Supplementary Information

to

On the heteroatom incorporation effect in σ- and π-electron systems.

The sEDA(II) and pEDA(II) descriptors.

by

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

C4H4Al2 Gibbs Free Energy = -639.505039 a.u.

0 1

C	0.00000000	1.70975700	0.71054900
C	0.00000000	1.70975700	-0.71054900
Al	0.00000000	0.00000000	-1.50279800
C	0.00000000	-1.70975700	-0.71054900
C	0.00000000	-1.70975700	0.71054900
Al	0.00000000	0.00000000	1.50279800
H	0.00000000	2.67408400	1.22866300
H	0.00000000	2.67408400	-1.22866300
H	0.00000000	-2.67408400	-1.22866300
H	0.00000000	-2.67408400	1.22866300

C4H6Al2 Gibbs Free Energy = -640.845276 a.u.

0 1

C	0.00000000	1.66904600	0.68266200
C	0.00000000	1.66904600	-0.68266200
Al	0.00000000	0.00000000	-1.72921600
C	0.00000000	-1.66904600	-0.68266200
C	0.00000000	-1.66904600	0.68266200
Al	0.00000000	0.00000000	1.72921600
H	0.00000000	2.64854500	1.18905000
H	0.00000000	2.64854500	-1.18905000
H	0.00000000	0.00000000	-3.31963900
H	0.00000000	-2.64854500	-1.18905000
H	0.00000000	-2.64854500	1.18905000
H	0.00000000	0.00000000	3.31963900

C4H4As2 Gibbs Free Energy = -4626.549931 a.u.

0 1

C	0.00000000	1.44535000	0.69162700
C	0.00000000	1.44535000	-0.69162700
As	0.00000000	0.00000000	-1.88518900
C	0.00000000	-1.44535000	-0.69162700
C	0.00000000	-1.44535000	0.69162700
As	0.00000000	0.00000000	1.88518900
H	0.00000000	2.42037300	1.19246900
H	0.00000000	2.42037300	-1.19246900
H	0.00000000	-2.42037300	-1.19246900
H	0.00000000	-2.42037300	1.19246900

C4H6As2 Gibbs Free Energy = -4627.586080 a.u.

0 1

C	0.00000000	1.60502200	0.67255200
C	0.00000000	1.60502200	-0.67255200
As	0.00000000	0.00000000	-1.70106400
C	0.00000000	-1.60502200	-0.67255200
C	0.00000000	-1.60502200	0.67255200
As	0.00000000	0.00000000	1.70106400
H	0.00000000	2.53668400	1.23849200
H	0.00000000	2.53668400	-1.23849200
H	0.00000000	0.00000000	-3.18125300
H	0.00000000	-2.53668400	-1.23849200
H	0.00000000	-2.53668400	1.23849200
H	0.00000000	0.00000000	3.18125300

C4H4B2 Gibbs Free Energy = -204.380684 a.u.

0 1

C	0.00000000	1.37103400	0.72246100
C	0.00000000	1.37103400	-0.72246100
B	0.00000000	0.00000000	-1.18864000
C	0.00000000	-1.37103400	-0.72246100
C	0.00000000	-1.37103400	0.72246100
B	0.00000000	0.00000000	1.18864000
H	0.00000000	2.31509400	1.26353900
H	0.00000000	2.31509400	-1.26353900
H	0.00000000	-2.31509400	-1.26353900
H	0.00000000	-2.31509400	1.26353900

C4H4Be2 Gibbs Free Energy = -184.248426 a.u.

0 1

C	0.00000000	1.59054000	0.68780100
C	0.00000000	1.59054000	-0.68780100
Be	0.00000000	0.00000000	-1.22116900
C	0.00000000	-1.59054000	-0.68780100
C	0.00000000	-1.59054000	0.68780100
Be	0.00000000	0.00000000	1.22116900
H	0.00000000	2.55150400	1.22201700
H	0.00000000	2.55150400	-1.22201700
H	0.00000000	-2.55150400	-1.22201700
H	0.00000000	-2.55150400	1.22201700

C4H6B2 Gibbs Free Energy = -205.651592 a.u.

0 1

C	-1.35514100	-0.67909900	0.00000000
C	-1.35522500	0.67937200	0.00000000
C	1.35516300	0.67911600	0.00000000
C	1.35521400	-0.67936300	0.00000000
B	-0.00001400	-1.47145900	0.00000000
B	0.00000000	1.47145100	0.00000000
H	2.31197400	-1.21436200	0.00000000
H	-2.31180200	-1.21429700	0.00000000
H	-2.31199500	1.21434600	0.00000000
H	2.31187800	1.21419600	0.00000000
H	0.00031100	2.67437800	0.00000000
H	-0.00036100	-2.67437700	0.00000000

C6H8 Gibbs Free Energy = -233.351363 a.u.

0 1

C	0.00000000	0.66916600	1.25478100
C	0.00000000	-0.66916600	1.25478100
C	0.00000000	-0.66909600	-1.25476000
C	0.00000000	0.66909600	-1.25476000
C	0.00000000	1.50285400	-0.00000200
C	0.00000000	-1.50285400	-0.00000200
H	0.00000000	-1.20642100	-2.20655600
H	0.00000000	1.20642100	-2.20655600
H	0.00000000	1.20659500	2.20652500
H	0.00000000	-1.20659500	2.20652500
H	-0.87313500	-2.18079000	-0.00003900
H	0.87313500	-2.18079000	-0.00003900
H	0.87313500	2.18079000	-0.00003900
H	-0.87313500	2.18079000	-0.00003900

C6H6 Gibbs Free Energy = -232.199770 a.u.

0 1

C	0.00000000	1.39943600	0.00000000
C	1.21194700	0.69971800	0.00000000
C	1.21194700	-0.69971800	0.00000000
C	0.00000000	-1.39943600	0.00000000
C	-1.21194700	-0.69971800	0.00000000
C	-1.21194700	0.69971800	0.00000000
H	0.00000000	2.49006900	0.00000000
H	2.15646300	1.24503400	0.00000000

H	2.15646300	-1.24503400	0.00000000
H	0.00000000	-2.49006900	0.00000000
H	-2.15646300	-1.24503400	0.00000000
H	-2.15646300	1.24503400	0.00000000

C4H6Ga2 Gibbs Free Energy = -4005.677384 a.u.

0 1

C	0.00000000	1.67456500	0.67923900
C	0.00000000	1.67456500	-0.67923900
C	0.00000000	-1.67456500	-0.67923900
C	0.00000000	-1.67456500	0.67923900
H	0.00000000	2.64626300	1.19711700
H	0.00000000	2.64626300	-1.19711700
H	0.00000000	0.00000000	-3.30802100
H	0.00000000	-2.64626300	-1.19711700
H	0.00000000	-2.64626300	1.19711700
H	0.00000000	0.00000000	3.30802100
Ga	0.00000000	0.00000000	1.73439300
Ga	0.00000000	0.00000000	-1.73439300

C4H8Ge2 Gibbs Free Energy = -4311.168847 a.u.

0 1

C	-0.67281800	1.60253700	0.00000000
C	0.67281800	1.60253700	0.00000000
C	0.67281800	-1.60253700	0.00000000
C	-0.67281800	-1.60253700	0.00000000
Ge	-1.80007400	0.00000000	0.00000000
Ge	1.80007400	0.00000000	0.00000000
H	1.19631500	-2.56693900	0.00000000
H	-1.19631500	-2.56693900	0.00000000
H	-1.19631500	2.56693900	0.00000000
H	1.19631500	2.56693900	0.00000000
H	2.71930700	0.00000000	1.24563400
H	2.71930700	0.00000000	-1.24563400
H	-2.71930700	0.00000000	-1.24563400
H	-2.71930700	0.00000000	1.24563400

C4H6Ge2 Gibbs Free Energy = -4309.948373 a.u.

0 1

C	0.00000000	1.56747200	0.69691900
C	0.00000000	1.56747200	-0.69691900
Ge	0.00000000	0.00000000	-1.70777700

C	0.00000000	-1.56747200	-0.69691900
C	0.00000000	-1.56747200	0.69691900
Ge	0.00000000	0.00000000	1.70777700
H	0.00000000	2.53019900	1.21662500
H	0.00000000	2.53019900	-1.21662500
H	0.00000000	0.00000000	-3.23199100
H	0.00000000	-2.53019900	-1.21662500
H	0.00000000	-2.53019900	1.21662500
H	0.00000000	0.00000000	3.23199100

C4H4Mg2 Gibbs Free Energy = -554.892203 a.u.

0 1

C	0.00000000	1.92036100	0.68514800
C	0.00000000	1.92036100	-0.68514800
Mg	0.00000000	0.00000000	-1.52690800
C	0.00000000	-1.92036100	-0.68514800
C	0.00000000	-1.92036100	0.68514800
Mg	0.00000000	0.00000000	1.52690800
H	0.00000000	2.90261700	1.19284600
H	0.00000000	2.90261700	-1.19284600
H	0.00000000	-2.90261700	-1.19284600
H	0.00000000	-2.90261700	1.19284600

C4H4N2 Gibbs Free Energy = -264.299876 a.u.

0 1

C	0.00000000	1.13479200	0.69970500
C	0.00000000	1.13479200	-0.69970500
C	0.00000000	-1.13479200	-0.69970500
C	0.00000000	-1.13479200	0.69970500
H	0.00000000	2.07424900	1.25804000
H	0.00000000	2.07424900	-1.25804000
H	0.00000000	-2.07424900	-1.25804000
H	0.00000000	-2.07424900	1.25804000
N	0.00000000	0.00000000	1.40944200
N	0.00000000	0.00000000	-1.40944200

C4H4N2F2 Gibbs Free Energy = -463.849612 a.u.

0 1

C	-0.02558300	0.67574200	1.17866400
C	0.02558300	-0.67574200	1.17866400
C	0.02558300	-0.67574200	-1.17866400

C	-0.02558300	0.67574200	-1.17866400
H	-0.08206700	1.24841600	2.10055700
H	0.08206700	-1.24841600	2.10055700
H	0.08206700	-1.24841600	-2.10055700
H	-0.08206700	1.24841600	-2.10055700
N	0.02558300	1.41874300	0.00000000
N	-0.02558300	-1.41874300	0.00000000
F	1.16797400	-2.32383400	0.00000000
F	-1.16797400	2.32383400	0.00000000

C4H6N2 Gibbs Free Energy = -265.442763 a.u.

0 1

C	0.00000000	1.21139500	0.67089400
C	0.00000000	1.21139500	-0.67089400
N	0.00000000	0.00000000	-1.40111200
C	0.00000000	-1.21139500	-0.67089400
C	0.00000000	-1.21139500	0.67089400
N	0.00000000	0.00000000	1.40111200
H	0.00000000	2.13589100	1.24071200
H	0.00000000	2.13589100	-1.24071200
H	0.00000000	0.00000000	-2.40411000
H	0.00000000	-2.13589100	-1.24071200
H	0.00000000	-2.13589100	1.24071200
H	0.00000000	0.00000000	2.40411000

C4H4N2O2 Gibbs Free Energy = -414.651112 a.u.

0 1

C	0.00000000	1.16741000	0.68745100
C	0.00000000	1.16741000	-0.68745100
C	0.00000000	-1.16741000	-0.68745100
C	0.00000000	-1.16741000	0.68745100
N	0.00000000	0.00000000	1.40647600
N	0.00000000	0.00000000	-1.40647600
H	0.00000000	-2.07740600	-1.27984100
H	0.00000000	-2.07740600	1.27984100
H	0.00000000	2.07740600	1.27984100
H	0.00000000	2.07740600	-1.27984100
O	0.00000000	0.00000000	-2.68463600
O	0.00000000	0.00000000	2.68463600

C4H4O2 Gibbs Free Energy = -305.193900 a.u.

0 1

C	0.00000000	1.15438800	0.66675200
C	0.00000000	1.15438800	-0.66675200
O	0.00000000	0.00000000	-1.44113700
C	0.00000000	-1.15438800	-0.66675200
C	0.00000000	-1.15438800	0.66675200
O	0.00000000	0.00000000	1.44113700
H	0.00000000	2.06481100	1.25773700
H	0.00000000	2.06481100	-1.25773700
H	0.00000000	-2.06481100	-1.25773700
H	0.00000000	-2.06481100	1.25773700

C4H4P2 Gibbs Free Energy = -837.519126 a.u.

0 1

C	0.00000000	1.36874500	0.69513300
C	0.00000000	1.36874500	-0.69513300
P	0.00000000	0.00000000	-1.79375400
C	0.00000000	-1.36874500	-0.69513300
C	0.00000000	-1.36874500	0.69513300
P	0.00000000	0.00000000	1.79375400
H	0.00000000	2.34352200	1.19481500
H	0.00000000	2.34352200	-1.19481500
H	0.00000000	-2.34352200	-1.19481500
H	0.00000000	-2.34352200	1.19481500

C4H4P2F2 Gibbs Free Energy = -1037.257558 a.u.

0 1

C	-0.06040000	0.67069700	1.42481100
C	0.06040000	-0.67069700	1.42481100
C	0.06040000	-0.67069700	-1.42481100
C	-0.06040000	0.67069700	-1.42481100
H	-0.09958600	1.19333400	2.38683400
H	0.09958600	-1.19333400	2.38683400
H	0.09958600	-1.19333400	-2.38683400
H	-0.09958600	1.19333400	-2.38683400
F	1.49796900	-2.43312500	0.00000000
F	-1.49796900	2.43312500	0.00000000
P	0.06040000	1.80633300	0.00000000
P	-0.06040000	-1.80633300	0.00000000

C4H6P2 Gibbs Free Energy = 0.147472 a.u.

0 1

C	0.03252200	-0.66032600	-1.32599500
C	-0.03252200	0.66032600	-1.32599500
P	0.03228000	1.69239700	-0.00002300
C	-0.03228000	0.66033300	1.32603100
C	0.03228000	-0.66033300	1.32603100
P	-0.03228000	-1.69239700	-0.00002300
H	0.06800900	-1.22688400	-2.27104000
H	-0.06800900	1.22688400	-2.27104000
H	-1.25209100	2.15320200	0.00012500
H	-0.06649200	1.22702600	2.27105000
H	0.06649200	-1.22702600	2.27105000
H	1.25209100	-2.15320200	0.00012500

C4H4P2O2 Gibbs Free Energy = -987.967697 a.u.

0 1

C	0.00000000	1.41195700	0.69715200
C	0.00000000	1.41195700	-0.69715200
C	0.00000000	-1.41195700	-0.69715200
C	0.00000000	-1.41195700	0.69715200
P	0.00000000	0.00000000	1.68603200
P	0.00000000	0.00000000	-1.68603200
H	0.00000000	-2.36632700	-1.22684200
H	0.00000000	-2.36632700	1.22684200
H	0.00000000	2.36632700	1.22684200
H	0.00000000	2.36632700	-1.22684200
O	0.00000000	0.00000000	-3.20136600
O	0.00000000	0.00000000	3.20136600

C4H4S2 Gibbs Free Energy = -951.185748 a.u.

0 1

C	0.66847600	-1.36917800	0.26303600
C	-0.66853900	-1.36924000	0.26310000
C	-0.66845600	1.36937100	0.26307200
C	0.66846100	1.36942100	0.26303800
H	-1.23500000	-2.21481100	0.65620400
H	1.23485100	-2.21484800	0.65610800
H	-1.23524100	2.21481500	0.65598300
H	1.23534300	2.21482000	0.65588800
S	1.67479900	-0.00009800	-0.27928600
S	-1.67477400	-0.00004100	-0.27931800

C4H4Se2 Gibbs Free Energy = -4957.882758 a.u.

0 1

C	0.66774800	-1.45317100	0.26849100
C	-0.66781700	-1.45314700	0.26850900
C	-0.66776600	1.45321000	0.26839900
C	0.66780000	1.45318600	0.26838100
H	-1.23528100	-2.28534500	0.68977400
H	1.23519500	-2.28538900	0.68974000
H	-1.23519900	2.28546000	0.68960200
H	1.23527400	2.28541600	0.68956900
Se	-1.75879300	0.00002700	-0.35729500
Se	1.75875800	-0.00003500	-0.35734400

C4H4Se2O2 Gibbs Free Energy = -5258.550060 a.u.

0 1

C	0.66409600	1.54713800	0.00000000
C	-0.66409600	1.54713800	0.00000000
C	-0.66409600	-1.54713800	0.00000000
C	0.66409600	-1.54713800	0.00000000
Se	1.83978500	0.00000000	0.00000000
Se	-1.83978500	0.00000000	0.00000000
H	-1.25350900	-2.46736600	0.00000000
H	1.25350900	-2.46736600	0.00000000
H	1.25350900	2.46736600	0.00000000
H	-1.25350900	2.46736600	0.00000000
O	-2.64288800	0.00000000	1.42779700
O	2.64288800	0.00000000	1.42779700
O	-2.64288800	0.00000000	-1.42779700
O	2.64288800	0.00000000	-1.42779700

C4H4Se2O2 Gibbs Free Energy = -5108.220308 a.u.

0 1

C	0.66300400	-1.44445200	0.42830200
C	-0.66299300	-1.44445200	0.42832000
C	-0.66299300	1.44448500	0.42821100
C	0.66300400	1.44448500	0.42819300
H	-1.28900300	-2.23306700	0.85260400
H	1.28902700	-2.23306700	0.85256900
H	-1.28900400	2.23313100	0.85243600
H	1.28902700	2.23313100	0.85240100
Se	-1.77281200	-0.00001300	-0.33853800
Se	1.77280200	-0.00001300	-0.33858600
O	-3.16778000	0.00002200	0.58342300
O	3.16779700	0.00002200	0.58333400

C4H8Si2 Gibbs Free Energy = -736.168412 a.u.

0 1

C	-0.67528300	1.54523000	0.00000000
C	0.67528300	1.54523000	0.00000000
C	0.67528300	-1.54523000	0.00000000
C	-0.67528300	-1.54523000	0.00000000
Si	-1.75362100	0.00000000	0.00000000
Si	1.75362100	0.00000000	0.00000000
H	1.19271300	-2.51378300	0.00000000
H	-1.19271300	-2.51378300	0.00000000
H	-1.19271300	2.51378300	0.00000000
H	1.19271300	2.51378300	0.00000000
H	2.64940500	0.00000000	1.20113400
H	2.64940500	0.00000000	-1.20113400
H	-2.64940500	0.00000000	-1.20113400
H	-2.64940500	0.00000000	1.20113400

C4H6Si2 Gibbs Free Energy = -734.940750 a.u.

0 1

C	0.00000000	1.51483100	0.70120000
C	0.00000000	1.51483100	-0.70120000
Si	0.00000000	0.00000000	-1.66242700
C	0.00000000	-1.51483100	-0.70120000
C	0.00000000	-1.51483100	0.70120000
Si	0.00000000	0.00000000	1.66242700
H	0.00000000	2.48196800	1.21416400
H	0.00000000	2.48196800	-1.21416400
H	0.00000000	0.00000000	-3.14368600
H	0.00000000	-2.48196800	-1.21416400
H	0.00000000	-2.48196800	1.21416400
H	0.00000000	0.00000000	3.14368600

C4H4S2O4 Gibbs Free Energy = -1251.933035 a.u.

0 1

C	0.66480900	1.43131400	0.00000000
C	-0.66480900	1.43131400	0.00000000
C	-0.66480900	-1.43131400	0.00000000
C	0.66480900	-1.43131400	0.00000000
S	1.74713600	0.00000000	0.00000000
S	-1.74713600	0.00000000	0.00000000
H	-1.25217000	-2.35207300	0.00000000
H	1.25217000	-2.35207300	0.00000000

H	1.25217000	2.35207300	0.00000000
H	-1.25217000	2.35207300	0.00000000
O	-2.48725600	0.00000000	1.28963900
O	2.48725600	0.00000000	1.28963900
O	-2.48725600	0.00000000	-1.28963900
O	2.48725600	0.00000000	-1.28963900

C4H4S2O2 Gibbs Free Energy = -1101.532495 a.u.

0 1

C	0.66415800	1.36144800	-0.23019200
C	-0.66427700	1.36153900	-0.22960200
C	-0.66428400	-1.36152900	-0.22968200
C	0.66415000	-1.36142900	-0.23025900
H	-1.28521600	2.18140600	-0.59469800
H	1.28472300	2.18137400	-0.59579600
H	-1.28521200	-2.18138200	-0.59483000
H	1.28472400	-2.18133400	-0.59590000
S	1.69355500	-0.00000700	0.42567600
S	-1.69344700	-0.00001600	0.42608700
O	3.00949800	0.00000100	-0.35817200
O	-3.00940300	0.00001700	-0.35790100

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

C4H5Al Gibbs Free Energy=-397.797414 a.u.

0 1

C	-1.42943100	-0.05138100	0.00000000
C	-0.75268700	-1.22449000	0.00000000
C	0.75276500	-1.22441700	0.00000000
C	1.42939800	-0.05133600	0.00000000
H	-2.52056200	-0.05254000	0.00000000
H	-1.25087600	-2.20129300	0.00000000
H	1.25115300	-2.20110700	0.00000000
H	2.52052300	-0.05256100	0.00000000
Al	0.00000000	1.30232300	0.00000000
H	-0.00050700	2.88704800	0.00000000

C4H5As Gibbs Free Energy = -2391.247444 a.u.

0 1

C	-0.08218400	0.48604700	1.32967900
C	-0.08218400	0.48604700	-1.32967900
C	-0.08218400	1.70132600	-0.73309300
C	-0.08218400	1.70132600	0.73309300
H	-0.06779100	0.32306900	-2.40638600
H	-0.08792500	2.63910900	-1.29371400
H	-0.06779100	0.32306900	2.40638600
H	-0.08792500	2.63910900	1.29371400
As	0.11029500	-0.93281000	0.00000000
H	-1.35588900	-1.39008400	0.00000000

C4H4Be Gibbs Free Energy=-169.483170 a.u.

0 1

C	0.00000000	1.43324700	0.47050500
C	0.00000000	0.76330800	-0.70948100
C	0.00000000	-0.76330800	-0.70948100
C	0.00000000	-1.43324700	0.47050500
H	0.00000000	2.52015300	0.50318300
H	0.00000000	1.25305600	-1.69166100
H	0.00000000	-1.25305600	-1.69166100
H	0.00000000	-2.52015300	0.50318300
Be	0.00000000	0.00000000	1.31116700

C4H4BF Gibbs Free Energy = -279.524119 a.u.

0 1

C	0.00000000	1.26781300	-0.15157100
C	0.00000000	0.75913500	-1.40041500
C	0.00000000	-0.75913500	-1.40041500
C	0.00000000	-1.26781300	-0.15157100
H	0.00000000	2.33173700	0.07653900
H	0.00000000	1.33046300	-2.33121900
H	0.00000000	-1.33046300	-2.33121900
H	0.00000000	-2.33173700	0.07653900
B	0.00000000	0.00000000	0.79165600
F	0.00000000	0.00000000	2.13054500

C4H5B Gibbs Free Energy = -180.187970 a.u.

0 1

C	0.00020400	0.35193100	1.25560200
C	0.00020400	-0.90296300	0.76011900
C	0.00020400	-0.90296300	-0.76011900
C	0.00020400	0.35193100	-1.25560200
H	0.00012500	0.57722200	2.32100300
H	-0.00000600	-1.83150900	1.33651600
H	-0.00000600	-1.83150900	-1.33651600
H	0.00012500	0.57722200	-2.32100300
B	-0.00062900	1.32035300	0.00000000
H	-0.00197600	2.51919200	0.00000000

C5H6 Gibbs Free Energy = -194.058796 a.u.

0 1

C	1.20352600	-0.16652700	-0.00062800
C	0.63428400	1.06153800	0.00051700
C	-0.82942800	0.91729000	-0.00078500
C	-1.14778800	-0.39830500	0.00034300
H	2.26833300	-0.39088200	-0.00066600
H	1.16244600	2.01425000	0.00184900
H	-1.53353400	1.74846200	-0.00058100
H	-2.14827500	-0.82629300	0.00055200
H	0.18500300	-1.87323600	0.88213300
H	0.18471900	-1.87674300	-0.87949100
C	0.11962400	-1.21325700	-0.00007900

C4H5Ga Gibbs Free Energy = -2080.211673 a.u.

0 1

C	0.00000000	1.41883500	-0.46563900
C	0.00000000	-1.41883500	-0.46563900
C	0.00000000	-0.75271700	-1.63988300
C	0.00000000	0.75271700	-1.63988300
H	0.00000000	-2.50890100	-0.43273100
H	0.00000000	-1.25745400	-2.61238100
H	0.00000000	2.50890100	-0.43273100
H	0.00000000	1.25745400	-2.61238100
Ga	0.00000000	0.00000000	0.93104500
H	0.00000000	0.00000000	2.49410800

C4H6Ge Gibbs Free Energy = -2232.965404 a.u.

0 1

C	0.49857200	-1.37800100	0.00014900
C	1.69071300	-0.74304900	0.00001200
C	1.69065100	0.74313500	0.00004000
C	0.49844700	1.37797500	-0.00046800
H	0.40407800	-2.46299100	-0.00070200
H	2.64669800	-1.27464000	-0.00013400
H	2.64658700	1.27480800	0.00058600
H	0.40391400	2.46296600	0.00031400
Ge	-0.89945100	-0.00001000	0.00001700
H	-1.79390700	0.00052400	1.25805700
H	-1.79523700	-0.00071500	-1.25705000

C4H4Mg Gibbs Free Energy = -354.815771 a.u.

0 1

C	0.00000000	1.55349900	0.03836600
C	0.00000000	0.75765800	-1.05874300
C	0.00000000	-0.75765800	-1.05874300
C	0.00000000	-1.55349900	0.03836600
H	0.00000000	2.63630800	-0.09856500
H	0.00000000	1.19160100	-2.06883500
H	0.00000000	-1.19160100	-2.06883500
H	0.00000000	-2.63630800	-0.09856500
Mg	0.00000000	0.00000000	1.38161100

C4H4NF Gibbs Free Energy = -309.319651 a.u.

0 1

C	0.00000000	1.14378400	-0.11223500
C	0.00000000	0.71287800	-1.43214300
C	0.00000000	-0.71287800	-1.43214300
C	0.00000000	-1.14378400	-0.11223500
H	0.00000000	2.12244500	0.35068600
H	0.00000000	1.36425000	-2.30014900
H	0.00000000	-1.36425000	-2.30014900
H	0.00000000	-2.12244500	0.35068600
N	0.00000000	0.00000000	0.63127700
F	0.00000000	0.00000000	2.00139200

C4H5N Gibbs Free Energy = -210.142349 a.u.

0 1

C	-1.12728800	0.33346200	0.00000000
C	-0.71419300	-0.98587300	0.00000000
C	0.71417300	-0.98571200	0.00000000
C	1.12730500	0.33369000	0.00000000
H	-2.12008700	0.76947400	0.00000000
H	-1.36595200	-1.85411000	0.00000000
H	1.36600400	-1.85387900	0.00000000
H	2.12016500	0.76958800	0.00000000
H	-0.00010900	2.13155600	0.00000000
N	0.00000000	1.12342400	0.00000000

C4H4O Gibbs Free Energy = -230.008456 a.u.

0 1

C	-0.00004600	-0.34909200	1.09795000
C	-0.00004600	0.96143400	0.71919500
C	-0.00004600	0.96143400	-0.71919500
C	-0.00004600	-0.34909200	-1.09795000
H	0.00047500	-0.84923700	2.05904600
H	-0.00043000	1.82224500	1.38004600
H	-0.00043000	1.82224500	-1.38004600
H	0.00047500	-0.84923700	-2.05904600
O	0.00012600	-1.16176400	0.00000000

C4H4PF Gibbs Free Energy = -596.012621 a.u.

0 1

C	0.08989700	0.38503200	1.29872000

C	0.08989700	1.61586400	0.73903000
C	0.08989700	1.61586400	-0.73903000
C	0.08989700	0.38503200	-1.29872000
H	0.11600800	0.17760300	2.36659800
H	0.09668900	2.54785100	1.30797100
H	0.09668900	2.54785100	-1.30797100
H	0.11600800	0.17760300	-2.36659800
P	0.40654600	-0.87008200	0.00000000
F	-0.96456900	-1.82338200	0.00000000

C4H5P Gibbs Free Energy = -496.733682 a.u.

0 1

C	-0.04874500	0.04890000	1.29131300
C	-0.04874500	1.28721200	0.73007400
C	-0.04874500	1.28721200	-0.73007400
C	-0.04874500	0.04890000	-1.29131300
H	-0.03331800	-0.15416300	2.36040500
H	-0.04733100	2.21382800	1.30713500
H	-0.04733100	2.21382800	-1.30713500
H	-0.03331800	-0.15416300	-2.36040500
P	0.16415700	-1.22128800	0.00000000
H	-1.13117400	-1.83336900	0.00000000

C4H4S Gibbs Free Energy = -553.004733 a.u.

0 1

C	-0.01153700	-1.24569100	0.00004700
C	-1.27635900	-0.71547100	0.00002700
C	-1.27635800	0.71547100	0.00001500
C	-0.01153600	1.24569200	-0.00001800
S	1.20271800	0.00000000	-0.00003400
H	0.28462000	-2.29089100	0.00007100
H	-2.17899100	-1.32475400	0.00005300
H	-2.17899000	1.32475600	0.00002700
H	0.28462200	2.29089100	-0.00002800

C4H4Se Gibbs Free Energy = -2556.349224 a.u.

0 1

C	0.00014400	0.44481600	1.29408900
C	0.00014400	1.68490000	0.71778400
C	0.00014400	1.68490000	-0.71778400
C	0.00014400	0.44481600	-1.29408900

H	0.00025300	0.20265100	2.35335300
H	0.00029200	2.60247200	1.30652800
H	0.00029200	2.60247200	-1.30652800
H	0.00025300	0.20265100	-2.35335300
Se	-0.00013400	-0.91667200	0.00000000

C4H4SeO2 Gibbs Free Energy = -2706.666231 a.u.

0 1

C	0.00000000	1.35719500	-0.83960100
C	0.00000000	0.74408900	-2.02761000
C	0.00000000	-0.74408900	-2.02761000
C	0.00000000	-1.35719500	-0.83960100
H	0.00000000	2.41490000	-0.59399700
H	0.00000000	1.28955200	-2.97214200
H	0.00000000	-1.28955200	-2.97214200
H	0.00000000	-2.41490000	-0.59399700
Se	0.00000000	0.00000000	0.56720000
O	-1.42165200	0.00000000	1.39087600
O	1.42165200	0.00000000	1.39087600

C4H4SeO Gibbs Free Energy = -2631.496762 a.u.

0 1

C	-0.70682500	1.32452800	0.02699900
C	-0.70739100	-1.32455200	0.02769000
Se	0.69397100	-0.00025300	-0.31710200
H	-0.47637300	-2.38652100	-0.00887700
C	-1.90513400	-0.73673900	0.18433700
C	-1.90483900	0.73743700	0.18438900
H	-2.83242700	-1.29842500	0.31444000
H	-0.47491900	2.38629300	-0.01005200
H	-2.83182700	1.29948300	0.31497600
O	1.79570900	0.00046400	0.95381100

C4H6Si Gibbs Free Energy = -445.464396 a.u.

0 1

C	0.09372500	-1.35810000	-0.00031000
C	1.29995700	-0.74348200	-0.00014700
C	1.29980800	0.74364700	0.00015300
C	0.09352500	1.35810700	0.00022100
H	-0.00844900	-2.44268100	0.00025200
H	2.25144400	-1.28279600	0.00040300

H	2.25128300	1.28301500	-0.00022000
H	-0.00888100	2.44265600	-0.00059500
Si	-1.21622400	-0.00006600	0.00000800
H	-2.09053300	0.00099900	-1.21293800
H	-2.08981900	-0.00130400	1.21348700

C4H4SO2 Gibbs Free Energy = -703.354992 a.u.

0 1

C	0.00000000	1.30241300	-0.56996800
C	0.00000000	0.74335200	-1.78502900
C	0.00000000	-0.74335200	-1.78502900
C	0.00000000	-1.30241300	-0.56996800
H	0.00000000	2.34495900	-0.26587500
H	0.00000000	1.31344600	-2.71333000
H	0.00000000	-1.31344600	-2.71333000
H	0.00000000	-2.34495900	-0.26587500
O	-1.28761300	0.00000000	1.44567400
O	1.28761300	0.00000000	1.44567400
S	0.00000000	0.00000000	0.69297500

C4H4SO Gibbs Free Energy = -628.154290 a.u.

0 1

C	-0.39677500	1.27565500	-0.01013700
C	-0.39677500	-1.27565100	-0.01010400
S	0.82060100	-0.00000500	-0.38667600
H	-0.10221400	-2.32020500	-0.06510200
C	-1.62223200	-0.73358200	0.13657800
C	-1.62222300	0.73358600	0.13663300
H	-2.53823800	-1.31703000	0.23454000
H	-0.10221000	2.32020700	-0.06516300
H	-2.53822400	1.31703400	0.23462000
O	2.04741300	0.00000300	0.54126300