Supplementary Information to

The sEDA(=) and pEDA(=) Descriptors of the Double Bonded Substituent Effect

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1. FA molecules optimized at the DFT/B3LYP/aug-cc-pVDZ level.

C1H3Al Gibbs Free Energy=-282.264570 a.u.

0 1

C	0.00344300	1.17020800	0.00000000
H	0.23723900	1.72603300	0.91535700
H	0.23723900	1.72603300	-0.91535700
Al	0.00344300	-0.64250300	0.00000000
H	-0.53989800	-2.12078000	0.00000000

CH2Be Gibbs Free Energy=-53.905600 a.u.

0 1

C	0.00000000	0.00000000	0.41274200
H	0.00000000	0.92338600	1.00092000
H	0.00000000	-0.92338600	1.00092000
Be	0.00000000	0.00000000	-1.11957300

C2H4 Gibbs Free Energy=-78.568408 a.u.

0 1

C	0.00000000	0.00000000	0.66759600
H	0.00000000	0.92887300	1.24079900
H	0.00000000	-0.92887300	1.24079900
C	0.00000000	0.00000000	-0.66759600
H	0.00000000	-0.92887300	-1.24079900
H	0.00000000	0.92887300	-1.24079900

CH3B Gibbs Free Energy=-64.683737 a.u.

0 1

C	0.00000000	0.00000000	0.59259300
H	0.00000000	0.92179300	1.17984500
H	0.00000000	-0.92179300	1.17984500
B	0.00000000	0.00000000	-0.78951400
H	0.00000000	0.00000000	-1.96768000

C2H2Cl2 Gibbs Free Energy=-997.828843 a.u.

0 1

C	0.00000000	0.00000000	1.75932400
H	0.00000000	0.93874000	2.30887100
H	0.00000000	-0.93874000	2.30887100
C	0.00000000	0.00000000	0.42812500
Cl	0.00000000	1.46559500	-0.52183600
Cl	0.00000000	-1.46559500	-0.52183600

CH2Mg Gibbs Free Energy=-239.261146 a.u.

0 1

C	0.00000000	0.00000000	-1.12273900
H	0.00000000	0.97225500	-1.61389200

H	0.00000000	-0.97225500	-1.61389200
Mg	0.00000000	0.00000000	0.83035100

CH3Ga Gibbs Free Energy=-1964.697388 a.u.

0 1

C	-0.00159800	1.45374100	0.00000000
H	0.24099700	1.98558100	0.92466000
H	0.24099700	1.98558100	-0.92466000
H	-0.42285000	-1.83516100	0.00000000
Ga	-0.00159800	-0.35027300	0.00000000

C2H3Cl Gibbs Free Energy=-538.203167 a.u.

0 1

C	1.29985700	1.05030700	0.00000000
H	2.06536500	0.27591100	0.00000000
H	1.61833200	2.09288800	0.00000000
C	0.00000000	0.76838200	0.00000000
H	-0.79286300	1.51460800	0.00000000
Cl	-0.62882200	-0.87032600	0.00000000

CH4Ge Gibbs Free Energy=-2117.454781 a.u.

0 1

C	0.00000000	0.00000000	-1.45574100
H	0.00000000	0.93002700	-2.02362100
H	0.00000000	-0.93002700	-2.02362100
Ge	0.00000000	0.00000000	0.32763600
H	0.00000000	1.29317900	1.14866600
H	0.00000000	-1.29317900	1.14866600

CH3As Gibbs Free Energy=-2275.753080 a.u.

0 1

C	0.03519900	1.42720900	0.00000000
H	0.98874500	1.95966400	0.00000000
H	-0.86350300	2.04520600	0.00000000
H	-1.49801600	-0.52439100	0.00000000
As	0.03519900	-0.36496200	0.00000000

CH2NBF Gibbs Free Energy=-318.747508 a.u.

0 1

C	-0.47567500	-1.96878900	0.00000000
H	-0.01419600	-2.96662200	0.00000000
H	-1.57820000	-1.93930800	0.00000000
N	0.24455000	-0.93592500	0.00000000
B	0.11889500	0.46460200	0.00000000
F	0.11889500	1.16372900	1.14807700
F	0.11889500	1.16372900	-1.14807700

CH2S Gibbs Free Energy=-437.486582 a.u.

0 1

C	0.00000000	0.00000000	-1.03366300
H	0.00000000	0.93113200	-1.61368500
H	0.00000000	-0.93113200	-1.61368500
S	0.00000000	0.00000000	0.58933400

CH4Si Gibbs Free Energy=-329.947314 a.u.

0 1

C	0.00000000	0.00000000	-1.16368900
H	0.00000000	0.92503400	-1.74246100
H	0.00000000	-0.92503400	-1.74246100
Si	0.00000000	0.00000000	0.55449900
H	0.00000000	-1.25251300	1.35203300
H	0.00000000	1.25251300	1.35203300

CH2NF -193.836360

0 1

C	1.09388900	-0.06047400	0.00000000
H	1.99203500	0.55929600	0.00000000
H	1.14898300	-1.15191000	0.00000000
N	0.00000000	0.58279800	0.00000000
F	-1.07826100	-0.34712600	0.00000000

CH2NCl Gibbs Free Energy=-554.231227 a.u.

0 1

C	1.27135200	0.89714900	0.00000000
H	1.71012200	1.90098200	0.00000000
H	1.92864500	0.02082000	0.00000000
N	0.00000000	0.86633400	0.00000000
Cl	-0.66275800	-0.78641400	0.00000000

CH3NO Gibbs Free Energy=-169.824787 a.u.

0 1

C	1.14173600	-0.02747800	0.00000000
H	2.00855200	0.63237200	0.00000000
H	1.26410700	-1.11586200	0.00000000
N	0.00000000	0.53737900	0.00000000
O	-1.03632600	-0.40669000	0.00000000
H	-1.83246700	0.14022400	0.00000000

CH3P Gibbs Free Energy=-381.235508 a.u.

0 1

C	0.05705700	1.08046000	0.00000000
H	1.01141300	1.61223500	0.00000000
H	-0.83747900	1.70518000	0.00000000
P	0.05705700	-0.60064600	0.00000000
H	-1.37214000	-0.79048600	0.00000000

CH4N2 Gibbs Free Energy=-149.956582 a.u.

0 1

C	-1.15770600	0.16969700	0.00837200
H	-2.10530700	-0.36728500	0.03159500
H	-1.16948100	1.27073000	-0.02124500
N	-0.08058700	-0.51843600	0.00704100
N	1.11464200	0.14421200	-0.09391600
H	1.11761900	1.10748900	0.24698200
H	1.86502400	-0.40954600	0.30056000

CH3N Gibbs Free Energy=-94.627768 a.u.

0 1

C	0.05646600	0.58699500	0.00000000
H	-0.85017500	1.21361300	0.00000000
H	1.01889300	1.11465700	0.00000000
N	0.05646600	-0.68565800	0.00000000
H	-0.90277600	-1.05063600	0.00000000

CH4NB Gibbs Free Energy=-120.096750 a.u.

0 1

C	-0.26727700	-1.20016200	0.00000000
H	-1.30609900	-1.56033000	0.00000000
H	0.52692700	-1.96109200	0.00000000
N	0.00000000	0.02352000	0.00000000
B	0.30371600	1.34755400	0.00000000
H	0.43212600	1.90999200	1.05332800
H	0.43212600	1.90999200	-1.05332800

CH2SO Gibbs Free Energy=-512.690631 a.u.

0 1

C	1.25469900	-0.59335100	0.00000000
H	2.24812500	-0.14389200	0.00000000
H	1.11883500	-1.67493300	0.00000000
O	-1.36189500	-0.22751000	0.00000000
S	0.00000000	0.44993800	0.00000000

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2. CPDA molecules optimized at the DFT/B3LYP/aug-cc-pVDZ level.

C5H6 Gibbs Free Energy=-194.058127 a.u.

0 1

C	0.00000000	0.00000000	1.21900300
H	0.88054400	0.00000000	1.88431400
H	-0.88054400	0.00000000	1.88431400
C	0.00000000	1.18149600	0.28374900
H	0.00000000	2.21928400	0.61139200
C	0.00000000	0.73551800	-0.99409000
H	0.00000000	1.35440800	-1.89066800
C	0.00000000	-1.18149600	0.28374900
H	0.00000000	-2.21928400	0.61139200
C	0.00000000	-0.73551800	-0.99409000
H	0.00000000	-1.35440800	-1.89066800

C5H4SeO2 -2744.760459

0 1

C	-1.53582400	-1.19440700	-0.00011200
H	-1.17463300	-2.21694000	-0.00014200
C	-2.82452200	-0.73266300	-0.00016000
H	-3.71694100	-1.35495000	-0.00030300
C	-1.53534400	1.19412000	0.00027100
H	-1.17360800	2.21645700	0.00049400
C	-2.82421200	0.73293400	0.00007800
H	-3.71643600	1.35549900	0.00026000
C	-0.70859200	-0.00035300	0.00041700
O	1.86088100	-1.43908800	0.00070800
O	1.85994000	1.43951600	0.00019000
Se	1.07605900	-0.00003700	-0.00030800

C5H5NO -323.401589

0 1

C	0.86670400	-1.19616100	-0.00002100
H	0.76165100	-2.27690500	-0.00011100
C	2.00014500	-0.45415200	0.00019100
H	3.02019400	-0.83262800	0.00018600
C	0.28566100	1.11549500	-0.00016500
H	-0.29825400	2.02923600	-0.00013400
C	1.63636900	0.98285400	0.00001000
H	2.35809800	1.79823000	0.00031500
C	-0.27053600	-0.25100400	-0.00024300
N	-1.48975900	-0.67512000	-0.00007200
O	-2.40804500	0.36483500	0.00012700
H	-3.25907300	-0.09296500	0.00060100

C5H4SO Gibbs Free Energy=-666.273710 a.u.

0 1

C	0.50381000	1.52416400	0.00000000
H	-0.11282600	2.41833300	0.00000000
C	1.86215500	1.44058600	0.00000000
H	2.55631000	2.27837000	0.00000000
C	1.13854900	-0.76556800	0.00000000

H	1.06755500	-1.84803600	0.00000000
C	2.25600200	0.01788600	0.00000000
H	3.28472100	-0.33831800	0.00000000
C	0.00000000	0.14113600	0.00000000
S	-1.62484400	-0.19643200	0.00000000
O	-1.92016800	-1.68958200	0.00000000

C5H5As Gibbs Free Energy=-2429.337002 a.u.

0 1

C	1.25232800	1.03991400	0.00000000
H	2.24930100	0.60612700	0.00000000
C	0.92664100	2.36233700	0.00000000
H	1.62278700	3.19938800	0.00000000
C	-1.09619000	1.24477500	0.00000000
H	-2.15142500	0.98574100	0.00000000
C	-0.54439400	2.49022600	0.00000000
H	-1.08464000	3.43569300	0.00000000
C	0.00000000	0.26808700	0.00000000
H	-1.60613500	-1.63010100	0.00000000
As	-0.06849100	-1.54633000	0.00000000

C5H4NCl Gibbs Free Energy=-707.806680 a.u.

0 1

C	0.69909000	1.68645600	0.00000000
H	0.18227000	2.64092400	0.00000000
C	2.02500700	1.43251300	0.00000000
H	2.82433200	2.17056600	0.00000000
C	1.04643400	-0.67985600	0.00000000
H	0.85499000	-1.74698000	0.00000000
C	2.23899100	-0.04045400	0.00000000
H	3.21818500	-0.51639600	0.00000000
C	0.00000000	0.36715800	0.00000000
N	-1.28681000	0.34572300	0.00000000
Cl	-2.00760200	-1.26841700	0.00000000

C5H4NBr Gibbs Free Energy=-2821.751725 a.u.

0 1

C	-0.20416100	2.37048400	0.00000000
H	-1.18218600	2.84130600	0.00000000
C	1.01883200	2.94124200	0.00000000
H	1.23333400	4.00798900	0.00000000
C	1.46393400	0.65698400	0.00000000
H	1.93308600	-0.32076000	0.00000000
C	2.05555500	1.87334400	0.00000000
H	3.12789700	2.06181600	0.00000000
C	0.00000000	0.88828200	0.00000000
N	-1.03268000	0.12336200	0.00000000
Br	-0.68252400	-1.76674000	0.00000000

C5H4Se Gibbs Free Energy=-2594.416356 a.u.

0 1

C	0.00000000	1.18667800	-1.12976500
H	0.00000000	2.21008000	-0.76659400
C	0.00000000	0.74631300	-2.41116700
H	0.00000000	1.36201300	-3.30924700

C	0.00000000	-1.18667800	-1.12976500
H	0.00000000	-2.21008000	-0.76659400
C	0.00000000	-0.74631300	-2.41116700
H	0.00000000	-1.36201300	-3.30924700
C	0.00000000	0.00000000	-0.24927500
Se	0.00000000	0.00000000	1.53348600

C5H4Be Gibbs Free Energy=-207.503114 a.u.

0 1

C	0.00000000	1.17128400	0.11680100
H	0.00000000	2.20747600	0.44734700
C	0.00000000	0.72179300	-1.18894900
H	0.00000000	1.35310900	-2.07682100
C	0.00000000	-1.17128400	0.11680100
H	0.00000000	-2.20747600	0.44734700
C	0.00000000	-0.72179300	-1.18894900
H	0.00000000	-1.35310900	-2.07682100
C	0.00000000	0.00000000	0.98638800
Be	0.00000000	0.00000000	2.55159900

C5H6Ge Gibbs Free Energy=-2271.043021 a.u.

0 1

C	0.00000000	1.17486000	-1.15516900
H	0.00000000	2.20756800	-0.81556000
C	0.00000000	0.73041100	-2.45212300
H	0.00000000	1.35527100	-3.34358100
C	0.00000000	-1.17486000	-1.15516900
H	0.00000000	-2.20756800	-0.81556000
C	0.00000000	-0.73041100	-2.45212300
H	0.00000000	-1.35527100	-3.34358100
C	0.00000000	0.00000000	-0.28784800
H	0.00000000	-1.29571100	2.33740400
H	0.00000000	1.29571100	2.33740400
Ge	0.00000000	0.00000000	1.52056500

C6H4Cl2 Gibbs Free Energy=-1151.406659 a.u.

0 1

C	0.00000000	1.18303200	-1.45550800
H	0.00000000	2.21157200	-1.10979200
C	0.00000000	0.73655900	-2.73959200
H	0.00000000	1.35840000	-3.63286000
C	0.00000000	-1.18303200	-1.45550800
H	0.00000000	-2.21157200	-1.10979200
C	0.00000000	-0.73655900	-2.73959200
H	0.00000000	-1.35840000	-3.63286000
C	0.00000000	0.00000000	-0.57853800
C	0.00000000	0.00000000	0.77355400
Cl	0.00000000	1.45496600	1.72518800
Cl	0.00000000	-1.45496600	1.72518800

C5H6Si Gibbs Free Energy=-483.533146 a.u.

0 1

C	0.00000000	1.17404800	-0.58932100
H	0.00000000	2.20744100	-0.25125200
C	0.00000000	0.73057700	-1.88497000

H	0.00000000	1.35577600	-2.77625500
C	0.00000000	-1.17404800	-0.58932100
H	0.00000000	-2.20744100	-0.25125200
C	0.00000000	-0.73057700	-1.88497000
H	0.00000000	-1.35577600	-2.77625500
C	0.00000000	0.00000000	0.28685600
Si	0.00000000	0.00000000	2.02766200
H	0.00000000	-1.25489300	2.81904600
H	0.00000000	1.25489300	2.81904600

C5H4NBF2 Gibbs Free Energy=-472.325355 a.u.

0 1

C	1.46813600	1.50654600	0.00000000
H	2.52141200	1.24172000	0.00000000
C	0.90357600	2.73023600	0.00000000
H	1.42304000	3.68666100	0.00000000
C	-0.91448700	1.28213300	0.00000000
H	-1.90454300	0.83420600	0.00000000
C	-0.58649600	2.58932900	0.00000000
H	-1.27684900	3.43113200	0.00000000
C	0.36345900	0.50040900	0.00000000
N	0.52235300	-0.75861400	0.00000000
B	-0.25354600	-1.93028600	0.00000000
F	-0.58649600	-2.54910600	1.14664500
F	-0.58649600	-2.54910600	-1.14664500

C5H4SeO Gibbs Free Energy=-2669.612202 a.u.

0 1

C	-0.97973200	1.60127200	0.00000000
H	-2.05988500	1.48305100	0.00000000
C	-0.26544200	2.76194000	0.00000000
H	-0.67652900	3.76944200	0.00000000
C	1.33495500	1.08031400	0.00000000
H	2.25504800	0.50521700	0.00000000
C	1.17475800	2.43722600	0.00000000
H	1.97487600	3.17547600	0.00000000
C	0.00000000	0.50703600	0.00000000
O	0.88966700	-2.18262100	0.00000000
Se	-0.47641400	-1.22938100	0.00000000

C5H4Mg Gibbs Free Energy=-392.879603 a.u.

0 1

C	0.00000000	1.17958800	-0.41026500
H	0.00000000	2.21373300	-0.07750000
C	0.00000000	0.71177500	-1.73583600
H	0.00000000	1.35043500	-2.61897200
C	0.00000000	-1.17958800	-0.41026500
H	0.00000000	-2.21373300	-0.07750000
C	0.00000000	-0.71177500	-1.73583600
H	0.00000000	-1.35043500	-2.61897200
C	0.00000000	0.00000000	0.39207800
Mg	0.00000000	0.00000000	2.39947500

C5H6B Gibbs Free Energy=-273.674969 a.u.

0 1

C	1.19633900	-0.56510300	0.00000000
H	2.22061700	-0.20395200	0.00000000
C	0.74932500	-1.84005900	0.00000000
H	1.36237600	-2.73950500	0.00000000
C	-1.19259100	-0.57075600	0.00000000
H	-2.21813000	-0.21320500	0.00000000
C	-0.73992400	-1.84362600	0.00000000
H	-1.34858100	-2.74603600	0.00000000
C	0.00000000	0.32471000	0.00000000
N	-0.00368700	1.58791100	0.00000000
B	-0.00913100	2.94132600	0.00000000
H	-0.01186000	3.52484800	1.05215500
H	-0.01186000	3.52484800	-1.05215500

C5H4O Gibbs Free Energy=-268.092798 a.u.

0 1

C	0.00000000	1.20725200	-0.08704300
H	0.00000000	2.23317900	0.27078400
C	0.00000000	0.75245900	-1.35171000
H	0.00000000	1.35291700	-2.26023600
C	0.00000000	-1.20725200	-0.08704300
H	0.00000000	-2.23317900	0.27078400
C	0.00000000	-0.75245900	-1.35171000
H	0.00000000	-1.35291700	-2.26023600
C	0.00000000	0.00000000	0.82367400
O	0.00000000	0.00000000	2.03773800

C6H6 Gibbs Free Energy=-232.148398 a.u.

0 1

C	0.00000000	1.18135400	-0.12466500
H	0.00000000	2.21241700	0.22065000
C	0.00000000	0.73864700	-1.40887700
H	0.00000000	1.35646700	-2.30537400
C	0.00000000	-1.18135400	-0.12466500
H	0.00000000	-2.21241700	0.22065000
C	0.00000000	-0.73864700	-1.40887700
H	0.00000000	-1.35646700	-2.30537400
C	0.00000000	0.00000000	0.76085400
C	0.00000000	0.00000000	2.10898400
H	0.00000000	-0.93117600	2.67646400
H	0.00000000	0.93117600	2.67646400

C5H4NF Gibbs Free Energy=-347.410845 a.u.

0 1

C	1.47031200	0.17717200	0.00000000
H	2.20411900	0.97672000	0.00000000
C	1.66507500	-1.15988900	0.00000000
H	2.62558900	-1.67071600	0.00000000
C	-0.65176200	-0.93323700	0.00000000
H	-1.72310500	-1.09698400	0.00000000
C	0.34596500	-1.84815200	0.00000000
H	0.21974100	-2.92944700	0.00000000
C	0.00000000	0.39252700	0.00000000
N	-0.47290900	1.58648000	0.00000000
F	-1.88816800	1.53828200	0.00000000

C6H5Cl Gibbs Free Energy=-691.781624 a.u.

0 1

C	1.20817800	-0.45614700	0.00000000
H	1.21277600	-1.54166300	0.00000000
C	2.28095400	0.38050600	0.00000000
H	3.32720100	0.07969900	0.00000000
C	0.45221700	1.78603000	0.00000000
H	-0.20766300	2.64956900	0.00000000
C	1.81088100	1.77802600	0.00000000
H	2.45968600	2.65182200	0.00000000
C	0.00000000	0.37938800	0.00000000
C	-1.29641700	0.01248300	0.00000000
H	-2.11667400	0.72853800	0.00000000
Cl	-1.84765900	-1.63821600	0.00000000

C5H5Al Gibbs Free Energy=-435.860099 a.u.

0 1

C	0.00000000	1.16853500	-0.52197000
H	0.00000000	2.20651000	-0.19488500
C	0.00000000	0.72105600	-1.82980500
H	0.00000000	1.35185000	-2.71750100
C	0.00000000	-1.16853500	-0.52197000
H	0.00000000	-2.20651000	-0.19488500
C	0.00000000	-0.72105600	-1.82980500
H	0.00000000	-1.35185000	-2.71750100
C	0.00000000	0.00000000	0.34627500
H	0.00000000	0.00000000	3.74194700
Al	0.00000000	0.00000000	2.17126700

C5H5B Gibbs Free Energy=-218.265145 a.u.

0 1

C	0.00000000	1.17716800	-0.02557300
H	0.00000000	2.21006600	0.31188000
C	0.00000000	0.72718200	-1.31805700
H	0.00000000	1.35543300	-2.20722000
C	0.00000000	-1.17716800	-0.02557300
H	0.00000000	-2.21006600	0.31188000
C	0.00000000	-0.72718200	-1.31805700
H	0.00000000	-1.35543300	-2.20722000
C	0.00000000	0.00000000	0.86203000
H	0.00000000	0.00000000	3.43763300
B	0.00000000	0.00000000	2.26088400

....

3. BQA molecules optimized at the DFT/B3LYP/aug-cc-pVDZ level.

C6H8N2B2 Gibbs Free Energy=-392.609709 a.u.

0 1

C	-2.39900200	0.17439800	-0.00015400
C	-1.51959800	1.19793400	-0.00026700
C	0.38534100	-0.43858800	0.00056700
C	-0.49406300	-1.46212400	0.00068600
C	-1.94609200	-1.22533200	0.00026400
C	-0.06757200	0.96114400	-0.00006000
H	-3.47513200	0.34611000	-0.00036000
H	-1.85146800	2.23594900	-0.00053500
H	1.46147100	-0.61030300	0.00090600
H	-0.16219100	-2.50013900	0.00109900
N	0.76200200	1.92735400	-0.00046700
N	-2.77569400	-2.19151900	0.00025300
B	1.64669900	2.95032200	-0.00079000
H	2.03169100	3.39608500	-1.05171500
H	2.03149800	3.39687800	1.04987300
B	-3.65914000	-3.21554700	0.00023800
H	-4.04330500	-3.66231700	-1.05056800
H	-4.04388900	-3.66184400	1.05103100

C6H4S2 Gibbs Free Energy=-1027.403199 a.u.

0 1

C	0.00000000	1.24284800	0.67956400
H	0.00000000	2.17517300	1.24372600
C	0.00000000	1.24284800	-0.67956400
H	0.00000000	2.17517300	-1.24372600
C	0.00000000	0.00000000	-1.43721200
C	0.00000000	-1.24284800	-0.67956400
H	0.00000000	-2.17517300	-1.24372600
C	0.00000000	-1.24284800	0.67956400
H	0.00000000	-2.17517300	1.24372600
C	0.00000000	0.00000000	1.43721200
S	0.00000000	0.00000000	-3.10579500
S	0.00000000	0.00000000	3.10579500

C6H4S2O2 Gibbs Free Energy=-1177.814994 a.u.

0 1

C	1.24162600	-0.69248900	0.00000000
H	2.16673300	-1.26690800	0.00000000
C	1.24162600	0.67612300	0.00000000
H	2.18296400	1.22785600	0.00000000
C	0.00250100	1.39842400	0.00000000
C	-1.24162600	0.69248900	0.00000000
H	-2.16673300	1.26690800	0.00000000
C	-1.24162600	-0.67612300	0.00000000
H	-2.18296400	-1.22785600	0.00000000
C	-0.00250100	-1.39842400	0.00000000
O	-1.33936000	3.69369200	0.00000000
O	1.33936000	-3.69369200	0.00000000
S	-0.07442100	-3.10206600	0.00000000
S	0.07442100	3.10206600	0.00000000

C8H8 Gibbs Free Energy=-309.551101 a.u.

0 1

C	-1.63953900	0.21433800	0.00000000
C	-0.96392200	1.38619800	0.00000000
C	1.18758000	0.14565800	0.00000000
C	0.51197300	-1.02621000	0.00000000
C	-0.94953600	-1.07501600	0.00000000
C	0.49758900	1.43502200	0.00000000
H	-2.73080000	0.20827000	0.00000000
H	-1.50573200	2.33348900	0.00000000
H	2.27884500	0.15173000	0.00000000
H	1.05377900	-1.97349800	0.00000000
C	1.17609200	2.61145900	0.00000000
H	2.26548000	2.63714800	0.00000000
H	0.65303700	3.56741000	0.00000000
C	-1.62805900	-2.25144300	0.00000000
H	-2.71744800	-2.27710700	0.00000000
H	-1.10502100	-3.20740100	0.00000000

C6H4N2Cl2 Gibbs Free Energy=-1260.872503 a.u.

0 1

C	-2.43936900	-0.12711700	0.00000000
C	-1.78290100	1.05308800	0.00000000
C	0.42497200	-0.13482300	0.00000000
C	-0.23150000	-1.31502500	0.00000000
C	-1.69835600	-1.38533100	-0.00000100
C	-0.31604000	1.12343100	0.00000000
H	-3.52581900	-0.16278800	0.00000000
H	-2.31756700	2.00236000	0.00000000
H	1.51141500	-0.09918200	0.00000000
H	0.30313100	-2.26431500	0.00000000
N	0.14179200	2.34343600	0.00000000
N	-2.15629500	-2.60526800	0.00000000
Cl	1.89262500	2.51031300	0.00000000
Cl	-3.90717400	-2.77137700	0.00000000

C6H4N2Br2 Gibbs Free Energy=-5488.762002 a.u.

0 1

C	-2.43713700	-0.12822200	0.00000000
C	-1.78278800	1.05277400	0.00000000
C	0.42270500	-0.13365300	0.00000000
C	-0.23162100	-1.31467200	0.00000000
C	-1.70118900	-1.39008700	0.00000000
C	-0.31320400	1.12822200	0.00000000
H	-3.52432300	-0.16398400	0.00000000
H	-2.32070600	2.00035400	0.00000000
H	1.50989000	-0.09790900	0.00000000
H	0.30632100	-2.26223600	0.00000000
N	0.13836800	2.34874300	0.00000000
N	-2.15280700	-2.61058400	0.00000000
Br	2.03539900	2.58009000	0.00000000
Br	-4.04984800	-2.84177400	0.00000000

C6H6N2O2 Gibbs Free Energy=-492.062209 a.u.

0 1

C	-2.43774200	-0.18443300	-0.00013400
C	-1.82700200	1.02257600	-0.00013200
C	0.42419700	-0.07868000	-0.00013500
C	-0.18654600	-1.28568900	-0.00012800
C	-1.64079000	-1.40744100	-0.00036300

C	-0.37275500	1.14433500	-0.00036800
H	-3.52142100	-0.26602000	-0.00000700
H	-2.40041900	1.94948200	-0.00000200
H	1.50787300	0.00289500	-0.00000900
H	0.38686900	-2.21259600	0.00000500
N	0.08865300	2.36373200	-0.00040800
N	-2.10220600	-2.62682500	-0.00040600
O	1.48230600	2.39862400	-0.00034600
H	1.67323700	3.34514800	-0.00036200
O	-3.49585100	-2.66153900	-0.00034800
H	-3.68684700	-3.60804800	-0.00036600

C6H8Si2 Gibbs Free Energy=-812.316430 a.u.

0 1

C	0.01340900	-0.03589900	0.00983700
C	0.02350700	-0.08525000	1.45140600
C	1.31918500	-0.03225300	2.08319300
C	2.47553800	0.04119500	1.35470900
C	2.46543300	0.09043100	-0.08688700
C	1.16976200	0.03754800	-0.71866000
H	-0.94282000	-0.06278600	-0.51624200
H	1.38057600	-0.05587600	3.17293500
H	3.43177300	0.06803000	1.88078000
H	1.10836200	0.06114100	-1.80840400
Si	3.97279700	0.11331200	-1.03626000
H	5.26773400	0.35336100	-0.35391600
H	3.91625600	0.34988300	-2.49949800
Si	-1.48387400	-0.10799200	2.40083200
H	-2.77857200	-0.34896200	1.71831400
H	-1.42709900	-0.34523100	3.86396100

C6H4Se2O2 Gibbs Free Energy=-5184.498876 a.u.

0 1

C	1.29963700	-0.54729300	0.00000000
H	2.29669100	-0.99167300	0.00000000
C	1.15639000	0.82062100	0.00000000
H	2.01869700	1.48716300	0.00000000
C	-0.14775100	1.38811200	0.00000000
C	-1.29963700	0.54729300	0.00000000
H	-2.29669100	0.99167300	0.00000000
C	-1.15639000	-0.82062100	0.00000000
H	-2.01869700	-1.48716300	0.00000000
C	0.14775100	-1.38811200	0.00000000
Se	-0.38131200	3.23421900	0.00000000
Se	0.38131200	-3.23421900	0.00000000
O	1.15639000	3.90133100	0.00000000
O	-1.15639000	-3.90133100	0.00000000

C6H4S2O4 Gibbs Free Energy=-1328.161608 a.u.

0 1

C	0.03937300	-0.69055200	1.23404700
H	0.08235200	-1.24704300	2.16826800
C	-0.03937300	0.69055200	1.23404700
H	-0.08235200	1.24704300	2.16826800
C	-0.03087000	1.37857100	0.00000000
C	-0.03937300	0.69055200	-1.23404700
H	-0.08235200	1.24704300	-2.16826800

C	0.03937300	-0.69055200	-1.23404700
H	0.08235200	-1.24704300	-2.16826800
C	0.03087000	-1.37857100	0.00000000
S	-0.32527800	3.11631200	0.00000000
S	0.32527800	-3.11631200	0.00000000
O	0.03937300	3.74620100	1.31592700
O	0.03937300	3.74620100	-1.31592700
O	-0.03937300	-3.74620100	1.31592700
O	-0.03937300	-3.74620100	-1.31592700

C6H4Se2O4 Gibbs Free Energy=-5334.811426 a.u.

0 1

C	0.10054700	-0.69323700	1.22588800
H	0.18331400	-1.23736700	2.16576700
C	-0.10054700	0.69323700	1.22588800
H	-0.18331400	1.23736700	2.16576700
C	-0.14899800	1.35731400	0.00000000
C	-0.10054700	0.69323700	-1.22588800
H	-0.18331400	1.23736700	-2.16576700
C	0.10054700	-0.69323700	-1.22588800
H	0.18331400	-1.23736700	-2.16576700
C	0.14899800	-1.35731400	0.00000000
O	0.10054700	3.88628200	1.43262000
O	0.10054700	3.88628200	-1.43262000
O	-0.10054700	-3.88628200	1.43262000
O	-0.10054700	-3.88628200	-1.43262000
Se	-0.49777200	3.30127800	0.00000000
Se	0.49777200	-3.30127800	0.00000000

C6H6P2 Gibbs Free Energy=-914.894530 a.u.

0 1

C	-0.06717100	1.40369500	0.00000000
H	-0.10299500	2.49459800	0.00000000
C	-1.22880100	0.68966300	0.00000000
H	-2.18644800	1.21068300	0.00000000
C	-1.22880100	-0.75675200	0.00000000
C	0.06717100	-1.40369500	0.00000000
H	0.10299500	-2.49459800	0.00000000
C	1.22880100	-0.68966300	0.00000000
H	2.18644800	-1.21068300	0.00000000
C	1.22880100	0.75675200	0.00000000
P	-2.64978100	-1.75379200	0.00000000
H	-3.60511000	-0.67839600	0.00000000
P	2.64978100	1.75379200	0.00000000
H	3.60511000	0.67839600	0.00000000

C6H4Se2Gibbs Free Energy=-5034.104841 a.u.

0 1

C	0.00000000	1.23684700	0.68259700
H	0.00000000	2.17277600	1.24070000
C	0.00000000	1.23684700	-0.68259700
H	0.00000000	2.17277600	-1.24070000
C	0.00000000	0.00000000	-1.43082400
C	0.00000000	-1.23684700	-0.68259700
H	0.00000000	-2.17277600	-1.24070000
C	0.00000000	-1.23684700	0.68259700
H	0.00000000	-2.17277600	1.24070000
C	0.00000000	0.00000000	1.43082400
Se	0.00000000	0.00000000	-3.24981300
Se	0.00000000	0.00000000	3.24981300

C6H6N2 Gibbs Free Energy=-341.670729 a.u.

0 1

C	-0.08386100	1.42081200	0.00000000
H	-0.09631100	2.51293300	0.00000000
C	-1.23197000	0.71437300	0.00000000
H	-2.20922500	1.19776300	0.00000000
C	-1.23197000	-0.75771700	0.00000000
C	0.08386100	-1.42081200	0.00000000
H	0.09631100	-2.51293300	0.00000000
C	1.23197000	-0.71437300	0.00000000
H	2.20922500	-1.19776300	0.00000000
C	1.23197000	0.75771700	0.00000000
N	-2.37142300	-1.36774200	0.00000000
H	-2.23646000	-2.38454100	0.00000000
N	2.37142300	1.36774200	0.00000000
H	2.23646000	2.38454100	0.00000000

C8H4Cl4Gibbs Free Energy=-2148.063156 a.u.

0 1

C	0.00000000	1.23708700	0.67741100
H	0.00000000	2.18424100	1.21158900
C	0.00000000	1.23708700	-0.67741100
H	0.00000000	2.18424100	-1.21158900
C	0.00000000	0.00000000	-1.44655900
C	0.00000000	-1.23708700	-0.67741100
H	0.00000000	-2.18424100	-1.21158900
C	0.00000000	-1.23708700	0.67741100
H	0.00000000	-2.18424100	1.21158900
C	0.00000000	0.00000000	1.44655900
C	0.00000000	0.00000000	-2.81344800
C	0.00000000	0.00000000	2.81344800
Cl	0.00000000	1.45308900	-3.77345000
Cl	0.00000000	-1.45308900	3.77345000
Cl	0.00000000	-1.45308900	-3.77345000
Cl	0.00000000	1.45308900	3.77345000

C6H4Mg2 Gibbs Free Energy=-631.106848 a.u.

0 1

C	0.00000000	1.19006100	0.70701600
H	0.00000000	2.16608600	1.20042000
C	0.00000000	1.19006100	-0.70701600
H	0.00000000	2.16608600	-1.20042000
C	0.00000000	0.00000000	-1.44752000
C	0.00000000	-1.19006100	-0.70701600
H	0.00000000	-2.16608600	-1.20042000
C	0.00000000	-1.19006100	0.70701600
H	0.00000000	-2.16608600	1.20042000
C	0.00000000	0.00000000	1.44752000
Mg	0.00000000	0.00000000	-3.60385800
Mg	0.00000000	0.00000000	3.60385800

C6H6Ga2 Gibbs Free Energy=-4081.832828 a.u.

0 1

C	0.02872300	-0.69512500	1.20588300
H	0.03113500	-1.20813300	2.17063300
C	-0.02872300	0.69512500	1.20588300
H	-0.03113500	1.20813300	2.17063300
C	-0.10753800	1.43508100	0.00000000
C	-0.02872300	0.69512500	-1.20588300
H	-0.03113500	1.20813300	-2.17063300

C	0.02872300	-0.69512500	-1.20588300
H	0.03113500	-1.20813300	-2.17063300
C	0.10753800	-1.43508100	0.00000000
H	-1.21154500	4.40786800	0.00000000
H	1.21154500	-4.40786800	0.00000000
Ga	0.02872300	3.39876700	0.00000000
Ga	-0.02872300	-3.39876700	0.00000000

C8H6Cl2 Gibbs Free Energy=-1228.814446 a.u.

0 1

C	-0.07285800	1.40807700	0.00000000
H	-0.09770600	2.49859900	0.00000000
C	-1.23077100	0.70676800	0.00000000
H	-2.18706400	1.22674200	0.00000000
C	-1.23077100	-0.74995700	0.00000000
C	0.07285800	-1.40807700	0.00000000
H	0.09770600	-2.49859900	0.00000000
C	1.23077100	-0.70676800	0.00000000
H	2.18706400	-1.22674200	0.00000000
C	1.23077100	0.74995700	0.00000000
C	-2.35146800	-1.51947900	0.00000000
H	-2.32014500	-2.60673800	0.00000000
C	2.35146800	1.51947900	0.00000000
H	2.32014500	2.60673800	0.00000000
Cl	-3.97859100	-0.89265800	0.00000000
Cl	3.97859100	0.89265800	0.00000000

C6H4Be2 Gibbs Free Energy=-260.339772 a.u.

0 1

C	0.00000000	1.21005500	0.69703500
H	0.00000000	2.16675000	1.22850700
C	0.00000000	1.21005500	-0.69703500
H	0.00000000	2.16675000	-1.22850700
C	0.00000000	0.00000000	-1.43170300
C	0.00000000	-1.21005500	-0.69703500
H	0.00000000	-2.16675000	-1.22850700
C	0.00000000	-1.21005500	0.69703500
H	0.00000000	-2.16675000	1.22850700
C	0.00000000	0.00000000	1.43170300
Be	0.00000000	0.00000000	-3.11203000
Be	0.00000000	0.00000000	3.11203000

C6H8Ge2 Gibbs Free Energy=-4387.339488 a.u.

0 1

C	0.01223200	-0.01355500	0.01592600
C	0.03203100	-0.05532900	1.44598400
C	1.31279600	-0.00998900	2.08213700
C	2.47721700	0.01828600	1.34898800
C	2.45748000	0.06016300	-0.08101400
C	1.17667500	0.01473400	-0.71717200
H	-0.94542000	-0.01895600	-0.50795000
H	1.37111600	-0.01289200	3.17217500
H	3.43486200	0.02363500	1.87288400
H	1.11836800	0.01762800	-1.80721200
Ge	4.04503800	-0.04525600	-1.08107500
H	5.31103700	0.44104100	-0.34865300
H	3.92645600	0.43258400	-2.54175600
Ge	-1.55588900	0.04989600	2.44510200
H	-2.82217800	-0.43386900	1.71167000
H	-1.43985300	-0.42747200	3.90606300

C6H6B2 Gibbs Free Energy=-281.758280 a.u.

0 1

C	1.18916000	0.76320500	0.00000000
H	2.10770900	1.35154700	0.00000000
C	0.00000000	1.41272200	0.00000000
H	-0.00146700	2.50356000	0.00000000
C	-1.28325000	0.70067000	0.00000000
C	-1.18918800	-0.76330300	0.00000000
H	-2.10773200	-1.35165400	0.00000000
C	-0.00002700	-1.41282100	0.00000000
H	0.00143500	-2.50366000	0.00000000
C	1.28324500	-0.70077500	0.00000000
H	-3.54672500	1.95656500	0.00000000
H	3.54735600	-1.95520400	0.00000000
B	-2.51932700	1.38325800	0.00000000
B	2.51928400	-1.38312600	0.00000000

C6H6As2 Gibbs Free Energy=-4703.938159 a.u.

0 1

C	-0.05702800	1.40167000	0.00000000
H	-0.09281100	2.49290600	0.00000000
C	-1.22672000	0.68984400	0.00000000
H	-2.18100900	1.21688000	0.00000000
C	-1.22672000	-0.74875200	0.00000000
C	0.05702800	-1.40167000	0.00000000
H	0.09281100	-2.49290600	0.00000000
C	1.22672000	-0.68984400	0.00000000
H	2.18100900	-1.21688000	0.00000000
C	1.22672000	0.74875200	0.00000000
H	-3.73760700	-0.62193900	0.00000000
H	3.73760700	0.62193900	0.00000000
As	-2.75717100	-1.80691300	0.00000000
As	2.75717100	1.80691300	0.00000000

C6H6Al2Gibbs Free Energy=-716.974646 a.u.

0 1

C	0.02211600	-0.69548900	1.20325700
H	0.02162600	-1.20555900	2.17034100
C	-0.02211600	0.69548900	1.20325700
H	-0.02162600	1.20555900	2.17034100
C	-0.08486200	1.44485600	0.00000000
C	-0.02211600	0.69548900	-1.20325700
H	-0.02162600	1.20555900	-2.17034100
C	0.02211600	-0.69548900	-1.20325700
H	0.02162600	-1.20555900	-2.17034100
C	0.08486200	-1.44485600	0.00000000
H	-1.29173100	4.33070600	0.00000000
H	1.29173100	-4.33070600	0.00000000
Al	0.02211600	3.40175700	0.00000000
Al	-0.02211600	-3.40175700	0.00000000