Supporting Information

Probing Hyperconjugative Aromaticity of Cyclopentadiene and Pyrroliums Containing Groups 13, 15, 16 Substituents

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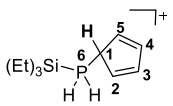


Figure S1. Structure of $C_{11}H_{22}PSi^{+}$.

Table S1. Comparison of bond lengths (Å) and relative deriviations (RD).

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C1	RD(%)
Exp.	1.462	1.348	1.466	1.337	1.516	0.0
B3LYP	1.519	1.352	1.475	1.352	1.518	1.2
PBE0	1.509	1.353	1.467	1.352	1.508	1.1
M06	1.506	1.35	1.466	1.349	1.505	1.0
M06L	1.508	1.355	1.464	1.354	1.507	1.1
M06-2X	1.512	1.348	1.474	1.348	1.511	1.0
TPSS	1.519	1.363	1.473	1.363	1.519	1.5
ωB97X-D	1.512	1.347	1.471	1.346	1.511	1.0

$$RD = \Sigma[(|BL_{func.} - BL_{exp.}|)/ BL_{exp.}]/n.$$

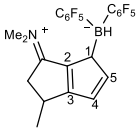


Figure S2. Structure of $C_{23}H_{26}BF_{10}$.

Table S2. Comparison of bond lengths (Å) and relative deriviations (RD).

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C1	RD(%)
Exp.	1.488	1.364	1.423	1.351	1.480	0.0
B3LYP	1.484	1.389	1.415	1.374	1.466	1.1
PBE0	1.476	1.386	1.412	1.372	1.459	1.2
M06	1.472	1.386	1.405	1.373	1.45	1.5
M06L	1.472	1.392	1.405	1.376	1.452	1.6
M06-2X	1.478	1.385	1.416	1.371	1.46	1.1
TPSS	1.484	1.399	1.416	1.383	1.466	1.3
ωB97X-D	1.48	1.379	1.416	1.366	1.464	0.9

$$RD = \Sigma[(|BL_{func.} - BL_{exp.}|)/ BL_{exp.}]/n.$$

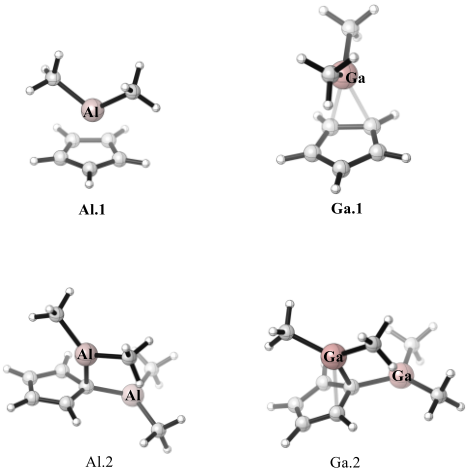


Figure S3. The distorted structures of **Al.1**, **Al.2**, **Ga.1**, **Ga.2**.

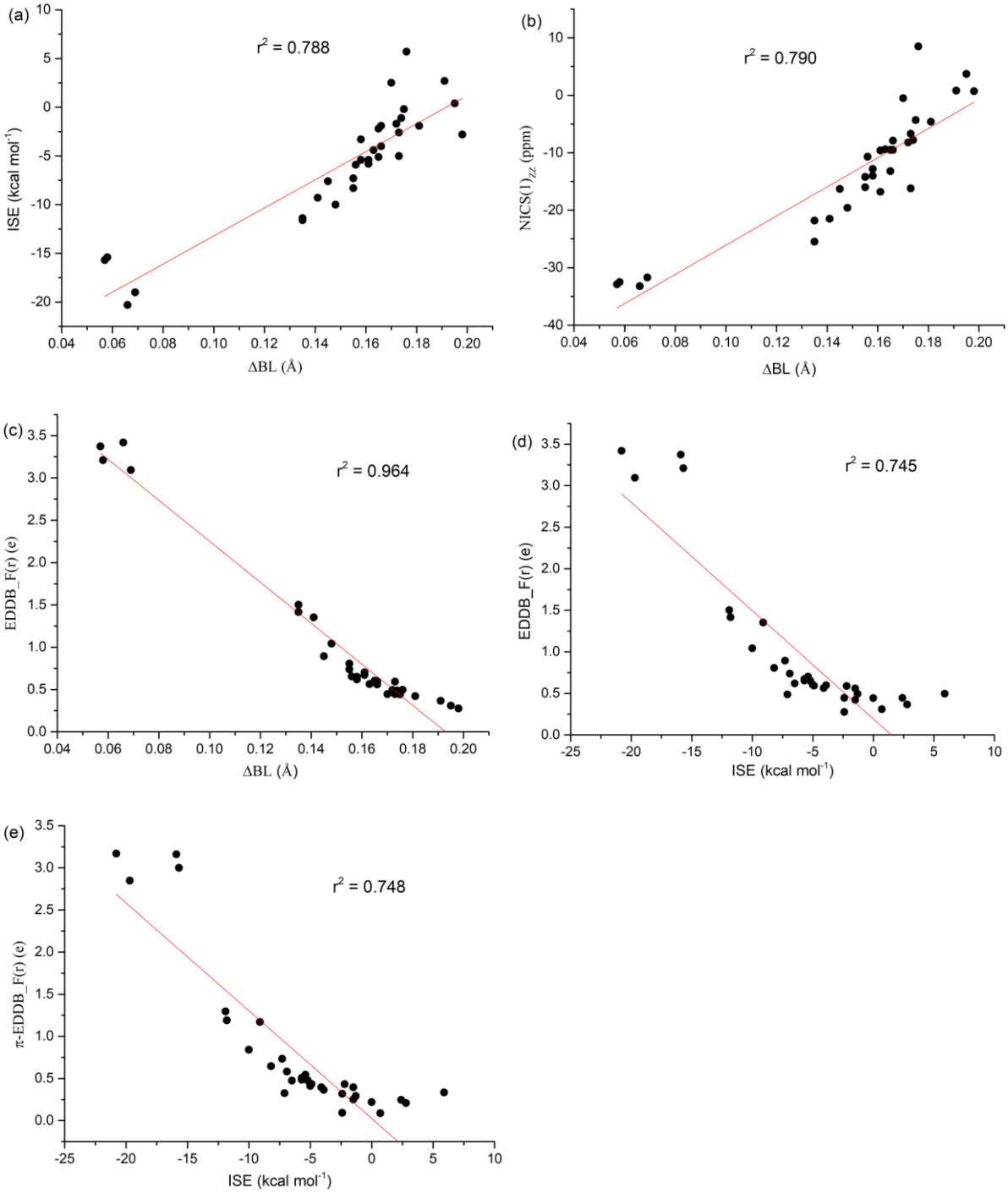


Figure S4. Correlation between (a) ΔBL vs. ISE, (b) ΔBL vs. NICS(1)$_{zz}$, (c) ΔBL vs. EDDB_F(r), (d) ISE vs. EDDB_F(r), and (e) ISE vs. π-EDDB_F(r) values for all the cyclopentadiene derivatives.

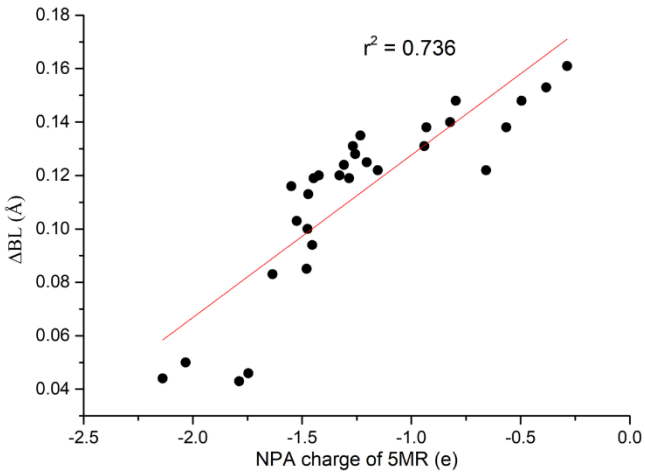
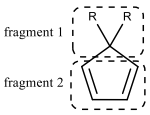
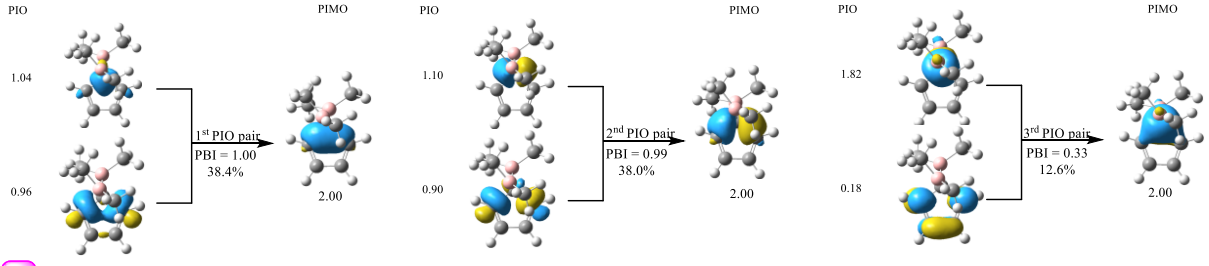


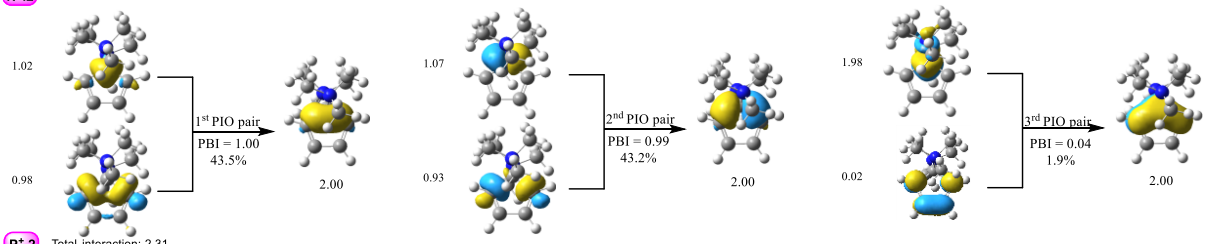
Figure S5. Correlation between NPA charge of 5 carbon atoms in 5MR vs. ΔBL for all the cyclopentadiene derivatives (1-R, 2-R and 3-R) considered here.



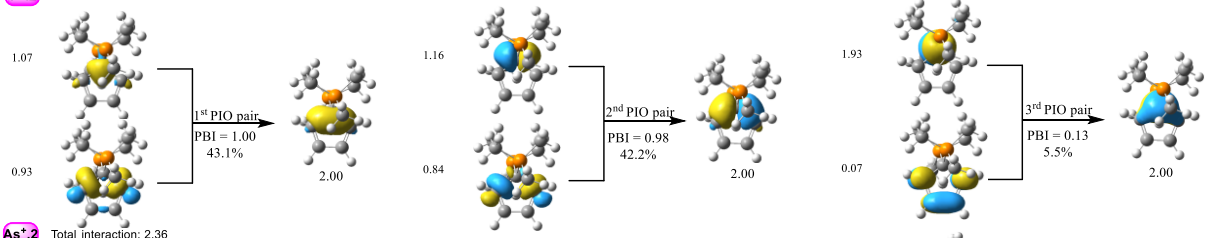
B.2 Total interaction: 2.60



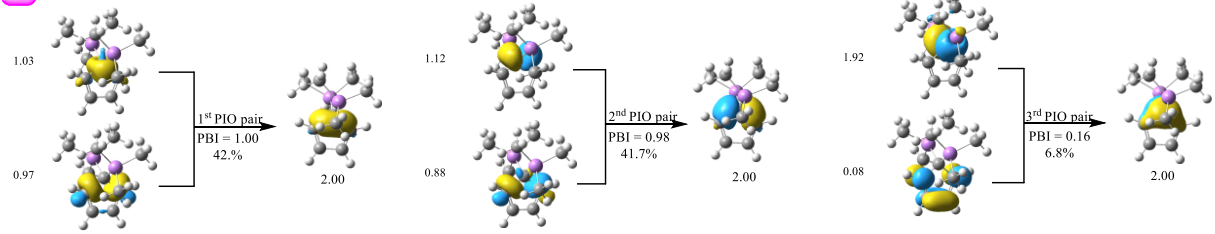
N⁺.2 Total interaction: 2.30



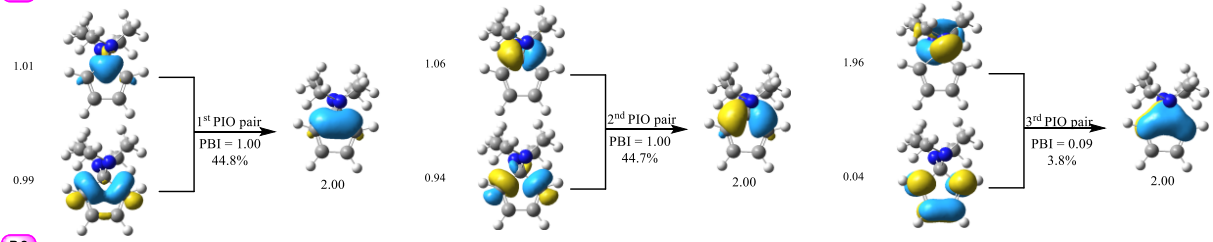
P⁺.2 Total interaction: 2.31



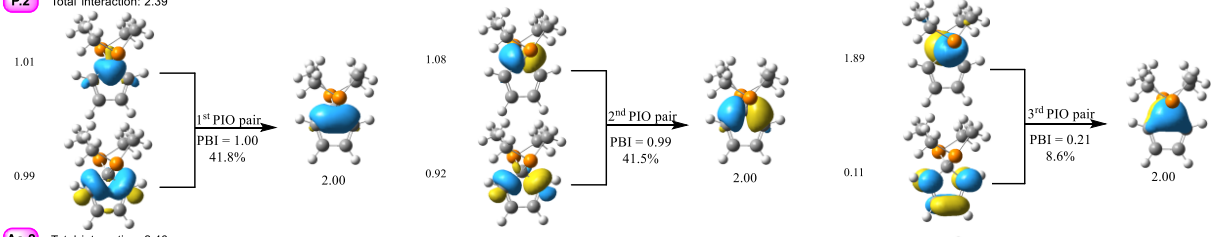
As⁺.2 Total interaction: 2.36



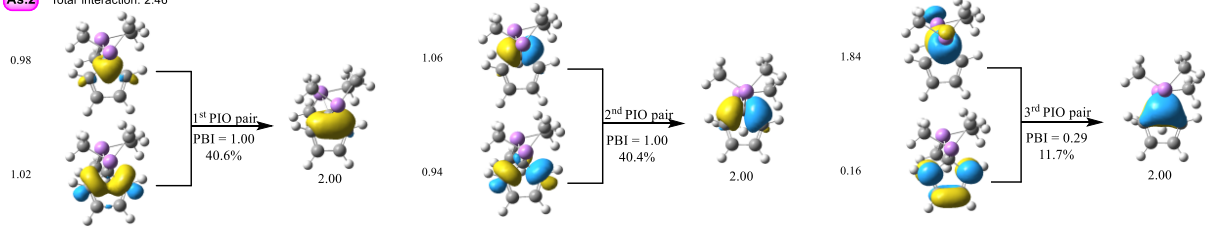
N.2 Total interaction: 2.23



P.2 Total interaction: 2.39



As.2 Total interaction: 2.46



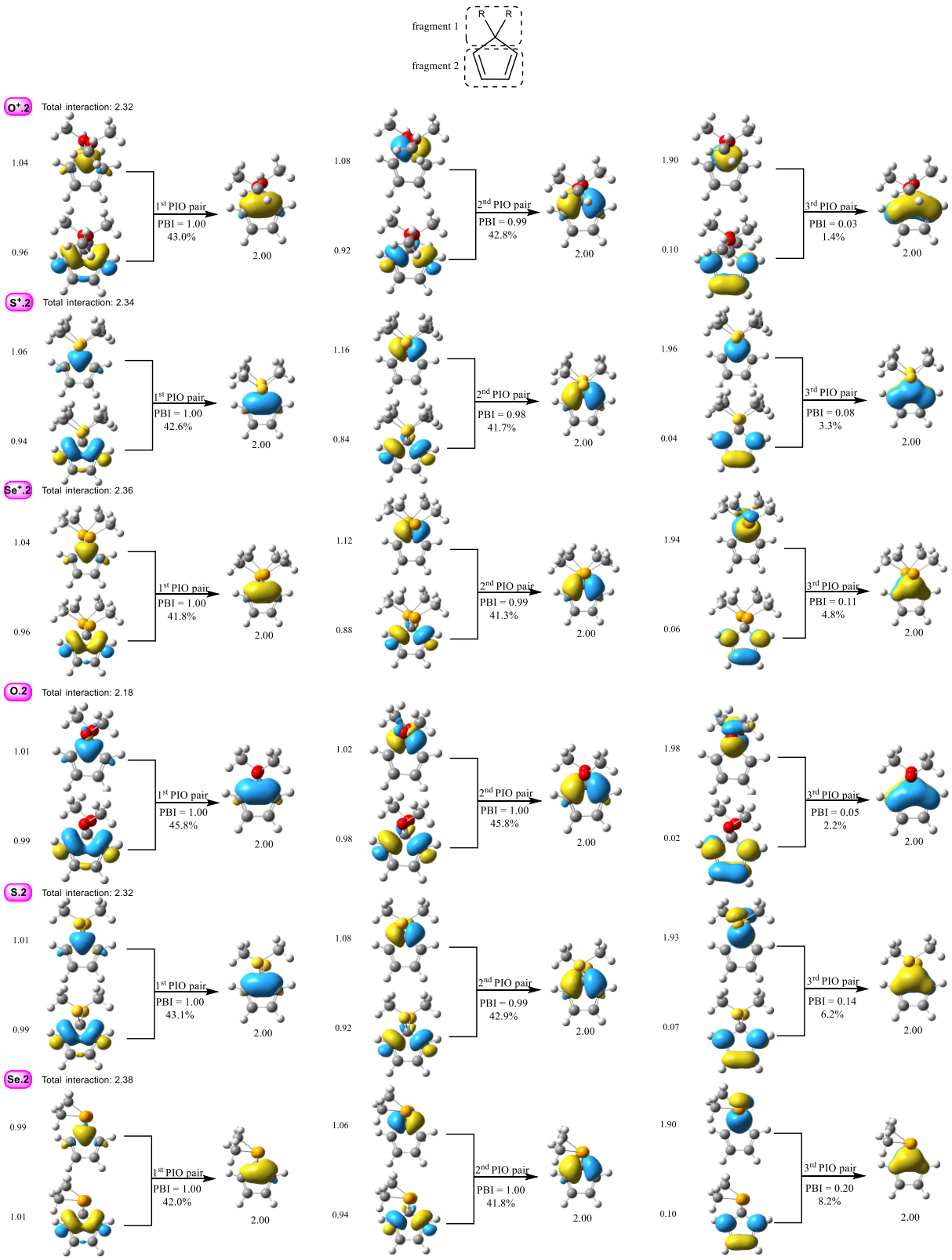


Figure S6. PIO analysis for the interaction of two fragments in **B.2**, **N**$^{+}$**.2**, **P**$^{+}$**.2**, **As**$^{+}$**.2**, **N.2**, **P.2**, **As.2**, **O**$^{+}$**.2**, **S**$^{+}$**.2**, **Se**$^{+}$**.2**, **O.2**, **S.2**, **Se.2**. PIO pairs, populations (Pop), PBI, and contribution (%) of each interaction are shown in blue and red (isovalue: 0.05 a.u).

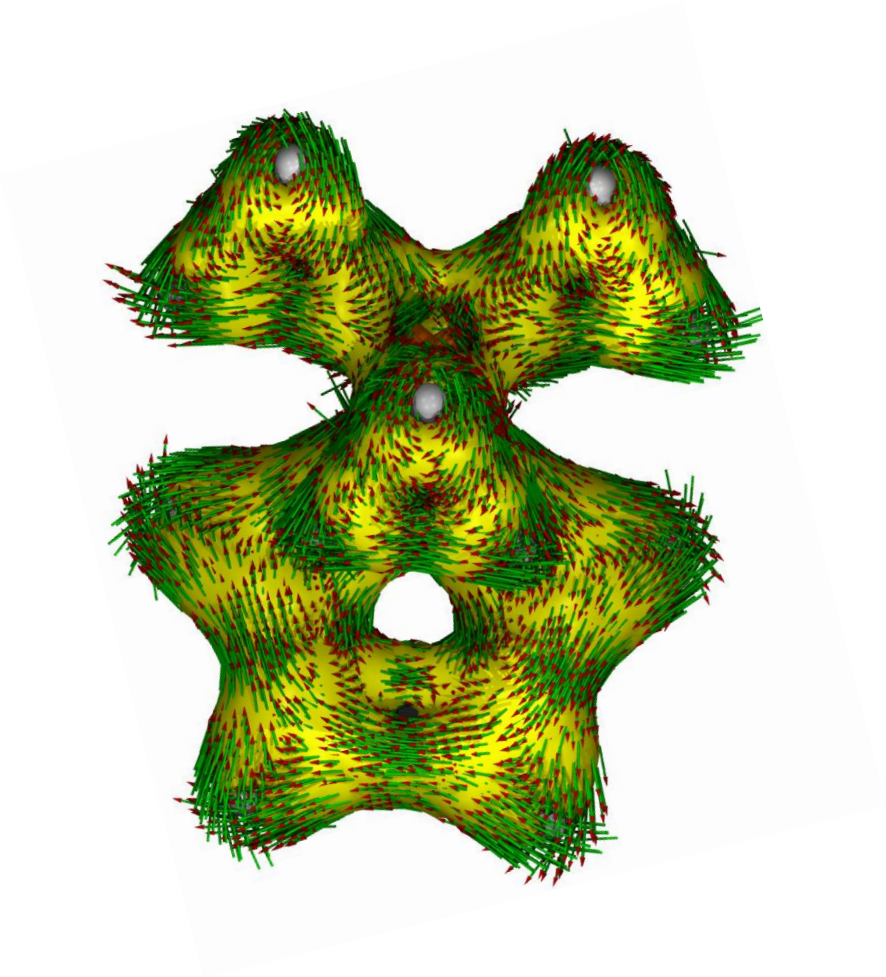


Figure S7. ACID plot of **B^{-}.1**. Isovalue: 0.030 a.u

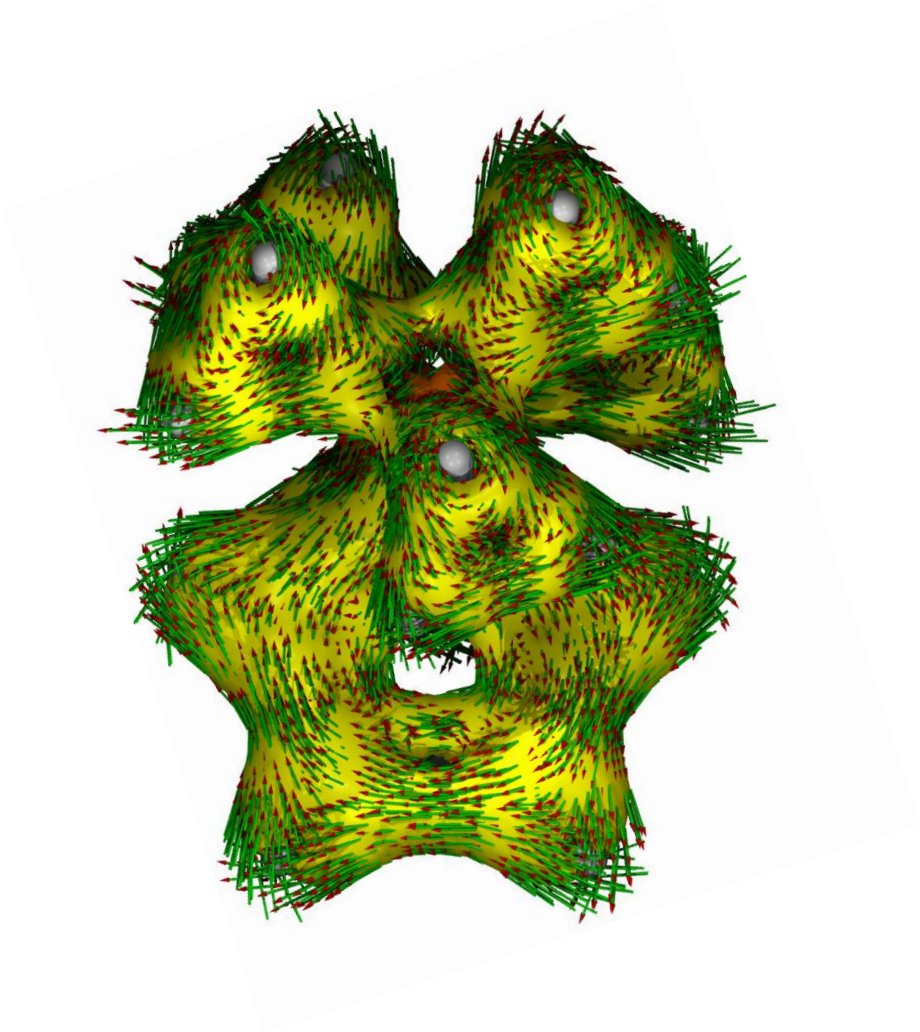


Figure S8. ACID plot of **B^{-}.2**. Isovalue: 0.030 a.u

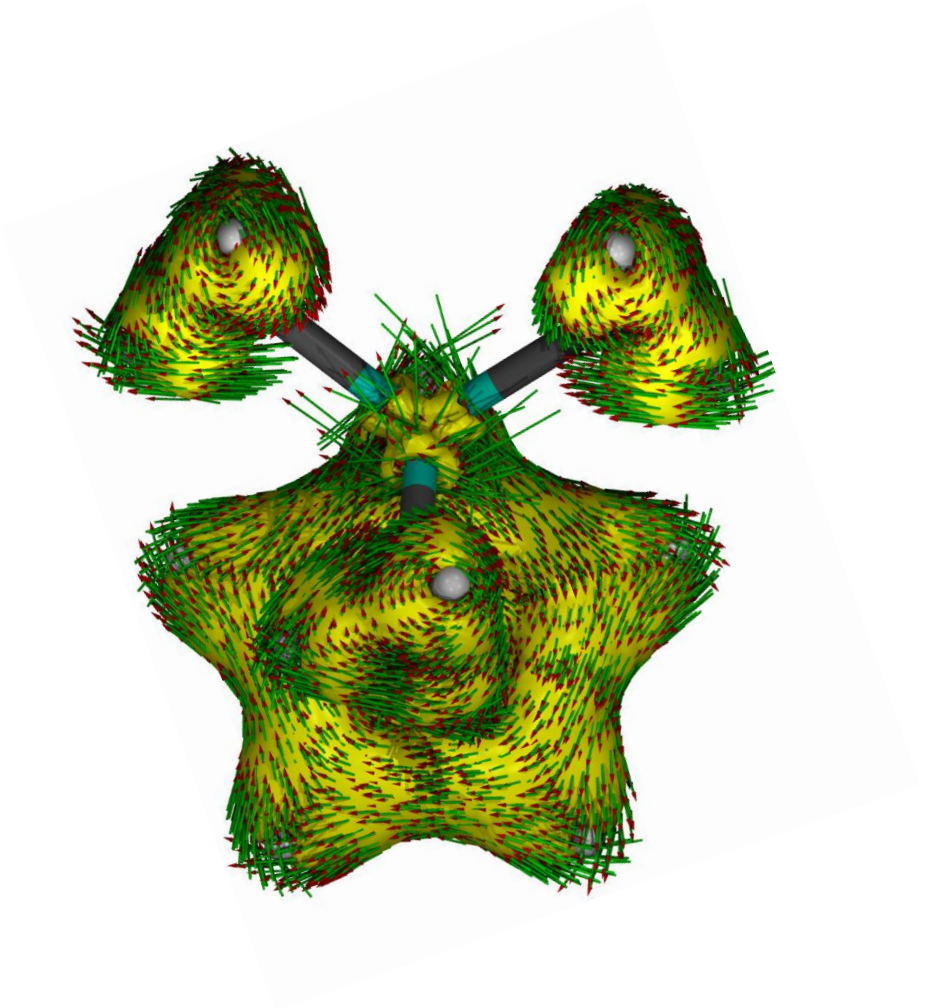


Figure S9. ACID plot of **Al$^-$.1**. Isovalue: 0.030 a.u

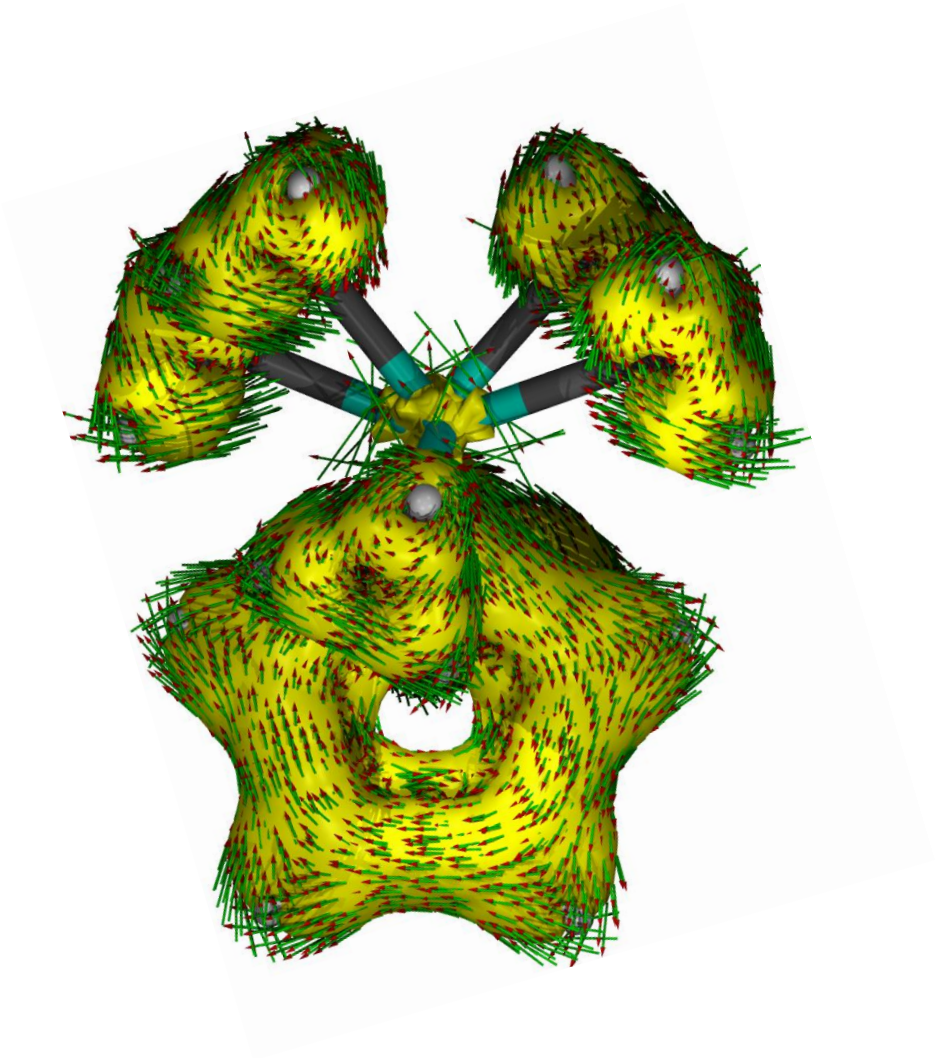


Figure S10. ACID plot of **Al**$^{-}$**.2**. Isovalue: 0.030 a.u.

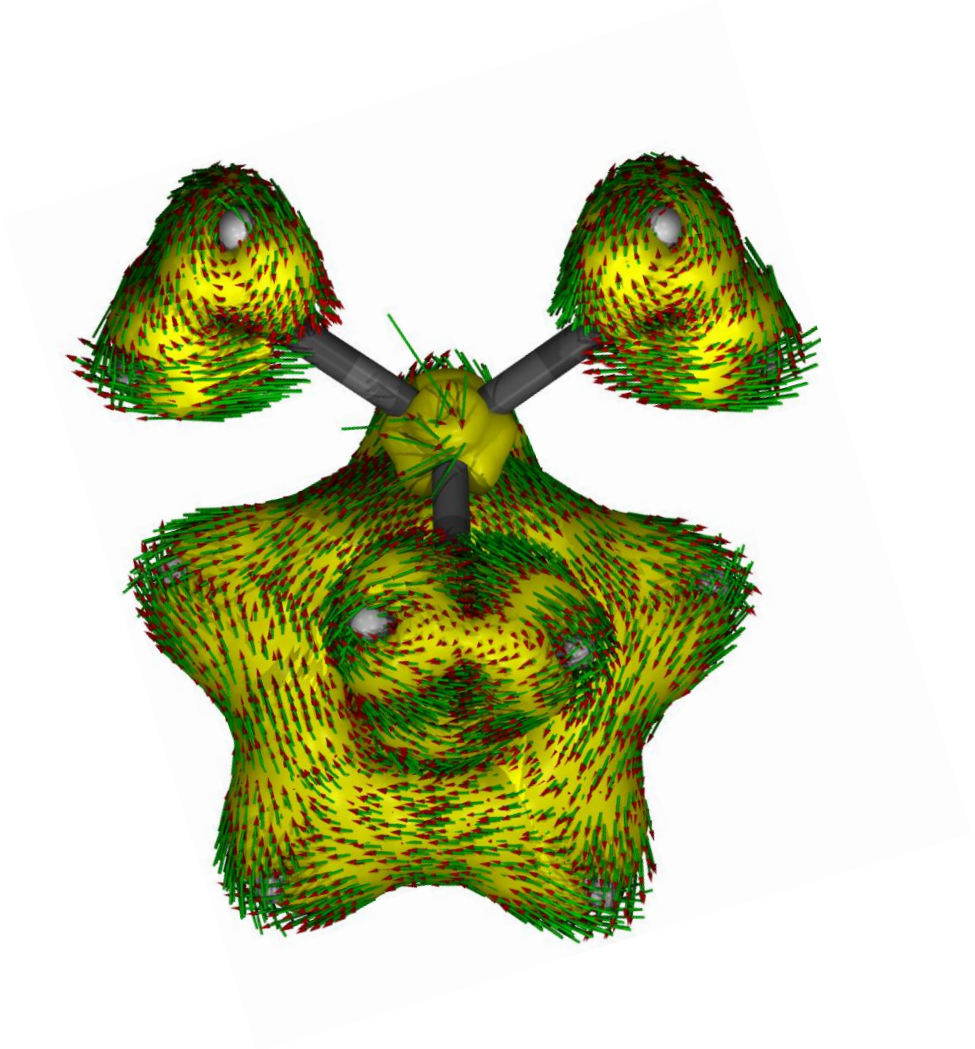


Figure S11. ACID plot of **Ga^{-}.1**. Isovalue: 0.030 a.u.

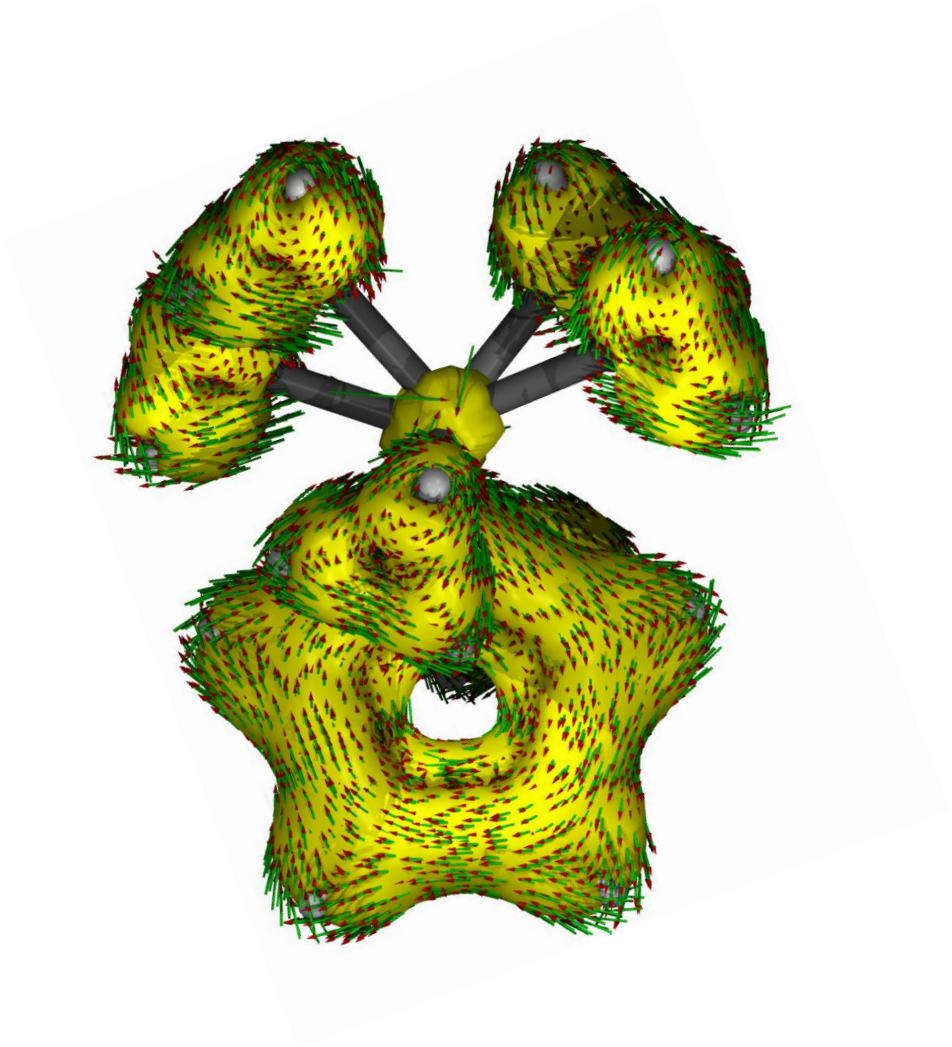


Figure S12. ACID plot of **Ga^{-}.2**. Isovalue: 0.030 a.u.

Cartesian coordinates and electronic energies of the species in this study

CPD Energy = -194.104500 a.u.

C	-0.00036400	-1.21070700	-0.00021000
H	-0.00056700	-1.86794200	-0.87685400
H	-0.00055900	-1.86854700	0.87595800
C	1.17244500	-0.28001500	0.00022000
H	2.20218400	-0.60592600	0.00032600
C	0.73255500	0.98466000	-0.00006500
H	1.34725300	1.87394600	-0.00014700
C	-1.17261200	-0.27931300	0.00023300
H	-2.20254700	-0.60460300	0.00035000
C	-0.73196300	0.98509600	-0.00008600
H	-1.34612700	1.87475200	-0.00018000

B.1 Energy = -298.210040 a.u.

C	0.08163400	-0.48837000	0.73094300
H	-0.21366800	-1.16938200	1.53199600
C	0.63977100	-1.16167700	-0.48277800
H	0.16201700	-1.97902100	-1.00325900
C	1.79246800	-0.55051300	-0.82856200
H	2.40132600	-0.79110900	-1.68898400
C	1.12839200	0.49523400	1.07983900
H	1.06912100	1.16357600	1.92678200
C	2.10087500	0.47481800	0.14629100
H	2.96551500	1.12250700	0.11061500
B	-1.22269900	0.14419000	0.04061300
C	-2.56102500	-0.67284800	0.15205700
H	-3.05526100	-0.34776900	1.07787800
H	-3.26561300	-0.48359900	-0.65958500
H	-2.40930100	-1.75001700	0.25442500
C	-1.17858800	1.53571800	-0.67760200
H	-1.52549800	2.28925200	0.04202500
H	-0.17715300	1.83879700	-0.98650700
H	-1.85915400	1.59164800	-1.52956800

B.2 Energy = -402.318970 a.u.

C	-0.06765600	-0.28585000	0.05058800
C	-0.94213900	-0.90380000	1.06116500
H	-0.71991200	-0.92658400	2.11808100
C	-2.06142600	-1.38639300	0.47111100
H	-2.88713300	-1.87117300	0.97224000
C	-0.81921800	-0.49200000	-1.21795800
H	-0.47018500	-0.19942200	-2.19739800
C	-1.99339000	-1.11339400	-0.93840900
H	-2.74917500	-1.38523200	-1.66227600
B	1.47177200	-0.57996500	0.17654900

B	-0.25562500	1.32208200	-0.05397900
C	-1.41734900	2.03883000	0.71789100
H	-1.69521000	2.99658200	0.27394700
H	-2.30573300	1.41550700	0.83177500
H	-1.06129400	2.25122200	1.73424900
C	0.79326900	2.18642900	-0.85281700
H	0.31119800	3.00639600	-1.39024200
H	1.45424300	2.66238500	-0.11631900
H	1.43153900	1.64015800	-1.54787600
C	2.18387600	-0.40699500	1.56855200
H	2.74568300	-1.30973400	1.82846400
H	2.93843100	0.38295700	1.47332400
H	1.53272300	-0.15146700	2.40535300
C	2.30795400	-1.05862100	-1.06274100
H	3.38678400	-0.93680700	-0.95044800
H	2.11230700	-2.13557600	-1.16001600
H	1.99146900	-0.61903300	-2.01000200

Al.1 Energy = -515.813810 a.u.

C	-1.14756400	-1.28736200	0.00090600
H	-1.01049800	-2.35623800	0.00171400
C	-1.19067200	-0.45756900	1.14190100
H	-1.16296600	-0.78939500	2.16831200
C	-1.35002300	0.88311200	0.69860000
H	-1.39424200	1.75533300	1.33117200
C	-1.19063200	-0.45928800	-1.14131000
H	-1.16282600	-0.79264100	-2.16722300
C	-1.34992300	0.88207500	-0.70002500
H	-1.39415400	1.75334800	-1.33390600
Al	0.71191000	0.01971900	-0.00001100
C	1.64354000	1.75529100	-0.00002600
H	2.72875300	1.62264300	-0.00065700
H	1.38281100	2.35693800	-0.87584100
H	1.38379900	2.35630200	0.87652700
C	2.00065800	-1.46871600	-0.00002300
H	2.65647200	-1.38837500	-0.87410800
H	2.65647000	-1.38841700	0.87406800
H	1.56924000	-2.47109900	-0.00004900

Al.2 Energy = -837.512938 a.u.

C	-0.00965000	0.70610400	-0.17813500
C	-0.80093900	1.62593100	0.57456300
H	-0.53593900	1.99558000	1.55597400
C	-1.96908500	1.93587300	-0.11120600
H	-2.75784300	2.58427400	0.24024700
C	-0.81657600	0.42974400	-1.37351000

H	-0.46427100	-0.09829800	-2.25112100
C	-1.98663500	1.19737500	-1.29981600
H	-2.77288100	1.20983900	-2.04131700
Al	-1.02252900	-1.06735000	0.16044500
C	-2.64177400	-1.20435100	1.23343500
H	-3.22983700	-0.28703500	1.24555100
H	-3.27740400	-2.01290300	0.86073700
H	-2.39124200	-1.45565100	2.26868700
C	0.11636800	-2.64141600	-0.13272200
H	-0.47862800	-3.53933200	-0.32281600
H	0.81027200	-2.52561900	-0.96985500
H	0.71962900	-2.86210400	0.75606800
Al	1.88614700	0.37525000	0.05998700
C	2.91758800	-0.41078100	-1.39831600
H	2.31183600	-0.60888200	-2.28537700
H	3.74328300	0.23984600	-1.70229400
H	3.36926800	-1.35879300	-1.08966600
C	2.70241000	0.84542400	1.77026900
H	3.17795000	-0.02636400	2.23073500
H	3.49282500	1.59141100	1.64199400
H	1.98570600	1.24790100	2.48945500

Ga.1 Energy = -2198.282439 a.u.

C	0.84000200	-1.10941200	0.72700600
C	0.83988300	-1.11013400	-0.72612300
H	0.37931300	-1.86419200	-1.34929400
C	1.80318600	-0.16612600	-1.13405100
H	2.02761800	0.08733600	-2.15959200
C	1.80330500	-0.16494100	1.13387000
H	2.02788200	0.08962000	2.15910400
C	2.38681700	0.40112400	-0.00041700
H	3.11949700	1.19422000	-0.00084100
Ga	-0.80387200	0.12451800	0.00015500
C	-0.61290900	2.07573300	-0.00047600
H	-1.10248500	2.49550500	0.88052600
H	-1.10327000	2.49493200	-0.88131200
H	0.43185600	2.37931200	-0.00099400
C	-2.50818300	-0.87388400	-0.00021400
H	-3.10389800	-0.61829300	0.87903300
H	-2.34482100	-1.95221600	-0.00044900
H	-3.10346100	-0.61780300	-0.87961500
H	0.37918700	-1.86263100	1.35105400

Ga.2 Energy = -4202.452193 a.u.

C	-0.00806400	0.79505800	-0.22536100
C	-0.83915600	0.61535300	-1.42079400

H	-0.59038800	-0.02227200	-2.25971700
C	-1.82734400	1.60448700	-1.41557500
H	-2.58612100	1.73403300	-2.17415600
C	-0.58931500	1.90833600	0.45293700
H	-0.25080500	2.28417900	1.40877200
C	-1.66462400	2.39964100	-0.27211700
H	-2.30245500	3.22163500	0.01827300
Ga	1.83108500	0.18580700	0.02814800
Ga	-1.30545900	-0.83262100	0.18719900
C	2.79231500	0.78674300	1.64103100
H	3.45717500	1.61657500	1.38612500
H	3.41542000	-0.00877900	2.05375400
H	2.11091200	1.13639700	2.41753700
C	2.65107600	-0.99778300	-1.31805700
H	3.65170400	-0.65482900	-1.58870800
H	2.05074400	-1.06626700	-2.22586400
H	2.75684100	-2.00552300	-0.90725800
C	-2.91060400	-0.49930300	1.26446400
H	-2.71053400	-0.73134100	2.31266200
H	-3.72604400	-1.14465000	0.93297900
H	-3.22745000	0.53962100	1.19304100
C	-0.49501200	-2.60669300	-0.14658400
H	0.11842800	-2.91117700	0.70644000
H	0.14507400	-2.60030900	-1.02979400
H	-1.26255800	-3.37110800	-0.27948500

B$^-$.1 Energy = -338.175464 a.u.

C	0.33823300	-0.00012400	-0.78491600
H	-0.03976400	-0.00016600	-1.81123900
C	1.17808900	1.15099400	-0.42806800
H	0.88190700	2.18189000	-0.56818300
C	2.30811700	0.72468800	0.18635100
H	3.07068300	1.35012000	0.63489500
C	1.17834600	-1.15102100	-0.42813300
H	0.88270600	-2.18201200	-0.56872300
C	2.30829800	-0.72450300	0.18628900
H	3.07115500	-1.34980700	0.63451200
B	-1.18601800	-0.00002400	0.08203600
C	-2.00705200	-1.34218300	-0.38686000
H	-3.01561700	-1.34581100	0.04984300
H	-2.13609900	-1.40254100	-1.47713700
H	-1.52353200	-2.27454400	-0.06775800
C	-2.00617800	1.34311100	-0.38568700
H	-2.13482300	1.40473300	-1.47593700
H	-3.01490000	1.34671200	0.05068100

H	-1.52240600	2.27494500	-0.06541500
C	-0.94685900	-0.00092600	1.69796300
H	-1.91118700	-0.00028400	2.22617300
H	-0.39287000	-0.88259000	2.04277500
H	-0.39113500	0.87925700	2.04369800

B^{-}.2 Energy = -482.107021 a.u.

C	0.00000000	0.00000000	0.30126000
C	-1.13450500	-0.01176300	1.23463200
H	-2.16863500	-0.00890400	0.90870500
C	-0.72320600	-0.00756100	2.53166200
H	-1.35762300	-0.00331800	3.41426400
C	1.13450500	0.01176300	1.23463200
H	2.16863500	0.00890400	0.90870500
C	0.72320600	0.00756100	2.53166200
H	1.35762300	0.00331800	3.41426400
B	0.00000000	1.49061800	-0.61000100
B	0.00000000	-1.49061800	-0.61000100
C	-1.09274100	1.48477000	-1.84441900
H	-1.12731700	2.48602900	-2.30659300
H	-0.85024300	0.76802100	-2.63771700
H	-2.11169200	1.25446500	-1.50349300
C	1.49865900	1.83322800	-1.22394800
H	1.43809900	2.73511800	-1.85623600
H	2.22659500	2.05296400	-0.42970200
H	1.92232300	1.03426100	-1.84068700
C	-0.39796500	2.75481200	0.38855400
H	0.17652700	2.74058400	1.32477800
H	-0.19178000	3.71614000	-0.11266700
H	-1.46116700	2.75684800	0.66668700
C	-1.49865900	-1.83322800	-1.22394800
H	-1.92232300	-1.03426100	-1.84068700
H	-1.43809900	-2.73511800	-1.85623600
H	-2.22659500	-2.05296400	-0.42970200
C	0.39796500	-2.75481200	0.38855400
H	0.19178000	-3.71614000	-0.11266700
H	1.46116700	-2.75684800	0.66668700
H	-0.17652700	-2.74058400	1.32477800
C	1.09274100	-1.48477000	-1.84441900
H	0.85024300	-0.76802100	-2.63771700
H	2.11169200	-1.25446500	-1.50349300
H	1.12731700	-2.48602900	-2.30659300

Al$^{\cdot}$.1 Energy = -555.785889 a.u.

C	-0.69951800	0.01935600	-1.09827100
H	-0.13835500	0.03186300	-2.02828900

C	-1.38478900	-1.13927400	-0.59894600
H	-1.11256700	-2.16348000	-0.81351900
C	-2.39545000	-0.71819200	0.23979300
H	-3.03269800	-1.35843900	0.83572100
C	-1.40671600	1.15642100	-0.58242900
H	-1.15336900	2.18845500	-0.78156400
C	-2.40968900	0.70378400	0.24911900
H	-3.06177500	1.32311000	0.85136700
Al	1.09102400	-0.00221300	0.13517800
C	2.13309000	-1.55985900	-0.59429100
H	2.28669300	-1.48808900	-1.67832900
H	3.12917100	-1.62152700	-0.13720800
H	1.63257700	-2.51602800	-0.40116200
C	2.01193600	1.72709000	-0.31455200
H	3.03888000	1.74735800	0.07261600
H	2.07813600	1.89291200	-1.39718200
H	1.48928300	2.59092300	0.11250600
C	0.64885600	-0.18195700	2.07067100
H	0.49091900	-1.22555800	2.36305100
H	1.45157000	0.21905200	2.70261800
H	-0.26809700	0.36400600	2.31550500

Al$^-$.2 Energy = -917.346859 a.u.

C	0.00000000	0.00000000	0.63102000
C	1.13218700	-0.05440800	1.52960400
H	2.16484300	-0.10476500	1.20248100
C	0.71108800	-0.03473800	2.84415100
H	1.34643400	-0.06209800	3.72389800
C	-1.13218700	0.05440800	1.52960400
H	-2.16484300	0.10476500	1.20248100
C	-0.71108800	0.03473800	2.84415100
H	-1.34643400	0.06209800	3.72389800
Al	0.00000000	1.68046200	-0.55631100
C	1.30119500	1.56013500	-2.10543300
H	1.03590200	0.77210400	-2.81984400
H	1.32288400	2.51335800	-2.65419700
H	2.32506500	1.35514700	-1.76730000
C	-1.86330600	2.03762500	-1.27337900
H	-1.85813800	2.89676000	-1.96023100
H	-2.27575500	1.18171900	-1.81945900
H	-2.56000500	2.27686600	-0.45902000
C	0.54020000	3.27348500	0.58139800
H	1.61975700	3.28677100	0.77977900
H	0.28031800	4.22803400	0.10002400
H	0.03478200	3.23994900	1.55480500

Al	0.00000000	-1.68046200	-0.55631100
C	1.86330600	-2.03762500	-1.27337900
H	1.85813800	-2.89676000	-1.96023100
H	2.27575500	-1.18171900	-1.81945900
H	2.56000500	-2.27686600	-0.45902000
C	-1.30119500	-1.56013500	-2.10543300
H	-1.32288400	-2.51335800	-2.65419700
H	-2.32506500	-1.35514700	-1.76730000
H	-1.03590200	-0.77210400	-2.81984400
C	-0.54020000	-3.27348500	0.58139800
H	-0.28031800	-4.22803400	0.10002400
H	-0.03478200	-3.23994900	1.55480500
H	-1.61975700	-3.28677100	0.77977900

Ga⁻.1 Energy = -2238.249249 a.u.

C	0.94264900	0.00864100	-1.10481900
H	0.39740900	0.01351100	-2.04340600
C	1.64589100	1.15168300	-0.59505500
H	1.38784000	2.18150000	-0.80071200
C	2.65001900	0.70986600	0.23926300
H	3.30031700	1.33561000	0.83702900
C	1.63570200	-1.14348600	-0.59998800
H	1.36855300	-2.17011500	-0.81015900
C	2.64348200	-0.71452200	0.23643800
H	3.28618900	-1.34861000	0.83345000
Ga	-0.92147100	-0.00122900	0.11307300
C	-1.89742400	-1.62500000	-0.60643200
H	-1.37768800	-2.55047700	-0.33960000
H	-2.91261200	-1.68593700	-0.19762200
H	-1.98633300	-1.59490000	-1.69766100
C	-1.83052900	1.72037600	-0.44801900
H	-1.87229600	1.81934900	-1.53799200
H	-2.86103700	1.76018100	-0.07651200
H	-1.30203600	2.59403300	-0.05431100
C	-0.43498300	-0.10113100	2.05849200
H	-1.00073300	0.62397900	2.65287400
H	-0.62064200	-1.09698100	2.47192200
H	0.62983800	0.11839200	2.17815900

Ga⁻.2 Energy = -4282.269992 a.u.

C	0.00401200	0.78730500	-0.00346300
C	0.09869500	1.68255400	-1.13618200
H	0.13168900	1.35092700	-2.16806000
C	0.14710400	2.99388500	-0.71535500
H	0.22096800	3.87209700	-1.34939100
C	-0.00356600	1.68647300	1.13023600

H	-0.06781700	1.35818800	2.16169600
C	0.08160000	2.99635400	0.71103800
H	0.10291900	3.87647200	1.34633800
Ga	1.67786400	-0.46531500	0.00814200
Ga	-1.70733700	-0.39865400	-0.00813700
C	2.00725400	-1.19778200	-1.87289700
H	2.82975700	-1.92591700	-1.86441300
H	1.12113800	-1.69425500	-2.27967900
H	2.28582600	-0.38734000	-2.55683000
C	1.49417100	-2.01004100	1.33302500
H	0.67698600	-2.68579900	1.06149100
H	2.42475700	-2.59314700	1.36067600
H	1.29708800	-1.64546800	2.34750900
C	3.29548100	0.67248700	0.54608300
H	3.36773100	0.77719600	1.63512800
H	4.23728600	0.23748600	0.18416000
H	3.19487800	1.67820000	0.12312000
C	-1.58809100	-1.97711500	-1.30156800
H	-1.38120400	-1.64289600	-2.32461400
H	-0.79643500	-2.67815800	-1.01845400
H	-2.54053300	-2.52434300	-1.31378800
C	-2.07953700	-1.08221500	1.88407200
H	-2.94543000	-1.75820800	1.88663500
H	-1.22524300	-1.62657800	2.29801200
H	-2.30647700	-0.24676900	2.55696300
C	-3.28474200	0.78160600	-0.57911500
H	-4.24809400	0.33137600	-0.30201700
H	-3.21268600	1.76279200	-0.09682600
H	-3.28775300	0.94612200	-1.66307000

N^+.1 Energy = -367.765694 a.u.

C	-0.26503400	-0.00006100	-0.62422400
H	-0.06909200	-0.00009000	-1.70217900
C	-1.12981500	-1.18336800	-0.27021100
H	-0.84787300	-2.21480200	-0.41364700
C	-2.32349500	-0.73544400	0.11930600
H	-3.17747000	-1.34690200	0.37126600
C	-1.12970100	1.18330900	-0.27018300
H	-0.84753000	2.21470500	-0.41342500
C	-2.32349700	0.73550800	0.11911200
H	-3.17742200	1.34703800	0.37106500
N	1.10525400	-0.00002000	0.03467800
C	1.86879100	-1.21062300	-0.39257400
H	2.87071400	-1.15541700	0.02644200
H	1.36960200	-2.10137000	-0.02464900

H	1.92293500	-1.23162900	-1.47880800
C	1.86805300	1.21147900	-0.39129400
H	1.92073000	1.23456800	-1.47755900
H	1.36921600	2.10144700	-0.02099400
H	2.87055100	1.15561800	0.02626600
C	0.97331300	-0.00081000	1.52318000
H	0.42801200	0.88777300	1.82864200
H	0.42925800	-0.89043100	1.82782500
H	1.96989100	-0.00030600	1.95832900

N^+.2 Energy = -541.263858 a.u.

C	0.00000000	0.00000000	0.24941100
C	-0.92373000	0.74556000	1.19972000
H	-1.74420400	1.37172600	0.88489200
C	-0.57514800	0.46439300	2.45226700
H	-1.05598300	0.84390800	3.34284700
C	0.92373000	-0.74556000	1.19972000
H	1.74420400	-1.37172600	0.88489200
C	0.57514800	-0.46439300	2.45226700
H	1.05598300	-0.84390800	3.34284700
N	0.82742900	1.04672400	-0.58016700
N	-0.82742900	-1.04672400	-0.58016700
C	0.00000000	2.16861700	-1.15803100
H	0.67258100	2.80690800	-1.72535000
H	-0.76463100	1.79307700	-1.82291200
H	-0.44031900	2.74288600	-0.34946000
C	1.80323000	1.72595600	0.36631000
H	2.58795600	1.03311900	0.64715900
H	2.23038500	2.56661000	-0.17366200
H	1.26875800	2.08575700	1.23911100
C	1.66802700	0.46424700	-1.67751500
H	2.26474200	-0.35593800	-1.28876300
H	1.04612500	0.14798600	-2.50855400
H	2.33633400	1.24663900	-2.02887200
C	-1.66802700	-0.46424700	-1.67751500
H	-2.33633400	-1.24663900	-2.02887200
H	-2.26474200	0.35593800	-1.28876300
H	-1.04612500	-0.14798600	-2.50855400
C	0.00000000	-2.16861700	-1.15803100
H	-0.67258100	-2.80690800	-1.72535000
H	0.76463100	-1.79307700	-1.82291200
H	0.44031900	-2.74288600	-0.34946000
C	-1.80323000	-1.72595600	0.36631000
H	-2.58795600	-1.03311900	0.64715900
H	-2.23038500	-2.56661000	-0.17366200

H	-1.26875800	-2.08575700	1.23911100

P^+.1 Energy = -654.430846 a.u.

C	0.55297000	0.00002700	-0.82966500
H	0.32874100	0.00000300	-1.90259000
C	1.38462700	1.18001700	-0.40957700
H	1.11328600	2.20905100	-0.59083700
C	2.50157000	0.73044200	0.17594900
H	3.29902200	1.34399700	0.56896600
C	1.38457100	-1.17999800	-0.40951500
H	1.11316800	-2.20903300	-0.59068100
C	2.50154000	-0.73044400	0.17597700
H	3.29895100	-1.34401700	0.56904900
P	-1.03656200	0.00000300	0.03896400
C	-1.97485700	1.45555600	-0.42504400
H	-2.95197400	1.42957300	0.05826400
H	-1.44609500	2.35449400	-0.10974600
H	-2.11321900	1.47933900	-1.50626300
C	-1.97524200	-1.45498400	-0.42604400
H	-2.95246200	-1.42898400	0.05705500
H	-2.11336600	-1.47810800	-1.50730800
H	-1.44683300	-2.35426900	-0.11114100
C	-0.77620500	-0.00060800	1.80955200
H	-0.21677300	-0.88934700	2.09863000
H	-0.21469200	0.88674600	2.09888300
H	-1.74317100	0.00046200	2.31346100

P^+.2 Energy = -1114.632652 a.u.

C	0.00000000	0.00000000	0.41113800
C	1.18075700	-0.01598200	1.35803100
H	2.21250100	-0.01929700	1.03811300
C	0.72821400	-0.00895400	2.62017400
H	1.34329900	-0.01313900	3.50897800
C	-1.18075700	0.01598200	1.35803100
H	-2.21250100	0.01929700	1.03811300
C	-0.72821400	0.00895400	2.62017400
H	-1.34329900	0.01313900	3.50897800
P	0.00000000	1.60111900	-0.50833100
P	0.00000000	-1.60111900	-0.50833100
C	1.26978900	1.62881100	-1.77348400
H	1.01686200	0.96594800	-2.60111700
H	1.33523800	2.64672300	-2.16375700
H	2.23971100	1.35810500	-1.35573400
C	0.32643500	2.90660900	0.66980200
H	0.15027600	3.85856900	0.16447400
H	-0.34858200	2.82658500	1.52137100

H	1.35904700	2.86882800	1.01218100
C	-1.58892900	1.91190300	-1.27689700
H	-1.51579100	2.85388800	-1.82478800
H	-1.86395900	1.12711300	-1.97890100
H	-2.36148100	2.01367100	-0.51502300
C	1.58892900	-1.91190300	-1.27689700
H	1.51579100	-2.85388800	-1.82478800
H	1.86395900	-1.12711300	-1.97890100
H	2.36148100	-2.01367100	-0.51502300
C	-1.26978900	-1.62881100	-1.77348400
H	-1.01686200	-0.96594800	-2.60111700
H	-1.33523800	-2.64672300	-2.16375700
H	-2.23971100	-1.35810500	-1.35573400
C	-0.32643500	-2.90660900	0.66980200
H	-0.15027600	-3.85856900	0.16447400
H	0.34858200	-2.82658500	1.52137100
H	-1.35904700	-2.86882800	1.01218100

As^{+}.1 Energy = -2548.983234 a.u.

C	-0.83668600	-0.00003200	-0.91470000
H	-0.60067700	-0.00004900	-1.98234700
C	-1.64038300	-1.17867300	-0.45749000
H	-1.37966500	-2.20712900	-0.65795200
C	-2.72175800	-0.73012600	0.19530200
H	-3.49375500	-1.34365600	0.63621400
C	-1.64019300	1.17873100	-0.45735400
H	-1.37928800	2.20717100	-0.65764900
C	-2.72164100	0.73027800	0.19538100
H	-3.49349400	1.34388400	0.63644100
As	0.85818000	0.00001500	0.03018200
C	1.86685600	-1.55730000	-0.45031700
H	2.83264700	-1.52571700	0.05204100
H	1.32188400	-2.44690600	-0.13990400
H	2.01622900	-1.57337200	-1.52877100
C	1.86626300	1.55809200	-0.44908900
H	2.83239800	1.52592900	0.05257700
H	2.01492400	1.57547900	-1.52762000
H	1.32143900	2.44726600	-0.13720900
C	0.53683300	-0.00095900	1.91584900
H	-0.03232700	0.88809600	2.17905600
H	-0.02995800	-0.89170300	2.17845100
H	1.49396300	0.00013500	2.43516500

As^{+}.2 Energy = -4903.744288 a.u.

C	0.00000000	0.00000000	0.59224000
C	0.88804900	0.77496800	1.52631800

H	1.67008300	1.44825900	1.20538000
C	0.54891300	0.47843700	2.79143200
H	1.01404500	0.88106200	3.67998100
C	-0.88804900	-0.77496800	1.52631800
H	-1.67008300	-1.44825900	1.20538000
C	-0.54891300	-0.47843700	2.79143200
H	-1.01404500	-0.88106200	3.67998100
As	-1.10063800	1.28919000	-0.40071300
As	1.10063800	-1.28919000	-0.40071300
C	2.16439000	-0.40281900	-1.72677800
H	2.89582800	-1.11927100	-2.10177800
H	1.53994400	-0.07249000	-2.55551100
H	2.68861500	0.44064800	-1.28000900
C	0.00000000	-2.61109500	-1.24495400
H	-0.68885300	-2.15122600	-1.95008400
H	0.65726800	-3.29548300	-1.78219000
H	-0.54932200	-3.16290700	-0.48406700
C	2.23853700	-2.13494100	0.88301400
H	2.69720300	-2.99855100	0.40124000
H	3.00749400	-1.43706000	1.20658700
H	1.64127300	-2.46003100	1.73308400
C	-2.16439000	0.40281900	-1.72677800
H	-2.89582800	1.11927100	-2.10177800
H	-1.53994400	0.07249000	-2.55551100
H	-2.68861500	-0.44064800	-1.28000900
C	0.00000000	2.61109500	-1.24495400
H	0.68885300	2.15122600	-1.95008400
H	-0.65726800	3.29548300	-1.78219000
H	0.54932200	3.16290700	-0.48406700
C	-2.23853700	2.13494100	0.88301400
H	-2.69720300	2.99855100	0.40124000
H	-3.00749400	1.43706000	1.20658700
H	-1.64127300	2.46003100	1.73308400

N.1 Energy = -328.066829 a.u.

C	0.05477200	0.00028900	0.38972300
C	0.96421500	-1.17315200	0.12392700
H	0.66289300	-2.20540200	0.21225900
C	2.19258600	-0.73318400	-0.15757400
H	3.06098800	-1.34876600	-0.34609100
C	0.96435600	1.17340800	0.12299400
H	0.66308600	2.20577000	0.21015800
C	2.19269900	0.73308100	-0.15805300
H	3.06114700	1.34840300	-0.34720800
C	-1.98716000	-1.18914100	-0.06453600

H	-2.92678600	-1.13778700	-0.61522500
H	-1.45975900	-2.08246400	-0.39447700
H	-2.22568700	-1.30109400	1.00866000
C	-1.98789700	1.18871200	-0.06346800
H	-1.46063300	2.08273700	-0.39170900
H	-2.92708000	1.13776800	-0.61495300
H	-2.22722600	1.29905800	1.00971600
N	-1.20589200	0.00015300	-0.33958800
H	-0.14112500	0.00062600	1.48790900

N.2 Energy = -462.028299 a.u.

C	0.00000000	0.00000000	0.24232000
C	-0.99013300	0.62859100	1.22155100
H	-1.89479400	1.13206200	0.91841200
C	-0.62600000	0.38338500	2.47676900
H	-1.17069900	0.67734900	3.36294100
C	0.99013300	-0.62859100	1.22155100
H	1.89479400	-1.13206200	0.91841200
C	0.62600000	-0.38338500	2.47676900
H	1.17069900	-0.67734900	3.36294100
C	0.00000000	2.18625100	-1.01123300
H	0.72252000	2.97241900	-1.24532100
H	-0.57691100	1.98881900	-1.92823100
H	-0.67253200	2.58380100	-0.25544200
C	1.67484900	0.55251800	-1.48136300
H	1.20751900	0.23000300	-2.42557100
H	2.38218400	1.35060700	-1.72027700
H	2.24531900	-0.28679600	-1.08717300
C	0.00000000	-2.18625100	-1.01123300
H	-0.72252000	-2.97241900	-1.24532100
H	0.57691100	-1.98881900	-1.92823100
H	0.67253200	-2.58380100	-0.25544200
C	-1.67484900	-0.55251800	-1.48136300
H	-2.24531900	0.28679600	-1.08717300
H	-1.20751900	-0.23000300	-2.42557100
H	-2.38218400	-1.35060700	-1.72027700
N	0.71759100	1.03346300	-0.51152100
N	-0.71759100	-1.03346300	-0.51152100

P.1 Energy = -614.708512 a.u.

C	0.35124400	-0.32590700	0.78225400
H	0.19019400	-0.85568100	1.72854300
C	0.88609800	-1.22842800	-0.27738500
H	0.38502400	-2.11997600	-0.62372200
C	2.05656000	-0.74850700	-0.72393000
H	2.66758800	-1.18367900	-1.50247300

C	1.41974100	0.71304500	0.90924100
H	1.37231300	1.53710800	1.60612800
C	2.38873700	0.46596700	0.01576100
H	3.27918800	1.05900600	-0.13826500
P	-1.30143800	0.49486400	0.43983200
C	-1.04394300	1.13091400	-1.26428000
H	-0.69710000	0.36160200	-1.95542100
H	-1.98976600	1.53802900	-1.62540200
H	-0.31434500	1.94049700	-1.24247000
C	-2.33632100	-0.98366400	0.07702400
H	-3.34330100	-0.64867100	-0.17691400
H	-1.95022100	-1.58384600	-0.74849700
H	-2.41069500	-1.60786600	0.96889500

P.2 Energy = -1035.301577 a.u.

C	0.00000000	0.00000000	0.51712900
C	0.00059700	1.16180000	1.46508700
H	-0.01252300	2.19284500	1.14307700
C	0.00000000	0.72370500	2.73606200
H	-0.00807200	1.34446900	3.62070100
C	-0.00059700	-1.16180000	1.46508700
H	0.01252300	-2.19284500	1.14307700
C	0.00000000	-0.72370500	2.73606200
H	0.00807200	-1.34446900	3.62070100
P	-1.70836500	-0.01020800	-0.27193900
P	1.70836500	0.01020800	-0.27193900
C	-1.80265800	-1.60472900	-1.18978500
H	-1.78325300	-2.43740700	-0.48700600
H	-2.77473900	-1.62324700	-1.68726900
H	-1.02876800	-1.74801600	-1.94113400
C	-1.56911500	1.14070700	-1.70179700
H	-2.55779500	1.21634200	-2.15825900
H	-1.28879500	2.13619400	-1.35626000
H	-0.86230000	0.81114100	-2.46356000
C	1.80265800	1.60472900	-1.18978500
H	1.78325300	2.43740700	-0.48700600
H	2.77473900	1.62324700	-1.68726900
H	1.02876800	1.74801600	-1.94113400
C	1.56911500	-1.14070700	-1.70179700
H	2.55779500	-1.21634200	-2.15825900
H	1.28879500	-2.13619400	-1.35626000
H	0.86230000	-0.81114100	-2.46356000

As.1 Energy = -2509.286938 a.u.

C	0.68858100	-0.31032800	0.86440600
H	0.50426400	-0.67890500	1.87680000

C	1.27321700	-1.32070800	-0.04959000
H	0.84832500	-2.29752600	-0.22558900
C	2.37947500	-0.81472600	-0.62221000
H	3.00189200	-1.31138800	-1.35337200
C	1.65761700	0.81809700	0.79727300
H	1.55898200	1.73319100	1.36334300
C	2.61730500	0.52299100	-0.09588200
H	3.43814600	1.16443800	-0.38377400
As	-1.11599500	0.38488300	0.28996200
C	-1.97242200	-1.33981900	-0.11013100
H	-3.00207200	-1.15202700	-0.41548000
H	-1.45412000	-1.87210900	-0.90675400
H	-1.98981100	-1.95765500	0.78801500
C	-0.68305400	0.89200800	-1.55315800
H	-0.03961100	0.15170200	-2.02788600
H	-1.61733600	0.97422600	-2.10963800
H	-0.18512900	1.85982900	-1.55867100

O⁺.1 Energy = -348.262314 a.u.

C	-0.08806500	-0.17950100	0.65985700
H	0.13790700	-0.58833100	1.64675200
C	-1.08555000	0.93630000	0.74711700
H	-0.92879000	1.83601900	1.32180000
C	-2.18545900	0.54771800	0.10324800
H	-3.11688200	1.09196200	0.04928700
C	-0.72079400	-1.19395500	-0.24993100
H	-0.27097000	-2.13451300	-0.52906500
C	-1.95753100	-0.77627000	-0.51847100
H	-2.70248100	-1.31853600	-1.08231100
O	1.24106200	0.31960400	0.18216900
C	2.36051300	-0.58352800	0.43353300
H	3.26138300	-0.04331000	0.15817400
H	2.35545900	-0.80160000	1.49697300
H	2.23789500	-1.48487800	-0.16538500
C	1.24031500	0.88618100	-1.17018000
H	1.24281200	0.07429300	-1.89445200
H	0.34185400	1.48994000	-1.24923600
H	2.13274100	1.50045200	-1.24092400

O⁺.2 Energy = -502.276756 a.u.

C	0.00000000	0.00000000	0.11588400
C	-1.16916700	0.26031300	1.02893500
H	-2.17463000	0.46265400	0.69225100
C	-0.73077000	0.14817900	2.27931800
H	-1.32929800	0.25088900	3.17385800
C	1.16916700	-0.26031300	1.02893500

H	2.17463000	-0.46265400	0.69225100
C	0.73077000	-0.14817900	2.27931800
H	1.32929800	-0.25088900	3.17385800
O	0.24971100	1.10974500	-0.82112400
C	1.50378700	1.03693700	-1.62570000
H	1.64952900	-0.00227100	-1.89925700
H	1.31502400	1.64517300	-2.50520200
H	2.31951000	1.42642900	-1.02095400
C	0.00000000	2.48591300	-0.28922100
H	0.63556700	2.63329800	0.58138900
H	0.26399800	3.15144100	-1.10509300
H	-1.05597600	2.54922300	-0.05563900
O	-0.24971100	-1.10974500	-0.82112400
C	0.00000000	-2.48591300	-0.28922100
H	-0.63556700	-2.63329800	0.58138900
H	-0.26399800	-3.15144100	-1.10509300
H	1.05597600	-2.54922300	-0.05563900
C	-1.50378700	-1.03693700	-1.62570000
H	-1.31502400	-1.64517300	-2.50520200
H	-2.31951000	-1.42642900	-1.02095400
H	-1.64952900	0.00227100	-1.89925700

S$^+$.1 Energy = -671.287775 a.u.

C	-0.35972100	0.31858500	-0.76990000
H	-0.18873600	0.81451900	-1.73120400
C	-1.39494200	-0.77160400	-0.86883400
H	-1.32843100	-1.60365400	-1.55351800
C	-2.38619900	-0.48165200	-0.02274300
H	-3.29207800	-1.05451800	0.11087900
C	-0.89881800	1.24255000	0.28001300
H	-0.42661800	2.16353300	0.58497300
C	-2.08103200	0.76943100	0.68531000
H	-2.73721600	1.24049400	1.40278500
S	1.24846300	-0.44423400	-0.38404200
C	2.32711400	0.95652500	-0.10258100
H	3.31110300	0.56002800	0.14263500
H	2.38569600	1.51738400	-1.03401400
H	1.94718300	1.57717200	0.70558200
C	1.02489400	-1.09861400	1.26552500
H	0.64834300	-0.32567400	1.93160300
H	0.32182900	-1.92548800	1.19183800
H	1.99574200	-1.46737000	1.59237500

S$^+$.2 Energy = -1148.318863 a.u.

C	0.00000000	0.00000000	0.51106000
C	-1.18683900	0.00149400	1.44952400

H	-2.21676900	-0.00699300	1.12593900
C	-0.73036600	-0.00047000	2.70841100
H	-1.34387300	-0.00408100	3.59845600
C	1.18683900	-0.00149400	1.44952400
H	2.21676900	0.00699300	1.12593900
C	0.73036600	0.00047000	2.70841100
H	1.34387300	0.00408100	3.59845600
S	0.00000000	1.64142400	-0.29221700
S	0.00000000	-1.64142400	-0.29221700
C	-1.48058700	1.82227900	-1.28858200
H	-2.34279600	1.71340400	-0.63380900
H	-1.44895500	2.85020700	-1.65461600
H	-1.50730700	1.12899100	-2.12372600
C	1.30435500	1.69032500	-1.52231000
H	1.37959100	2.73653400	-1.82284400
H	2.23723700	1.39656700	-1.04454700
H	1.06922000	1.07206500	-2.38482000
C	1.48058700	-1.82227900	-1.28858200
H	2.34279600	-1.71340400	-0.63380900
H	1.44895500	-2.85020700	-1.65461600
H	1.50730700	-1.12899100	-2.12372600
C	-1.30435500	-1.69032500	-1.52231000
H	-1.37959100	-2.73653400	-1.82284400
H	-2.23723700	-1.39656700	-1.04454700
H	-1.06922000	-1.07206500	-2.38482000

Se^{+}.1 Energy = -2674.700236 a.u.

C	-0.68977700	0.32054500	-0.83264200
H	-0.51251300	0.70005800	-1.84225300
C	-1.64669900	-0.83689400	-0.77830300
H	-1.54300900	-1.73629400	-1.36682000
C	-2.63250200	-0.52302700	0.06803800
H	-3.48708600	-1.14059900	0.30229500
C	-1.27062700	1.32478300	0.10759100
H	-0.86088200	2.30771100	0.28086700
C	-2.40290100	0.82094800	0.61211000
H	-3.07200700	1.32759700	1.29251100
Se	1.07684900	-0.35686000	-0.27559400
C	2.01574700	1.29445100	0.08265800
H	1.49861000	1.84447300	0.86405600
H	3.02458200	1.02816300	0.39095600
H	2.04903100	1.86198400	-0.84500100
C	0.69181100	-0.90631600	1.53411000
H	0.03938200	-0.16954000	1.99706900
H	0.21432000	-1.88082200	1.48357800

H	1.64637200	-0.97643500	2.05155700

Se^{+}.2 Energy = -5155.150970 a.u.

C	0.00000000	0.00000000	0.66290600
C	-1.18433000	-0.00767700	1.59335700
H	-2.21467100	-0.00340200	1.26894900
C	-0.72994800	-0.00388400	2.85546000
H	-1.34331100	-0.00397600	3.74545400
C	1.18433000	0.00767700	1.59335700
H	2.21467100	0.00340200	1.26894900
C	0.72994800	0.00388400	2.85546000
H	1.34331100	0.00397600	3.74545400
Se	0.00000000	1.77626900	-0.19644000
Se	0.00000000	-1.77626900	-0.19644000
C	1.63385100	1.88043400	-1.22946000
H	1.62891400	2.87976100	-1.66579300
H	2.46843000	1.79326900	-0.53745700
H	1.66408100	1.12610400	-2.00854900
C	-1.29468300	1.68266400	-1.63174700
H	-2.24482300	1.36028600	-1.21105300
H	-1.39146000	2.70318200	-2.00244400
H	-0.94691300	1.02634400	-2.42452300
C	1.29468300	-1.68266400	-1.63174700
H	2.24482300	-1.36028600	-1.21105300
H	1.39146000	-2.70318200	-2.00244400
H	0.94691300	-1.02634400	-2.42452300
C	-1.63385100	-1.88043400	-1.22946000
H	-1.66408100	-1.12610400	-2.00854900
H	-1.62891400	-2.87976100	-1.66579300
H	-2.46843000	-1.79326900	-0.53745700

O.1 Energy = -308.624068 a.u.

C	-0.23088400	-0.21018700	0.35982200
H	-0.46748500	-0.25110900	1.44129600
C	0.89534100	-1.17369200	0.10990400
H	0.77067200	-2.24473600	0.15872300
C	2.01601400	-0.49054600	-0.12507600
H	2.99781400	-0.91066300	-0.29165200
C	0.41427400	1.13516300	0.10374800
H	-0.10319200	2.08028300	0.17157500
C	1.71546100	0.95151200	-0.12641500
H	2.45089800	1.72760900	-0.28736100
O	-1.37631700	-0.53255200	-0.38267600
C	-2.50664800	0.22299500	-0.03525400
H	-2.37933000	1.28562700	-0.27202200
H	-3.34311300	-0.16548700	-0.61378400

H	-2.73707600	0.12742700	1.03425000

O.2 Energy = -423.158769 a.u.

C	0.00000000	0.00000000	-0.03729100
C	-0.00273700	1.18532800	0.91971200
H	0.03831800	2.21105800	0.58724500
C	0.00000000	0.74048000	2.17083900
H	0.01377500	1.34933800	3.06379200
C	0.00273700	-1.18532800	0.91971200
H	-0.03831800	-2.21105800	0.58724500
C	0.00000000	-0.74048000	2.17083900
H	-0.01377500	-1.34933800	3.06379200
O	1.15338200	0.11937000	-0.82662300
O	-1.15338200	-0.11937000	-0.82662300
C	1.44974600	-0.99277800	-1.64467700
H	0.58238200	-1.29948100	-2.23549200
H	2.24786400	-0.68022900	-2.31563700
H	1.79967100	-1.84229200	-1.05029600
C	-1.44974600	0.99277800	-1.64467700
H	-1.79967100	1.84229200	-1.05029600
H	-0.58238200	1.29948100	-2.23549200
H	-2.24786400	0.68022900	-2.31563700

S.1 Energy = -631.616895 a.u.

C	0.11493500	-0.11150800	0.54713100
H	-0.16987500	-0.07296400	1.60498300
C	1.22964900	-1.09274800	0.33457500
H	1.13938500	-2.14773000	0.54539000
C	2.30170000	-0.44574900	-0.13442200
H	3.25771100	-0.88980300	-0.37312700
C	0.71979600	1.18682700	0.10493900
H	0.19072800	2.12778700	0.11029000
C	1.98398000	0.97753500	-0.27797800
H	2.67098800	1.72649600	-0.64592900
S	-1.35045200	-0.62906300	-0.39823700
C	-2.53316800	0.61214900	0.15349800
H	-2.24490100	1.61287600	-0.16645500
H	-3.48783700	0.36122600	-0.30719200
H	-2.65031600	0.58808700	1.23736800

S.2 Energy = -1069.132422 a.u.

C	0.00000000	0.00000000	0.25816000
C	0.00000000	1.17262100	1.19912200
H	0.00476800	2.19816300	0.86268000
C	-0.00100900	0.73086600	2.46078800
H	-0.00710500	1.34775200	3.34794900
C	0.00000000	-1.17262100	1.19912200

H	-0.00476800	-2.19816300	0.86268000
C	0.00100900	-0.73086600	2.46078800
H	0.00710500	-1.34775200	3.34794900
S	1.53733300	0.10960400	-0.72183400
S	-1.53733300	-0.10960400	-0.72183400
C	1.49235600	-1.43575300	-1.64324100
H	0.53226000	-1.55003000	-2.14609700
H	2.28185900	-1.37007700	-2.39084900
H	1.68472700	-2.29224700	-0.99883400
C	-1.49235600	1.43575300	-1.64324100
H	-0.53226000	1.55003000	-2.14609700
H	-2.28185900	1.37007700	-2.39084900
H	-1.68472700	2.29224700	-0.99883400

Se.1 Energy = -2635.031991 a.u.

C	0.53323400	0.07292600	-0.67905400
H	0.26824800	0.23222400	-1.72723900
C	1.17862200	1.26594900	-0.05583100
H	0.71587800	2.23971600	-0.00089700
C	2.38531800	0.92061900	0.41147300
H	3.08014900	1.57048900	0.92416900
C	1.55623600	-1.00355500	-0.50324300
H	1.42148100	-2.01799500	-0.84774600
C	2.62002900	-0.49629900	0.13278500
H	3.51617600	-1.03679600	0.40255200
Se	-1.12417000	-0.47159400	0.23518000
C	-2.19671100	1.07344800	-0.25926100
H	-2.23258300	1.17970800	-1.34195000
H	-3.20226400	0.88912400	0.11495900
H	-1.80566900	1.97920000	0.19882700

Se.2 Energy = -5075.956888 a.u.

C	0.05207200	0.52977700	-0.05441400
C	0.14550200	1.73646600	-0.94003800
H	0.25779100	1.67408800	-2.01238600
C	0.06361800	2.84285900	-0.19007000
H	0.09671800	3.85919800	-0.55514500
C	-0.09551500	1.12630800	1.30539700
H	-0.17168700	0.54102000	2.20864000
C	-0.08436200	2.46272500	1.21066300
H	-0.15578900	3.15720400	2.03543900
Se	-1.54659800	-0.50067000	-0.59700500
Se	1.76101700	-0.43529700	-0.25463800
C	-2.17636900	-1.16832400	1.12027100
H	-2.54720800	-0.35426600	1.73693500
H	-2.99432600	-1.84803200	0.88465600

H	-1.39691900	-1.71946100	1.64054000
C	1.37133300	-1.97608800	0.85770600
H	2.25898000	-2.60589600	0.82969500
H	1.17750200	-1.67865000	1.88662000
H	0.52700300	-2.52466800	0.44380000

Mn.2 Energy = -5926.556318 a.u.

C	-0.00350200	1.80471500	1.12220000
H	0.02084100	1.51454100	2.16745500
C	-0.01130400	3.12339400	0.71012500
C	0.01063400	3.12365100	-0.70877100
C	0.00339400	1.80509700	-1.12130700
H	-0.02180800	1.51527400	-2.16666400
H	0.00407500	3.99730100	-1.34823000
H	-0.00531800	3.99682700	1.34988400
C	0.00023500	0.88220100	0.00028900
P	4.15509700	-1.05800300	0.22290500
P	-4.15502500	-1.05776500	-0.22388700
Mn	2.14967800	-0.20679200	0.02632300
Mn	-2.14963300	-0.20671600	-0.02648000
H	-5.24596900	-0.31040500	-0.73973700
H	-4.40131400	-2.20682600	-1.02139600
H	-4.86495800	-1.54694600	0.90694400
H	4.86494600	-1.54646100	-0.90828500
H	5.24606000	-0.31086500	0.73905500
H	4.40160300	-2.20749700	1.01972400
P	2.92908000	1.79050500	0.72145600
P	2.56260300	0.47299500	-2.06540300
P	1.64204500	-0.76992700	2.11339300
P	1.56194700	-2.18347200	-0.78799500
P	-1.56215100	-2.18398100	0.78647600
P	-1.64178300	-0.76803500	-2.11404000
P	-2.56209200	0.47060300	2.06612500
P	-2.92941400	1.79108000	-0.71984900
H	4.32611200	2.01464300	0.59625200
H	2.50429000	2.97189300	0.08843700
H	2.83393300	2.22009700	2.06231000
H	3.69774900	-0.06014000	-2.73473300
H	1.67133600	0.24107300	-3.13737600
H	2.82260500	1.82510100	-2.37689800
H	2.19991300	-0.05655800	3.20363900
H	0.32072700	-0.75779100	2.60381000
H	1.97098600	-2.05564200	2.61856700
H	1.82943800	-3.35883200	-0.03791300
H	0.28223900	-2.61525300	-1.21548500

H	2.22090100	-2.64266500	-1.95897700
H	-0.28244700	-2.61581700	1.21381800
H	-2.22092600	-2.64329300	1.95752300
H	-1.82991400	-3.35914800	0.03621000
H	-0.32039700	-0.75631900	-2.60443900
H	-1.97140000	-2.05312000	-2.62039400
H	-2.19915800	-0.05341600	-3.20372100
H	-1.67094100	0.23698000	3.13795000
H	-2.82269700	1.82208900	2.37978800
H	-3.69699900	-0.06403500	2.73469900
H	-2.83427000	2.22184000	-2.06032900
H	-4.32653600	2.01462200	-0.59464700
H	-2.50516900	2.97211700	-0.08582000