.000000000
H	4.047638000	-2.543267000	0.000000000
N	1.548073000	1.072369000	0.000000000
C	-1.678635000	-2.734455000	0.000000000
C	3.766655000	0.858368000	0.000000000
C	1.122710000	3.436268000	0.000000000
H	1.482055000	4.458378000	0.000000000
H	4.171821000	3.047612000	0.000000000
H	4.761360000	0.433801000	0.000000000
C	2.572033000	0.125695000	0.000000000
C	-0.556067000	-3.571706000	0.000000000
H	-0.698622000	-4.645737000	0.000000000
C	2.235613000	-1.276888000	0.000000000
C	-3.719532000	-1.718885000	0.000000000
C	-2.742846000	-0.681807000	0.000000000
C	2.070724000	-3.558621000	0.000000000
N	-1.505165000	-1.351063000	0.000000000
C	-3.090805000	-2.950908000	0.000000000
B	-0.218587000	-0.775534000	0.000000000
B	0.157694000	0.790259000	0.000000000

[B₂(corrole)]⁻ dipyrromethene/dipyrromethene

C	-2.545566000	3.217758000	0.000000000
C	-2.145837000	1.852459000	0.000000000
H	-3.582294000	3.543506000	0.000000000
N	-0.722966000	1.889794000	0.000000000
C	-2.966366000	0.710223000	0.000000000
H	-4.028827000	0.965535000	0.000000000
C	-1.428509000	4.042926000	0.000000000
N	0.896785000	-1.669091000	0.000000000
C	0.763996000	-3.067560000	0.000000000
H	-3.592704000	-3.927911000	0.000000000
H	-1.423786000	5.128255000	0.000000000
H	-4.800249000	-1.537935000	0.000000000
C	2.975352000	-2.474999000	0.000000000
C	-0.252872000	3.214961000	0.000000000
H	2.331751000	-4.634130000	0.000000000
C	3.464746000	2.259205000	0.000000000
C	2.071854000	2.389449000	0.000000000
H	4.058892000	-2.544697000	0.000000000
N	1.557212000	1.082317000	0.000000000
C	-1.682530000	-2.752084000	0.000000000
C	3.775019000	0.858741000	0.000000000
C	1.119322000	3.462980000	0.000000000
H	1.474764000	4.490834000	0.000000000
H	4.179984000	3.075129000	0.000000000
H	4.772686000	0.430175000	0.000000000
C	2.589780000	0.132957000	0.000000000
C	-0.571023000	-3.593995000	0.000000000
H	-0.719877000	-4.671241000	0.000000000
C	2.247745000	-1.290981000	0.000000000
C	-3.728194000	-1.716032000	0.000000000
C	-2.753492000	-0.680126000	0.000000000
C	2.064199000	-3.582594000	0.000000000
N	-1.501843000	-1.357564000	0.000000000
C	-3.105762000	-2.957909000	0.000000000
B	-0.215730000	-0.781224000	0.000000000
B	0.163810000	0.793872000	0.000000000