Supporting Information

Computational Insight into Gold(I)-Catalyzed Intramolecular Regioselectivity of Tryptamine-Ynamide Cycloisomerizations

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1. Computational Data

Table S1. Absolute values of distortion/interaction and energy decomposition analysis of transition state structures at the M06-2X/DEF2-TZVP level

TS structures	ΔE_{act}	ΔE_{int}	ΔE_{Elstat}	ΔE_{Ind}	ΔE_{Disp}	ΔE_{Pauli}	ΔE_{dist}	$\Delta E_{dist,\ tryptamine\text{-}ynamide}$	$\Delta E_{dist,\ catalyst}$
1-1a-ts	1.37	-39.73	-71.87	-62.00	-32.41	126.55	41.10	38.69	2.41
1-1b-ts	6.80	-20.64	-54.96	-50.24	-30.17	114.73	27.44	25.20	2.24
2-1a-ts	2.92	-37.15	-70.76	-61.12	-44.08	138.81	40.07	36.97	3.10
2-1b-ts	10.63	-27.39	-65.42	-56.48	-40.76	135.27	38.02	35.89	2.13
3-1a-ts	12.74	-38.71	-75.48	-62.46	-31.76	130.99	51.45	48.66	2.79
3-1b-ts	6.93	-32.35	-72.02	-58.69	-36.56	134.92	39.28	36.99	2.29
4-1a-ts	9.62	-33.33	-68.12	-60.02	-30.85	125.66	42.95	40.56	2.39
4-1b-ts	8.43	-27.62	-65.92	-56.28	-35.17	129.75	36.05	34.02	2.03

The energies were given in kcal/mol.

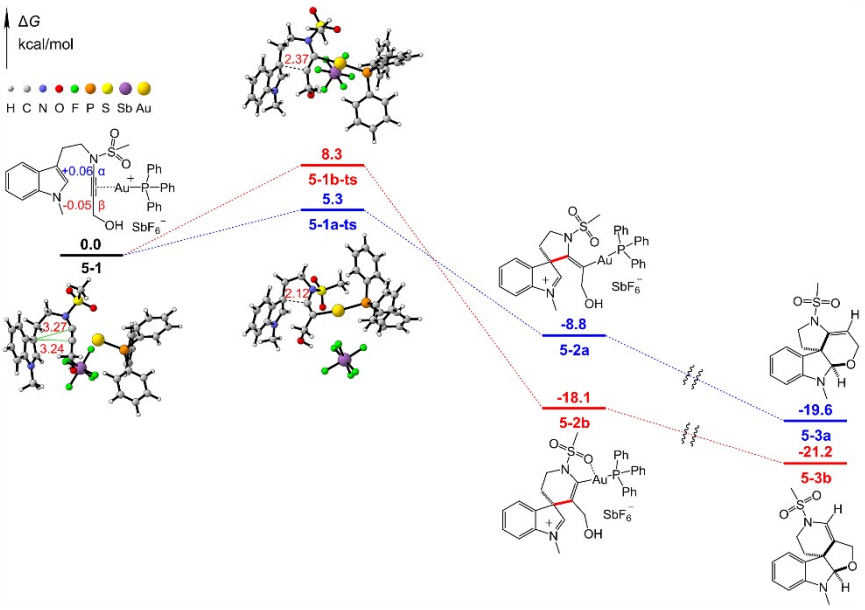

Figure S1. Free energy profiles (in kcal/mol) for the two possible cyclization pathways of **5-1** (containing complex **1-1** with SbF_6^- counterion). The blue lines represent the 5-*exo-dig* pathway and the red ones represent 6-*endo-dig* pathway. Bond lengths and natural atomic charges were shown in Å and *e*, respectively.

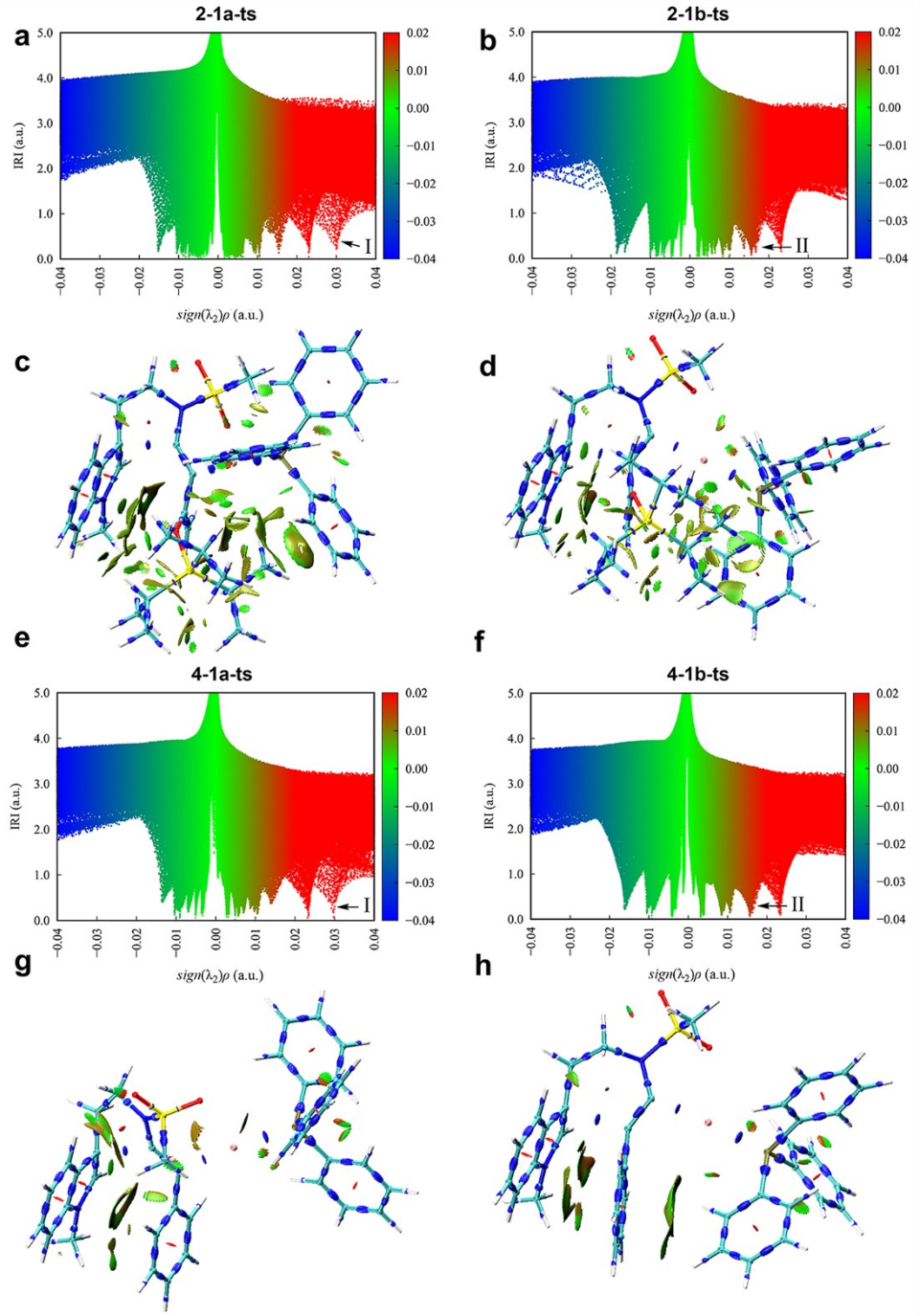

Figure S2. The IRI analysis of the TS structures of the first cyclization step. The scatter plots of IRI vs sign(λ2)ρ (a, b, e and f) and the corresponding 3D gradient isosurfaces (c, d, g and h).

2. Cartesian coordinates for all optimized geometries

1-1

E_{sol} = -2487.273332 Hartree
Thermal correction to Free Energy = 0.499113 Hartree
Sum of electronic and thermal Free Energies = -2486.774219 Hartree
Number of Imaginary Frequencies = 0

C	-6.84230700	-1.30113000	1.84201500
C	-6.69424500	0.05282100	2.16255200
C	-5.95490500	0.90021300	1.36407000
C	-5.34813300	0.38898600	0.21517800
C	-5.52419500	-0.98029100	-0.09382800
C	-6.26341000	-1.83823300	0.70959800
H	-7.43292200	-1.94561100	2.49926800
H	-7.17614100	0.44243200	3.06350700
H	-5.85327400	1.95915400	1.62479700
C	-4.53675700	0.94315200	-0.81810700
C	-4.27517000	-0.08511300	-1.68037400
N	-4.86014500	-1.23295300	-1.25144000
C	-4.10617300	2.35653000	-0.94984300
H	-3.65028200	2.53223400	-1.93869900
H	-4.99278100	3.01554500	-0.90719800
C	-1.40100700	1.23633300	0.07792300
C	-1.67300300	0.04554100	0.27108900
H	-3.68527400	-0.09040000	-2.59621600
Au	0.75839700	0.41704900	0.01571400
P	2.86845200	-0.59598900	0.00262100
C	4.18709900	0.54759100	-0.44102000
C	5.38302300	0.10269300	-0.99910500
C	4.00040300	1.90585200	-0.19853600
C	6.38451700	1.01049600	-1.29412700
H	5.53343900	-0.96231500	-1.20553800
C	5.00623700	2.80806400	-0.49573500
H	3.05053300	2.25934200	0.22194500
C	6.19751300	2.36019300	-1.04185000
H	7.32247900	0.65838600	-1.73158200
H	4.85358500	3.87363300	-0.30672000
H	6.98973000	3.07372000	-1.28287100
C	3.27789500	-1.28154800	1.61862300
C	2.26815500	-1.93993100	2.31680200
C	4.54797000	-1.18578200	2.17787400
C	2.52714800	-2.50953600	3.54883600
H	1.26072700	-2.00558200	1.88616000
C	4.79942500	-1.75002800	3.41758400

H	5.35107000	-0.66504700	1.64677300
C	3.79472700	-2.41214900	4.10108700
H	1.72908400	-3.02712200	4.08767300
H	5.79841800	-1.66870600	3.85413300
H	3.99938000	-2.85409300	5.07994300
C	2.97538600	-1.96761300	-1.16346200
C	2.34112700	-1.83718100	-2.39699700
C	3.69412100	-3.12332100	-0.87571400
C	2.43775100	-2.84699300	-3.33675100
H	1.76768600	-0.92964300	-2.62305900
C	3.78167300	-4.13321200	-1.81894700
H	4.19436800	-3.23642800	0.09178300
C	3.15676400	-3.99570600	-3.04690200
H	1.93986600	-2.73864300	-4.30392900
H	4.34753500	-5.03990900	-1.58912600
H	3.22627800	-4.79677700	-3.78768200
C	-1.93352000	-1.38198900	0.30973600
H	-2.99149200	-1.48632500	0.62178300
H	-1.34538900	-1.84640700	1.12606500
O	-1.79202100	-2.03560200	-0.89615700
H	-0.85561900	-2.04862300	-1.11250800
C	-3.16000500	2.87287400	0.11582700
H	-3.18926100	3.97181000	0.11904900
N	-1.76284800	2.50790400	-0.12737300
H	-3.45201600	2.51965500	1.12301800
S	-0.60223700	3.69659100	0.13786700
O	0.63734700	3.12490800	-0.29801300
O	-1.11234800	4.88126700	-0.46569000
C	-0.56830300	3.88704400	1.87296000
H	-1.55627700	4.21053600	2.22575600
H	-0.28209600	2.93570900	2.34122500
H	0.17531100	4.65733900	2.11468200
C	-4.78554600	-2.50031600	-1.88997200
H	-4.35286600	-3.25829000	-1.21772600
H	-5.78215700	-2.84532600	-2.20960400
H	-4.14221300	-2.42548400	-2.77388300
H	-6.38700500	-2.89473700	0.45549700

1-1a-ts

E_{sol} = -2487.267598 Hartree

Thermal correction to Free Energy = 0.504286 Hartree

Sum of electronic and thermal Free Energies = -2486.763312 Hartree

Number of Imaginary Frequencies = 1

C	5.19878300	0.76592000	2.99146000

C	4.17181300	0.07145400	3.62799900
C	3.50783400	-0.96527300	2.99678300
C	3.89308600	-1.31144000	1.71076500
C	4.94403400	-0.61556900	1.10242200
C	5.60555300	0.43413500	1.71131900
H	5.69564200	1.58772300	3.51389100
H	3.88521400	0.35639800	4.64380000
H	2.69368300	-1.49605100	3.50108100
H	6.41115000	0.97745300	1.21055100
C	3.39776500	-2.26444000	0.73651100
C	4.25738900	-2.10945600	-0.36596800
N	5.14306800	-1.15247300	-0.14988800
C	2.75720200	-3.57196200	1.05555500
H	2.92995600	-4.27770700	0.22687500
H	3.19960900	-4.01517500	1.96136600
C	1.56503400	-1.38300200	0.07608400
C	1.36033600	-0.11092300	-0.10409900
H	4.26042800	-2.66818000	-1.30180300
Au	-0.70295300	0.37185800	-0.02335000
P	-3.02350800	0.73094600	0.09190600
C	-3.50929900	2.04796800	1.22146700
C	-4.65079000	1.98230200	2.01452100
C	-2.70403600	3.18324900	1.26762400
C	-4.98134300	3.04663700	2.83624500
H	-5.28943000	1.09291300	1.98969400
C	-3.04478300	4.24713900	2.08170700
H	-1.79719700	3.23094800	0.65259800
C	-4.18230100	4.17742000	2.86908200
H	-5.87787900	2.99017300	3.45954200
H	-2.40851700	5.13578900	2.11009100
H	-4.44738900	5.01425400	3.52086400
C	-3.80165500	1.10006800	-1.49160900
C	-3.24555100	0.54346200	-2.64121900
C	-4.94739300	1.88273900	-1.59333600
C	-3.83390900	0.75629600	-3.87447800
H	-2.33648600	-0.06671700	-2.56421500
C	-5.52617700	2.10152000	-2.83111300
H	-5.39362600	2.32861700	-0.69863000
C	-4.97313100	1.53902300	-3.96973100
H	-3.39196900	0.31380100	-4.77096000
H	-6.42292200	2.72230800	-2.90619500
H	-5.43432700	1.71694200	-4.94522500
C	-3.80386300	-0.78142700	0.69208100
C	-3.36834400	-1.27930700	1.91944500

C	-4.70078300	-1.52268600	-0.06853500
C	-3.83709300	-2.49213100	2.38547000
H	-2.64853000	-0.70505600	2.51505500
C	-5.15576900	-2.74661000	0.39692200
H	-5.04711800	-1.14832400	-1.03731300
C	-4.72585900	-3.23234400	1.61909300
H	-3.49635500	-2.87079600	3.35301300
H	-5.85980900	-3.32528500	-0.20695200
H	-5.08675400	-4.19872400	1.98185400
C	1.26536000	-3.38320000	1.22934800
H	0.70850800	-4.32913300	1.19517600
N	0.84853900	-2.51091700	0.16167800
H	1.02753800	-2.87453100	2.17898100
S	0.23102300	-3.23755300	-1.25211000
O	0.52836600	-2.36107900	-2.33789300
O	0.67050300	-4.59995300	-1.25793300
C	-1.48246400	-3.18440400	-0.91132800
H	-1.69225600	-3.71557700	0.02708700
H	-1.78767900	-2.13097800	-0.83705400
H	-2.00686900	-3.67524600	-1.74205400
C	6.08585700	-0.64630000	-1.08935700
H	5.86954100	0.40906800	-1.30869100
H	7.10544300	-0.72968300	-0.68590600
H	6.02276600	-1.22509400	-2.01679500
C	2.34992400	0.97714300	-0.33599300
H	2.83265000	1.22366800	0.63166700
H	1.80777400	1.89733100	-0.63527800
O	3.36927900	0.68802000	-1.22686300
H	2.96349700	0.52832600	-2.08114000

1-1b-ts

E_{sol} = -2487.260938 Hartree

Thermal correction to Free Energy = 0.502863 Hartree

Sum of electronic and thermal Free Energies = -2486.758075 Hartree

Number of Imaginary Frequencies = 1

C	-6.61677100	-1.30845200	2.14371800
C	-6.25642600	-0.01462000	2.52833200
C	-5.50913100	0.79926600	1.70119200
C	-5.11940100	0.31054100	0.45669100
C	-5.52055000	-0.98561200	0.08273200
C	-6.25506900	-1.81750600	0.91191600
H	-7.20146200	-1.92787400	2.82883900
H	-6.57501600	0.35722600	3.50582500
H	-5.23875900	1.81212300	2.01559700

C	-4.37235700	0.84772100	-0.64511800
C	-4.42265000	-0.12860800	-1.63150200
N	-5.07515700	-1.21223600	-1.19411200
C	-4.06330800	2.28304500	-0.88756600
H	-3.75983800	2.43035100	-1.93743200
H	-4.99111600	2.86625200	-0.75084400
C	-1.38359200	1.15886600	-0.25437500
C	-2.11835300	0.10900700	-0.22144500
H	-4.00853400	-0.10581700	-2.63812700
Au	0.63215800	0.31764200	-0.11887000
P	2.78424500	-0.59403400	0.03545700
C	4.07219500	0.61997500	-0.30404800
C	5.30850400	0.25253600	-0.82982600
C	3.81777200	1.95698000	-0.01137700
C	6.28050700	1.21364500	-1.04212300
H	5.51363700	-0.79445800	-1.07743000
C	4.79437200	2.91275800	-0.22333000
H	2.83312200	2.25252700	0.37261500
C	6.02584300	2.54088100	-0.73750400
H	7.24957000	0.92106600	-1.45454900
H	4.58764200	3.96155700	0.00555700
H	6.79572200	3.29792900	-0.91103300
C	3.12785000	-1.27714700	1.66904200
C	2.09989300	-1.95934000	2.31552500
C	4.37046300	-1.16623000	2.28412600
C	2.31451600	-2.53375400	3.55430500
H	1.11483800	-2.03828700	1.83753000
C	4.57771500	-1.73643000	3.52871600
H	5.18696600	-0.63033500	1.79002800
C	3.55431600	-2.41945600	4.16275200
H	1.50263100	-3.06919800	4.05381800
H	5.55546000	-1.64361100	4.00915300
H	3.72268100	-2.86599700	5.14677400
C	3.06219100	-1.94278100	-1.13344000
C	2.50752300	-1.82544200	-2.40601700
C	3.81860000	-3.06526100	-0.81419800
C	2.71365500	-2.81400600	-3.34945100
H	1.90873200	-0.94144200	-2.65877000
C	4.01766300	-4.05468500	-1.76198000
H	4.25959700	-3.16991200	0.18255100
C	3.46661600	-3.93120300	-3.02604400
H	2.27608700	-2.71454800	-4.34646500
H	4.61220600	-4.93606900	-1.50638500
H	3.62295300	-4.71774800	-3.76942300

C	-2.20580900	-1.34132200	-0.17885100
H	-3.14492900	-1.65542700	0.31007100
H	-1.40853200	-1.68727400	0.51410800
O	-2.14972200	-1.97654700	-1.40407500
H	-1.36559200	-1.65819900	-1.85890200
C	-3.01836500	2.90325500	0.00565200
H	-3.05692200	3.99443700	-0.09834200
N	-1.68530000	2.48067900	-0.37537200
H	-3.19935900	2.64620100	1.06898100
S	-0.43359700	3.57020200	-0.19178100
O	0.65399300	3.05379000	-0.96456100
O	-0.98845000	4.85206100	-0.48196100
C	-0.00992900	3.49290200	1.50392500
H	-0.87035700	3.80486700	2.11057100
H	0.28760500	2.46597900	1.76376800
H	0.82945200	4.17766800	1.68041100
C	-5.23213300	-2.43708200	-1.90323000
H	-4.72652500	-3.26274600	-1.37969800
H	-6.29862000	-2.68591700	-2.00822800
H	-4.79213700	-2.33640600	-2.90097100
H	-6.54445300	-2.82539900	0.60321100

1-2a

E_{sol} = -3092.058716 Hartree

Thermal correction to Free Energy = 0.509411 Hartree

Sum of electronic and thermal Free Energies = -3091.549305 Hartree

Number of Imaginary Frequencies = 0

C	-6.50665900	-0.16972900	-3.08224400
C	-5.55971900	-1.16847500	-3.26314500
C	-4.72710100	-1.56812400	-2.22613100
C	-4.86197100	-0.94346700	-1.00603500
C	-5.81487400	0.05032200	-0.85072800
C	-6.65517100	0.46690100	-1.85890300
H	-7.14295800	0.12827700	-3.91891400
H	-5.46367900	-1.64320900	-4.24303500
H	-3.96974900	-2.34223000	-2.38226700
H	-7.39366900	1.25849900	-1.71311200
C	-4.15829200	-1.13395100	0.30416600
C	-4.78660400	-0.06568800	1.10318300
N	-5.73570300	0.52797000	0.46481600
C	-4.46004200	-2.50065700	0.96188000
H	-4.58176100	-2.37632300	2.05095300
H	-5.37564500	-2.95929900	0.56325400
C	-2.61244900	-1.10907900	0.25204200

C	-1.81479800	-0.24179700	-0.37603700
H	-4.55393400	0.19092100	2.13931300
Au	0.23831300	-0.52433900	-0.41715700
P	2.56147500	-0.99570700	-0.42174800
C	3.50064100	-0.25898400	-1.77909100
C	4.34373500	-0.99420200	-2.60489000
C	3.35980400	1.11288700	-1.98599900
C	5.03624400	-0.36395900	-3.62572700
H	4.46506500	-2.07140900	-2.45182200
C	4.06148300	1.73659500	-3.00011300
H	2.69762800	1.69862500	-1.33889800
C	4.89804400	0.99912700	-3.82339000
H	5.69636700	-0.94869500	-4.27272000
H	3.94865600	2.81345500	-3.15208000
H	5.44637900	1.49354000	-4.63037500
C	3.46417800	-0.51930700	1.06918800
C	2.78842000	-0.49632000	2.28646500
C	4.81995500	-0.20662600	1.03306400
C	3.46442100	-0.17829700	3.45106700
H	1.71339600	-0.71353300	2.31861900
C	5.49051400	0.11695800	2.19975000
H	5.36072700	-0.21565200	0.08093800
C	4.81459900	0.12931500	3.40862800
H	2.92566500	-0.15597600	4.40195400
H	6.55449200	0.36660000	2.16197100
H	5.34488300	0.38969500	4.32884700
C	2.82219900	-2.78045200	-0.57110300
C	2.02091300	-3.47885500	-1.47491100
C	3.75438000	-3.48055000	0.18819600
C	2.16129800	-4.84603600	-1.62621000
H	1.27469800	-2.93676200	-2.06870600
C	3.88200400	-4.85252700	0.04328700
H	4.39027600	-2.95429000	0.90667600
C	3.08990900	-5.53674700	-0.86262300
H	1.53092100	-5.37989600	-2.34220600
H	4.61386200	-5.39278500	0.64973800
H	3.19240700	-6.62003000	-0.97212800
C	-2.41391400	1.00642200	-0.95251800
H	-3.00601400	0.74654500	-1.85540600
H	-1.62121500	1.68970900	-1.30120500
O	-3.28616200	1.68187200	-0.09139700
H	-2.71674000	2.12146800	0.54608900
C	-3.19872400	-3.28831700	0.69730100
H	-3.07437700	-4.13937400	1.37935800

N	-2.13951000	-2.31594000	0.83922600
H	-3.16990100	-3.66880500	-0.33858200
S	-1.45823700	-2.25173700	2.37640100
O	-1.02792200	-0.91052200	2.62772500
O	-2.32150300	-2.90544000	3.32381800
C	-0.06160000	-3.27210000	2.13253200
H	-0.38815400	-4.27850500	1.84027400
H	0.56072500	-2.83684200	1.33799800
H	0.49638900	-3.32730800	3.07629100
C	-6.51016700	1.62749600	0.94453700
H	-6.28934000	1.79314900	2.00293900
H	-6.25837000	2.52964400	0.36897400
H	-7.57932700	1.40975800	0.82200400
Sb	0.62064000	3.57946100	0.38762500
F	0.46973600	2.81397000	-1.28659800
F	2.03040100	4.58333500	-0.23431800
F	-0.57321400	4.88232200	-0.12521900
F	-0.79609900	2.55820900	1.01377300
F	0.76948800	4.35402400	2.04858400
F	1.79189500	2.25286600	0.90079400

1-2b

E_{sol} = -3092.074708 Hartree

Thermal correction to Free Energy = 0.510612 Hartree

Sum of electronic and thermal Free Energies = -3091.564096 Hartree

Number of Imaginary Frequencies = 0

C	7.12446500	-1.20072200	2.50772500
C	6.25876200	-2.23368000	2.17875800
C	5.23054100	-2.04757200	1.26263600
C	5.09332400	-0.81076600	0.67056100
C	5.96440000	0.20704000	1.03152800
C	6.98933500	0.05635200	1.93715200
H	7.91869300	-1.37283000	3.23812000
H	6.38116000	-3.20848800	2.65806000
H	4.53596300	-2.86128700	1.03572100
C	4.11238600	-0.26908200	-0.33649900
C	4.54114200	1.15327400	-0.37686800
N	5.59375700	1.36928900	0.33659700
C	4.30043800	-0.83167500	-1.75158200
H	3.92382300	-0.10052300	-2.48707000
H	5.36702300	-0.99917800	-1.96282100
C	1.71469100	-1.06764100	-0.64457000
C	2.65226400	-0.39140900	0.05751300
H	4.12142000	1.93248800	-1.01450000

Au	-0.31598600	-0.90504700	-0.10791700
P	-2.56981100	-0.78710100	0.58029300
C	-3.39187200	-2.39785900	0.44078700
C	-4.74655000	-2.53834700	0.15115900
C	-2.62593700	-3.53885300	0.67031600
C	-5.31797300	-3.79781500	0.08814900
H	-5.36373200	-1.65414900	-0.03773500
C	-3.20215100	-4.79560000	0.61682300
H	-1.55777100	-3.43375400	0.89929800
C	-4.54924200	-4.92626300	0.32096300
H	-6.38094300	-3.89735800	-0.14763600
H	-2.59051400	-5.68303300	0.80075300
H	-5.00450500	-5.91897300	0.26685000
C	-2.81781800	-0.32776700	2.31126000
C	-1.71508500	-0.02424900	3.09999700
C	-4.09089500	-0.30929700	2.88014600
C	-1.87733700	0.29636100	4.43765100
H	-0.71409200	-0.04173200	2.65454200
C	-4.25051600	0.01461200	4.21454800
H	-4.96918200	-0.54771800	2.26899500
C	-3.14424200	0.31643800	4.99412600
H	-1.00281700	0.53476600	5.04919000
H	-5.25172500	0.02946700	4.65314300
H	-3.27365300	0.56972600	6.04988900
C	-3.59585900	0.33860900	-0.38642600
C	-3.84869000	0.01149900	-1.71782800
C	-4.02647100	1.56303900	0.10800100
C	-4.54934300	0.88198700	-2.52977800
H	-3.48799200	-0.93997500	-2.12620700
C	-4.72318900	2.43492600	-0.71270100
H	-3.80767100	1.85318900	1.13989800
C	-4.98939600	2.09637700	-2.02696400
H	-4.74594600	0.61225200	-3.57111700
H	-5.05363600	3.39865400	-0.31621100
H	-5.53661800	2.79024900	-2.67083200
C	2.34109600	0.39968500	1.28092900
H	2.88398500	-0.00642200	2.15851000
H	1.25946600	0.33182000	1.51011800
O	2.76344600	1.72938300	1.18026200
H	2.16006000	2.15087400	0.55734000
C	3.52899200	-2.10594200	-1.91040300
H	3.70207400	-2.51918600	-2.91125900
N	2.12261900	-1.81256800	-1.75686000
H	3.86374500	-2.86156400	-1.16725300

S	1.09788400	-2.98012200	-2.33624200
O	-0.18303100	-2.38248000	-2.56079400
O	1.78728900	-3.61062700	-3.42112300
C	0.94504500	-4.14030900	-1.03049600
H	1.92295700	-4.60023900	-0.83284000
H	0.57443200	-3.62875000	-0.13120900
H	0.23023900	-4.91374800	-1.33993300
C	6.24911000	2.62733500	0.51200700
H	6.12760300	2.96122500	1.55186000
H	7.31942600	2.52157700	0.29199500
H	5.80755400	3.36631600	-0.16338600
H	7.65679200	0.87844700	2.20452300
Sb	-0.56373500	3.29471500	-0.63686900
F	0.30643500	4.48198500	0.47027500
F	-2.13881800	4.21592000	-0.42867700
F	-0.11786300	4.32789100	-2.09145800
F	1.05364400	2.38377100	-0.82711000
F	-1.35756600	2.07111800	-1.75447500
F	-0.94339000	2.24944900	0.83542400

1-3a

E_{sol} = -1315.608984 Hartree

Thermal correction to Free Energy = 0.266412 Hartree

Sum of electronic and thermal Free Energies = -1315.342572 Hartree

Number of Imaginary Frequencies = 0

C	3.06121000	2.67225200	-0.57911000
C	1.72065100	3.00928700	-0.47063300
C	0.79434100	2.05075900	-0.05975200
C	1.22937000	0.78153100	0.25401400
C	2.58384600	0.45381400	0.14120700
C	3.51586200	1.39172400	-0.28557300
H	3.78084600	3.42596300	-0.91706600
H	1.38728600	4.02094600	-0.71770900
H	-0.27050700	2.30794000	-0.00655200
H	4.57318100	1.13385600	-0.39515500
C	0.48035100	-0.44357300	0.72524800
C	1.55566800	-1.55549500	0.60815800
N	2.79665800	-0.84146800	0.51633600
C	-0.14068100	-0.29365900	2.11267300
H	-0.25700800	-1.29321600	2.56798900
H	0.45653900	0.33083700	2.79270600
C	-0.71647900	-0.74160900	-0.13127400
C	-0.56850200	-1.33428200	-1.31513600
H	1.56287900	-2.20691700	1.50356200

C	0.81539600	-1.81105800	-1.59639700
H	1.49656400	-1.00514300	-1.95638800
H	0.81135200	-2.58594800	-2.37954400
O	1.35957100	-2.42602900	-0.44988100
C	-1.50365600	0.29496700	1.83225100
H	-2.25300200	0.04278700	2.59560700
N	-1.84986100	-0.33448800	0.56622600
H	-1.46805400	1.40062900	1.74503900
S	-3.25721200	0.07514800	-0.18221200
O	-3.57558600	-0.97553200	-1.09625400
O	-4.15523200	0.43218600	0.86983000
C	-2.87428700	1.51251900	-1.11285500
H	-2.61276800	2.33438900	-0.43189400
H	-2.04456500	1.29537400	-1.80086000
H	-3.76756300	1.78783000	-1.69110600
C	3.97219100	-1.54863500	0.14992200
H	3.94673900	-2.55356800	0.59606000
H	4.09182000	-1.66759200	-0.94752000
H	4.86834600	-1.03561700	0.53596700
H	-1.39598900	-1.57948700	-1.98168200

1-3b

E_{sol} = -1315.611088 Hartree

Thermal correction to Free Energy = 0.265910 Hartree

Sum of electronic and thermal Free Energies = -1315.345178 Hartree

Number of Imaginary Frequencies = 0

C	3.33055600	2.68198500	-0.37031900
C	1.98982100	2.92707600	-0.62370300
C	1.04835100	1.91678100	-0.43149700
C	1.46796200	0.68651900	0.02416800
C	2.82587100	0.44655400	0.26205500
C	3.77448000	1.43780100	0.06633100
H	4.06461800	3.47817300	-0.53589300
H	1.67261900	3.90828000	-0.98871300
H	-0.00967100	2.09460600	-0.66609800
C	0.70601500	-0.57814600	0.35092500
C	1.85911900	-1.58280000	0.32089200
N	3.01019800	-0.84574300	0.70153900
C	-0.09306500	-0.51310700	1.64086600
H	-0.30209500	-1.54171600	1.98840800
H	0.46334600	0.00206900	2.44054400
C	-1.49086500	-1.08156400	-0.66651100
C	-0.16190400	-1.10986100	-0.73128200
H	1.72128600	-2.46801500	0.97853300

C	0.70703200	-1.89051600	-1.65831000
H	0.85893900	-1.39771200	-2.63974100
H	0.29658800	-2.90175800	-1.86504400
O	1.95704800	-1.97315000	-1.02862300
C	-1.39470600	0.21023100	1.40507000
H	-1.99707900	0.25144500	2.32427400
N	-2.17102100	-0.48822300	0.39561800
H	-1.18711600	1.25724300	1.09565000
S	-3.65994200	0.14077600	0.05434400
O	-4.31462700	-0.80578500	-0.79356900
O	-4.22597700	0.51779400	1.31094300
C	-3.35158600	1.59291900	-0.88222400
H	-2.81697000	2.33100200	-0.26858400
H	-2.76663700	1.33617400	-1.77695900
H	-4.32005300	2.01244600	-1.18783800
C	4.28979900	-1.46541200	0.62016900
H	4.68735600	-1.52400800	-0.41357400
H	5.01968300	-0.91619400	1.23640500
H	4.22276300	-2.48725600	1.02233600
H	4.83979100	1.25099100	0.23167200
H	-2.13537500	-1.58206100	-1.39475100

2-1

E_{sol} = -3169.846158 Hartree

Thermal correction to Free Energy = 0.757478 Hartree

Sum of electronic and thermal Free Energies = -3169.088680 Hartree

Number of Imaginary Frequencies: 0

C	6.02873900	-0.22414300	-1.01733600
C	6.02149100	-0.73886800	0.28484200
C	5.21682200	-1.80710100	0.62729900
C	4.39848100	-2.37729300	-0.35018300
C	4.41636800	-1.83105300	-1.65375200
C	5.22837300	-0.76222300	-2.00618300
H	6.68158200	0.62091900	-1.25704400
H	6.66765300	-0.28282000	1.04098800
H	5.22788900	-2.20418600	1.64815000
C	3.46420700	-3.45355500	-0.36877100
C	2.96426700	-3.49556500	-1.63981100
N	3.52831100	-2.52578700	-2.40812500
C	3.02548800	-4.27226200	0.78357900
H	2.48572900	-5.16949100	0.43755300
H	3.89080700	-4.63311300	1.36868400
C	0.84270000	-1.89457200	0.49667900
C	1.32147400	-0.89279400	-0.03989600

H	2.22116600	-4.16467400	-2.07286200
Au	-1.08381500	-0.62852900	0.07404300
P	-3.12038100	0.45559100	-0.29066500
C	-2.86175900	2.07798600	-1.03762000
C	-3.60953300	3.19034900	-0.66655000
C	-1.86417400	2.20895200	-2.00043300
C	-3.35308800	4.42028800	-1.24958200
H	-4.39673600	3.10235000	0.08908900
C	-1.61696300	3.43760400	-2.58409200
H	-1.26216600	1.33645500	-2.28584000
C	-2.35714500	4.54645900	-2.20335300
H	-3.94223500	5.29194900	-0.95163000
H	-0.82954800	3.53200700	-3.33734600
H	-2.15440200	5.52037500	-2.65728300
C	-4.21528200	-0.44941900	-1.39510000
C	-4.09344400	-1.83326100	-1.48103300
C	-5.18276200	0.20963700	-2.14943900
C	-4.93550200	-2.55232300	-2.31094300
H	-3.32597500	-2.35048800	-0.89206800
C	-6.01877400	-0.51515200	-2.97942100
H	-5.28067600	1.29878000	-2.09080700
C	-5.89524600	-1.89297200	-3.06119900
H	-4.83449500	-3.63865800	-2.37760000
H	-6.77408100	0.00441800	-3.57441100
H	-6.55389200	-2.46017900	-3.72445900
C	-4.02769800	0.74727600	1.23914600
C	-3.35233900	1.36972700	2.28824900
C	-5.35248800	0.36118400	1.40538200
C	-4.00120100	1.61387200	3.48334400
H	-2.30402000	1.67279100	2.16244700
C	-5.99310600	0.59789900	2.61113000
H	-5.89342500	-0.13000400	0.59078700
C	-5.32239500	1.22368700	3.64636800
H	-3.46880000	2.10938600	4.29962500
H	-7.03383300	0.28923800	2.73761200
H	-5.83283100	1.40905400	4.59515800
C	2.13195600	-3.51287600	1.73905600
H	1.86007200	-4.13956600	2.60347800
N	0.89176800	-3.08424900	1.08933300
H	2.62682700	-2.60708800	2.12875100
S	-0.52570100	-3.90199900	1.43368500
O	-1.44996600	-3.53097400	0.40827600
O	-0.13632600	-5.25749600	1.63375600
C	-1.04717300	-3.21476300	2.95092500

H	-0.27354100	-3.37772400	3.71223700
H	-1.23961600	-2.14067200	2.81974900
H	-1.97335100	-3.72101900	3.25376700
C	3.26459400	-2.28693400	-3.78282400
H	2.98423900	-1.23320100	-3.95059100
H	4.14162000	-2.51371400	-4.41100400
H	2.43180500	-2.92089400	-4.11007500
C	1.85644100	0.28934300	-0.64346700
C	1.61635600	0.54237600	-1.93994000
H	1.04453900	-0.17862100	-2.52527900
H	5.23995700	-0.36080800	-3.02383100
O	2.57956300	1.00689000	0.19129600
H	1.97085300	1.45107300	-2.42888900
Si	2.79826100	2.63956100	0.55141800
C	1.27348100	3.53316400	-0.04706700
C	2.91733600	2.55060000	2.40918600
C	4.41028300	3.13045500	-0.24321200
H	1.08969000	3.16236800	-1.07885800
C	0.06311900	3.14488900	0.78309000
C	1.40071400	5.03980000	-0.14308400
H	2.02508200	1.95131200	2.69687300
C	4.14042900	1.76582400	2.84218000
C	2.83002600	3.86903800	3.15233900
H	5.10400600	2.31867000	0.06868600
C	5.00097800	4.43141400	0.26503600
C	4.35885600	3.11240300	-1.75715900
H	0.15161000	3.48236600	1.83037800
H	-0.85929400	3.60178600	0.38228000
H	-0.10114100	2.05056700	0.80753100
H	0.45726200	5.48767500	-0.50630200
H	1.61674600	5.50999700	0.83192600
H	2.19355000	5.35416300	-0.84020700
H	5.07389100	2.31324400	2.62084200
H	4.13489500	1.57987300	3.93044700
H	4.21483800	0.78338200	2.34333800
H	1.90902600	4.43074300	2.92739700
H	2.84504400	3.70672700	4.24445000
H	3.67633500	4.53939400	2.92755600
H	5.95548100	4.65044400	-0.24495800
H	4.34572900	5.30118300	0.08676100
H	5.22054000	4.40332800	1.34377900
H	3.63361300	3.84250300	-2.16053900
H	5.34038700	3.37462500	-2.19066400
H	4.09011300	2.12212100	-2.15940500

2-1a-ts

E_{sol} = -3169.843099 Hartree

Thermal correction to Free Energy = 0.764925 Hartree

Sum of electronic and thermal Free Energies = -3169.078174 Hartree

Number of Imaginary Frequencies: 1

C	-4.84538100	-1.15652900	2.45020700
C	-3.96267400	-0.35611900	3.17490200
C	-3.55272300	0.87651600	2.69770600
C	-4.04595100	1.31257700	1.47677600
C	-4.93314700	0.49071900	0.77081200
C	-5.34765800	-0.74563200	1.22866400
H	-5.14675600	-2.12671000	2.85404300
H	-3.58826900	-0.71326200	4.13830200
H	-2.85167600	1.49059300	3.27186700
H	-6.03424700	-1.37343700	0.65455600
C	-3.78522300	2.46934300	0.64299100
C	-4.59107900	2.26828600	-0.49043000
N	-5.26319800	1.12691700	-0.40421400
C	-3.43088300	3.83564100	1.12484400
H	-3.75758000	4.58166000	0.38161700
H	-3.95266300	4.06582400	2.06675200
C	-1.80245800	2.10447500	-0.09263400
C	-1.38928000	0.93314400	-0.46695900
H	-4.73124700	2.92973100	-1.34566000
Au	0.67188500	0.56081400	-0.08152000
P	2.93710900	-0.01216800	0.21712900
C	3.42034300	-1.25974800	-0.99164900
C	3.65151800	-2.58356200	-0.63200100
C	3.43962600	-0.90381200	-2.33956000
C	3.91185300	-3.53315000	-1.60758000
H	3.62212500	-2.88565000	0.42039900
C	3.71135300	-1.85255300	-3.30718200
H	3.23774200	0.13303700	-2.63398300
C	3.94676300	-3.17006000	-2.94227000
H	4.09124300	-4.57109100	-1.31405800
H	3.73288400	-1.56158200	-4.36098700
H	4.15316800	-3.92097300	-3.70966700
C	4.07184000	1.37769100	-0.00081600
C	3.67925700	2.60528100	0.52793700
C	5.31190800	1.26774600	-0.62350400
C	4.50987500	3.70642100	0.43789700
H	2.70444600	2.69417500	1.02357100
C	6.14001500	2.37394900	-0.71332600

H	5.63783100	0.30985400	-1.04148300
C	5.74113300	3.59156300	-0.18749500
H	4.19187000	4.66501400	0.85704600
H	7.11277000	2.28143300	-1.20395800
H	6.39826100	4.46171900	-0.26600300
C	3.34215300	-0.70561900	1.82995700
C	2.32071900	-0.95750400	2.73890500
C	4.65945300	-1.00292800	2.17343300
C	2.60862100	-1.51355200	3.97503000
H	1.28676600	-0.70774200	2.46851900
C	4.94236200	-1.55580800	3.40805400
H	5.47225600	-0.80638000	1.46485400
C	3.91802400	-1.81294000	4.30776000
H	1.80000400	-1.70875500	4.68487800
H	5.97696000	-1.78912200	3.67407800
H	4.14778100	-2.25032200	5.28311600
C	-1.93260100	3.95490600	1.31077800
H	-1.59378900	4.99481700	1.39539500
N	-1.34081100	3.32313100	0.15919100
H	-1.59059700	3.40232400	2.20257800
S	-0.80432800	4.29299900	-1.14529300
O	-1.10940600	3.58946500	-2.34748100
O	-1.30512700	5.60990800	-0.90459100
C	0.91732900	4.25438200	-0.87197000
H	1.13583400	4.68026800	0.11571900
H	1.24893900	3.20772600	-0.93260200
H	1.40172700	4.85107700	-1.65596200
C	-2.15476700	-0.18938400	-0.98780900
C	-2.82265200	-0.11606300	-2.14569100
H	-2.86776500	0.83085700	-2.68380300
C	-6.05333400	0.54525600	-1.43261100
H	-6.22894400	1.28557400	-2.22084500
H	-5.53520400	-0.32582000	-1.87096200
H	-7.02144700	0.21627100	-1.03011200
H	-3.31840800	-0.98623000	-2.58044900
O	-2.04005800	-1.28274000	-0.24171400
Si	-1.63306300	-2.88682300	-0.47591900
C	-1.12687500	-3.17123500	-2.25118200
C	-0.22726700	-3.08458600	0.74281800
C	-3.17447500	-3.79797000	0.04228600
H	-1.92588800	-2.72408900	-2.87810300
C	0.16623700	-2.45814800	-2.59301000
C	-1.04790500	-4.63998500	-2.62299800
H	0.44644200	-2.23051100	0.49372500

C	-0.72599400	-2.85515400	2.15792900
C	0.60622600	-4.34555900	0.66180300
H	-3.47196800	-3.27199700	0.97659200
C	-3.00600000	-5.26419900	0.38538300
C	-4.29763300	-3.59778700	-0.95527900
H	0.41509000	-2.56688500	-3.66370700
H	0.12809000	-1.37372500	-2.38409800
H	1.01902200	-2.87069000	-2.02647200
H	-0.70814700	-4.76450400	-3.66649400
H	-0.33542500	-5.20153400	-1.99403100
H	-2.02161300	-5.14962900	-2.54435800
H	-1.41239900	-3.65520300	2.48762100
H	0.10772000	-2.84569900	2.88333100
H	-1.26850300	-1.89817200	2.26507800
H	1.08850900	-4.47594200	-0.32090500
H	1.41484100	-4.32631200	1.41667500
H	0.01788400	-5.25861000	0.85857900
H	-3.95645500	-5.69963000	0.74205000
H	-2.69350300	-5.86956500	-0.48292000
H	-2.26183500	-5.43273500	1.18037500
H	-4.09195600	-4.10700200	-1.91402800
H	-5.25268100	-4.00807700	-0.58099000
H	-4.47371600	-2.53193100	-1.18403500

2-1b-ts

E_{sol} = -3169.829644 Hartree

Thermal correction to Free Energy = 0.758764 Hartree

Sum of electronic and thermal Free Energies = -3169.070880 Hartree

Number of Imaginary Frequencies: 1

C	6.58388100	-0.20673700	-0.75856100
C	6.32464800	-0.79820400	0.47989500
C	5.25884400	-1.65955700	0.65579100
C	4.43768500	-1.93120100	-0.43341000
C	4.72593300	-1.33103400	-1.67021900
C	5.78732900	-0.46343400	-1.85882100
H	7.43454000	0.47211400	-0.86050900
H	6.98212200	-0.57463900	1.32463200
H	5.06782600	-2.12134700	1.63006800
C	3.28872600	-2.77161300	-0.63118400
C	3.00870500	-2.67776100	-1.99699600
N	3.82253500	-1.80813000	-2.59014500
C	2.88713900	-3.92748700	0.22494800
H	2.47743800	-4.72835800	-0.41291600
H	3.79442400	-4.34071400	0.69893800

C	0.53099000	-1.99416900	0.26133200
C	1.46486100	-1.32627500	-0.32746800
H	2.23532400	-3.18951800	-2.56930400
Au	-1.24662200	-0.78421000	0.05033500
P	-3.15295400	0.53207100	-0.33726700
C	-2.73084300	2.09468600	-1.13707100
C	-3.38982600	3.28376800	-0.83859600
C	-1.66266500	2.10651900	-2.03160300
C	-2.97401700	4.46962300	-1.42128800
H	-4.22681800	3.28800800	-0.13268800
C	-1.25591100	3.29195900	-2.61628800
H	-1.12653200	1.17437300	-2.25368400
C	-1.90595900	4.47638300	-2.30411700
H	-3.49050600	5.40202600	-1.17868700
H	-0.41258500	3.29347000	-3.31292000
H	-1.57475600	5.41663700	-2.75342300
C	-4.35806200	-0.28878200	-1.39616500
C	-4.47480200	-1.67390300	-1.30659100
C	-5.17770000	0.41850600	-2.27146500
C	-5.41014500	-2.34283400	-2.07562300
H	-3.82070300	-2.23353700	-0.62572400
C	-6.10560500	-0.25815200	-3.04449800
H	-5.09118300	1.50742300	-2.35145200
C	-6.22366200	-1.63478600	-2.94564500
H	-5.49726500	-3.42995500	-2.00098000
H	-6.74477000	0.29900700	-3.73442800
H	-6.95577500	-2.16415000	-3.56100400
C	-4.03031800	0.97856500	1.17619000
C	-3.27212700	1.38663900	2.27128000
C	-5.41631600	0.93183400	1.28014900
C	-3.89270400	1.75052700	3.45166600
H	-2.17766700	1.41635200	2.19482500
C	-6.03233700	1.28885800	2.46880000
H	-6.02470100	0.61054500	0.42838700
C	-5.27428700	1.69629600	3.55262500
H	-3.29018400	2.07004100	4.30623200
H	-7.12189700	1.24413100	2.54610600
H	-5.76474800	1.97200600	4.48977400
C	1.89235500	-3.65060200	1.31648900
H	1.75166500	-4.56260800	1.91208700
N	0.60453300	-3.27313300	0.75404900
H	2.24663800	-2.83879900	1.98477500
S	-0.75692100	-3.88179900	1.49400300
O	-1.85696200	-3.54771900	0.64186100

O	-0.45828500	-5.24611000	1.79412200
C	-0.90357100	-2.98028500	2.98432600
H	-0.01278000	-3.14846600	3.60419800
H	-1.01718600	-1.91198700	2.74763900
H	-1.79466000	-3.33562400	3.51706000
C	3.79815700	-1.43968100	-3.96740500
H	3.66764700	-0.35260300	-4.07726000
H	4.73683000	-1.73326300	-4.46044300
H	2.96466600	-1.94871300	-4.46395600
C	1.93582800	-0.02084100	-0.69396200
C	1.76413700	0.40619200	-1.95590500
H	1.29212600	-0.26232300	-2.67732600
H	5.99598800	-0.00901800	-2.83116700
O	2.51756700	0.63512400	0.29758300
H	2.04163300	1.40755000	-2.29052100
Si	2.82015500	2.24023900	0.71910300
C	1.36568300	3.25339800	0.13821900
C	2.87587300	2.05628200	2.57516900
C	4.46990100	2.72714800	-0.00328800
H	1.20112200	2.97152100	-0.92352200
C	0.11249900	2.86354400	0.89956100
C	1.56342300	4.75533500	0.16062100
H	1.94718600	1.48666600	2.80194600
C	4.04099500	1.18950000	3.01153400
C	2.82031900	3.33787500	3.38305200
H	5.12670700	1.86446100	0.23784100
C	5.10176800	3.94643600	0.64329000
C	4.46358900	2.87393600	-1.51184400
H	0.17891900	3.13593400	1.96757300
H	-0.77812400	3.37810800	0.49736000
H	-0.08814200	1.77620400	0.85464600
H	0.65365000	5.27071100	-0.19952200
H	1.76460500	5.14255800	1.17462900
H	2.39412600	5.08445300	-0.48381200
H	5.01419000	1.67835400	2.82413400
H	3.99966500	0.97622200	4.09421500
H	4.05861800	0.21965700	2.48668500
H	1.92617400	3.94486100	3.16834800
H	2.80385600	3.11890000	4.46537800
H	3.69479100	3.98620000	3.21115300
H	6.07372200	4.17430300	0.17103400
H	4.48587300	4.85672100	0.54269500
H	5.29997200	3.80256900	1.71644600
H	3.79088900	3.68203100	-1.85214800

H	5.47140000	3.12725400	-1.88718100
H	4.16018000	1.95091100	-2.03056100

2-2a

E_{sol} = -3169.871076 Hartree
Thermal correction to Free Energy = 0.763636 Hartree
Sum of electronic and thermal Free Energies = -3169.107440 Hartree
Number of Imaginary Frequencies: 0

C	5.85088000	0.77775600	1.70160500
C	4.80432200	0.35081100	2.50921400
C	3.93983100	-0.65538600	2.09704600
C	4.14503600	-1.22433400	0.86020200
C	5.19588600	-0.77996900	0.07297500
C	6.06813700	0.21658700	0.45229300
H	6.50878900	1.57816600	2.04857000
H	4.65277900	0.82417000	3.48312300
H	3.10462600	-0.96795900	2.73122200
H	6.87932100	0.55845000	-0.19475300
C	3.40386000	-2.28691600	0.10328700
C	4.12725100	-2.25874700	-1.18005700
N	5.15132100	-1.46970000	-1.14429700
C	3.49122100	-3.68856700	0.73411600
H	3.48034800	-4.45534500	-0.05834400
H	4.40004400	-3.82090100	1.33669600
C	1.87598500	-2.05831300	0.00963400
C	1.27096700	-0.94725100	-0.40978100
H	3.91872800	-2.87390500	-2.05794500
Au	-0.75195300	-0.52404600	-0.19054100
P	-3.02385600	0.08869400	0.06050900
C	-3.40881200	1.68144200	-0.70503700
C	-3.45047900	2.84852000	0.05045700
C	-3.54867700	1.76006100	-2.09023300
C	-3.64079100	4.07341200	-0.56816700
H	-3.33414800	2.80633600	1.13891300
C	-3.74705100	2.98427100	-2.70113200
H	-3.50674100	0.85016300	-2.69973100
C	-3.79160600	4.14380300	-1.94247100
H	-3.67494500	4.98373500	0.03760600
H	-3.86437600	3.03335100	-3.78717800
H	-3.94538400	5.11082700	-2.42924700
C	-4.19779000	-1.07256000	-0.67267600
C	-3.77450200	-2.37683400	-0.91600800
C	-5.50651500	-0.71087900	-0.98879400
C	-4.65203800	-3.31062600	-1.43841300

H	-2.73303600	-2.65494100	-0.70742500
C	-6.38009100	-1.64735800	-1.50958300
H	-5.84505200	0.31961500	-0.83830600
C	-5.95648000	-2.94844000	-1.72968300
H	-4.30921600	-4.33083700	-1.63010500
H	-7.40515600	-1.35507200	-1.75319000
H	-6.64914200	-3.68523300	-2.14607100
C	-3.49342200	0.30526500	1.79438800
C	-2.48048900	0.51312200	2.72741800
C	-4.82096200	0.34081800	2.21168200
C	-2.78977900	0.76170600	4.05413300
H	-1.43245100	0.47991800	2.40242200
C	-5.12558900	0.57815800	3.53974400
H	-5.63157300	0.18033400	1.49442100
C	-4.11267200	0.79167400	4.46111500
H	-1.98632800	0.92525400	4.77809800
H	-6.17104700	0.59831100	3.85956500
H	-4.35912600	0.98093400	5.50952900
C	2.20366800	-3.77296300	1.51748800
H	1.92168700	-4.80465000	1.76758700
N	1.22583100	-3.13477500	0.66025800
H	2.26423000	-3.19719400	2.45705900
S	0.32420200	-4.21490800	-0.26237200
O	-0.19265700	-3.50873000	-1.39321300
O	1.06341100	-5.43027800	-0.46598700
C	-0.97520600	-4.54210500	0.85937900
H	-0.57348500	-5.00032500	1.77241800
H	-1.48476400	-3.60073300	1.10378100
H	-1.67145500	-5.24228200	0.37932100
C	2.08131900	0.09173800	-1.04776600
C	2.57665300	-0.00787200	-2.29178700
H	2.36664300	-0.89171400	-2.89477400
C	6.00503200	-1.16422100	-2.24551600
H	5.81371600	-0.12926300	-2.57183000
H	7.05551200	-1.25409000	-1.94077900
H	5.79939200	-1.85338200	-3.07020800
H	3.14199900	0.81007900	-2.74850100
O	2.28663600	1.15942400	-0.27942400
Si	1.83214800	2.75834700	-0.21254600
C	1.25344600	3.32646500	-1.89519200
C	0.49186500	2.79722700	1.08720300
C	3.43472100	3.52686900	0.34997200
H	1.98965200	2.90776700	-2.61455800
C	-0.10730700	2.75935600	-2.25026400

C	1.26214100	4.83314900	-2.07005900
H	-0.26385700	2.07470500	0.70122700
C	1.00819500	2.23243300	2.39607700
C	-0.22543300	4.11299900	1.30644700
H	3.75505800	2.84373500	1.16828900
C	3.36384100	4.92265300	0.93134900
C	4.48823200	3.43012300	-0.73555600
H	-0.39520100	3.02023200	-3.28492100
H	-0.15179000	1.65802700	-2.17306700
H	-0.89732100	3.16515700	-1.59363500
H	0.88839100	5.11714000	-3.06982100
H	0.61466400	5.34624000	-1.33759000
H	2.26962000	5.26734500	-1.97131500
H	1.78132200	2.87992300	2.84862100
H	0.19978600	2.14250500	3.14576200
H	1.45612100	1.23000600	2.27007200
H	-0.71866100	4.48824100	0.39496800
H	-1.01570800	4.00507600	2.07379100
H	0.44732400	4.91144600	1.66401400
H	4.36385500	5.27906000	1.23692200
H	2.97361100	5.66418300	0.21324700
H	2.72410700	4.97293300	1.82755300
H	4.28295600	4.11992600	-1.57364100
H	5.49278800	3.68790700	-0.35441400
H	4.55773800	2.41305300	-1.16183300

2-2b

E_{sol} = -3169.872749 Hartree

Thermal correction to Free Energy = 0.763671 Hartree

Sum of electronic and thermal Free Energies = -3169.109078 Hartree

Number of Imaginary Frequencies: 0

C	6.60228400	-0.78635300	-0.99292200
C	6.36150200	-0.86339500	0.37309200
C	5.17938600	-1.40059800	0.86493500
C	4.24823100	-1.86399000	-0.03675400
C	4.52879100	-1.80989600	-1.39362700
C	5.68337100	-1.26738400	-1.91341900
H	7.53919100	-0.35316300	-1.35172600
H	7.11347100	-0.48718300	1.07172400
H	4.99536800	-1.45676600	1.94149100
C	2.90174700	-2.48547600	0.14547600
C	2.60948800	-2.90942500	-1.24622700
N	3.47749300	-2.43207000	-2.08175800
C	2.80691900	-3.58123600	1.20028100

H	3.06812300	-4.54700100	0.73900400
H	3.54802600	-3.39212900	1.99264100
C	0.46578300	-1.96727400	0.37432800
C	1.72552100	-1.48593600	0.17544400
H	1.72125600	-3.44362800	-1.58908400
Au	-1.20822100	-0.74883900	0.09517400
P	-3.07868400	0.65468900	-0.25265700
C	-2.65020200	2.19113500	-1.10162600
C	-3.27789500	3.40265100	-0.82656100
C	-1.62293900	2.14929900	-2.04153100
C	-2.87860300	4.55447600	-1.48413100
H	-4.08190000	3.45131600	-0.08452100
C	-1.23131600	3.30063000	-2.70074800
H	-1.11129600	1.19948700	-2.24217800
C	-1.85500600	4.50601100	-2.41763700
H	-3.37327600	5.50361100	-1.26146800
H	-0.42066300	3.25859200	-3.43389300
H	-1.53871900	5.41902900	-2.92959000
C	-4.36025700	-0.13086600	-1.24986700
C	-4.51632300	-1.51057600	-1.13836300
C	-5.19642600	0.59005000	-2.09764800
C	-5.50576700	-2.15889000	-1.85536400
H	-3.84339100	-2.08216700	-0.48590500
C	-6.17893200	-0.06531400	-2.81934700
H	-5.07956400	1.67478600	-2.19645400
C	-6.33531300	-1.43660100	-2.69765300
H	-5.62165800	-3.24225600	-1.76413400
H	-6.83092900	0.50380900	-3.48752800
H	-7.11090500	-1.95002300	-3.27261800
C	-3.88745500	1.17258200	1.27709200
C	-3.07264700	1.61697800	2.31732300
C	-5.26692100	1.14707200	1.45075100
C	-3.63031700	2.03888600	3.50954200
H	-1.98334600	1.63287200	2.18407700
C	-5.82014300	1.56102900	2.65174600
H	-5.91954100	0.80063400	0.64329700
C	-5.00605900	2.00581900	3.67911800
H	-2.98377100	2.38877400	4.31857400
H	-6.90487700	1.53416000	2.78439000
H	-5.44794500	2.32942300	4.62544800
C	1.43663200	-3.62647100	1.81174200
H	1.22909800	-4.62340700	2.22228500
N	0.43856400	-3.29571300	0.80593600
H	1.36230000	-2.88607700	2.63305700

S	-1.02448800	-4.06904100	0.95560200
O	-1.80584100	-3.69171500	-0.18332000
O	-0.71418000	-5.44511200	1.19107100
C	-1.76732400	-3.41644400	2.39946200
H	-1.13658100	-3.63670000	3.27107100
H	-1.90724200	-2.33088000	2.28815100
H	-2.74379300	-3.90162500	2.52720000
C	3.38007400	-2.46183600	-3.50806000
H	3.32433400	-1.43329800	-3.89341200
H	4.26536800	-2.95486400	-3.93108100
H	2.48006000	-3.01190300	-3.79937500
C	1.95789400	-0.12894400	-0.37275700
C	1.57980700	0.16995700	-1.62209900
H	1.07843700	-0.59397500	-2.21848400
H	5.87823000	-1.22964500	-2.98731400
O	2.58347100	0.67719700	0.47948300
H	1.73351900	1.14495100	-2.08738200
Si	2.99235900	2.31358500	0.50706000
C	1.54365500	3.31185800	-0.12579000
C	3.23841000	2.53623400	2.34517000
C	4.58334900	2.49884100	-0.45648500
H	1.28726100	2.89855300	-1.12098100
C	0.32961600	3.09467800	0.75940000
C	1.80747600	4.78839700	-0.34562300
H	2.33625400	2.05651400	2.78465700
C	4.43748100	1.75715200	2.84657700
C	3.27459200	3.96340400	2.85313000
H	5.20734100	1.65977600	-0.07864200
C	5.35010200	3.77765100	-0.17524800
C	4.43191300	2.29329700	-1.95109100
H	0.48132800	3.48430400	1.78149700
H	-0.56150300	3.60758000	0.35458700
H	0.07346000	2.02336500	0.85481800
H	0.89445900	5.29145100	-0.71500800
H	2.10796600	5.31879300	0.57353600
H	2.59353800	4.96953400	-1.09651700
H	5.38844500	2.16100700	2.45564100
H	4.50818800	1.79182100	3.94810000
H	4.39119300	0.69538400	2.55795900
H	2.33707400	4.50945000	2.66541900
H	3.44002500	3.98527200	3.94498800
H	4.08862700	4.55682300	2.40441800
H	6.29491100	3.79791100	-0.74727200
H	4.79067100	4.68245300	-0.46813900

H	5.62040400	3.89164900	0.88621100
H	3.75958200	3.04155700	-2.41051900
H	5.40694500	2.39266500	-2.46197500
H	4.03987000	1.29624000	-2.20774900

2-2a-ts

E_{sol} = -3169.865581 Hartree

Thermal correction to Free Energy = 0.762387 Hartree

Sum of electronic and thermal Free Energies = -3169.103194 Hartree

Number of Imaginary Frequencies: 1

C	5.35513100	0.28821700	2.58908800
C	4.15341100	-0.22039800	3.06259500
C	3.40076400	-1.10593600	2.30056200
C	3.87168000	-1.46769200	1.05785300
C	5.06137100	-0.92374500	0.59359700
C	5.83480500	-0.05350000	1.33298900
H	5.92679500	0.98563700	3.20643500
H	3.79212100	0.08538300	4.04751600
H	2.44173100	-1.48432900	2.66948000
H	6.76572000	0.36746000	0.94435200
C	3.30510400	-2.35410700	-0.02093800
C	4.19240000	-1.98376600	-1.15174900
N	5.26046900	-1.34581500	-0.71674500
C	3.41660400	-3.85527200	0.28496300
H	3.47767400	-4.42004400	-0.66103300
H	4.29591900	-4.10103100	0.89623000
C	1.79050900	-2.17024800	-0.22219200
C	1.22473500	-1.00095700	-0.53292000
H	4.21821400	-2.49003100	-2.11752100
Au	-0.76166900	-0.45330000	-0.25884600
P	-2.99400800	0.19747700	0.16240300
C	-3.29863000	1.97092200	-0.01275200
C	-3.87838700	2.75012900	0.98235200
C	-2.93051300	2.56377800	-1.22076500
C	-4.10234900	4.10075000	0.76132300
H	-4.16841900	2.30227900	1.93823800
C	-3.16099800	3.90886300	-1.43745700
H	-2.46009400	1.95615500	-2.00484800
C	-3.74947100	4.67965200	-0.44540500
H	-4.56329100	4.70618200	1.54626900
H	-2.87474200	4.36271400	-2.39040200
H	-3.92935600	5.74459900	-0.61490700
C	-4.20189700	-0.56077700	-0.94659700
C	-3.86115900	-1.73716100	-1.60985300

C	-5.45431000	0.00923700	-1.16490100
C	-4.76557100	-2.34030900	-2.46702000
H	-2.86449300	-2.17524100	-1.46449900
C	-6.35542000	-0.59858700	-2.02039300
H	-5.72747500	0.94389500	-0.66311500
C	-6.01206700	-1.77284700	-2.67115800
H	-4.48808100	-3.25899600	-2.99041600
H	-7.33627300	-0.14425700	-2.18574800
H	-6.72259100	-2.24645600	-3.35406400
C	-3.50268400	-0.21962000	1.84553100
C	-2.52288600	-0.19994400	2.83800200
C	-4.81425000	-0.53079100	2.18967000
C	-2.85266500	-0.47263800	4.15336200
H	-1.48431600	0.03053500	2.56656700
C	-5.13720300	-0.81553100	3.50502300
H	-5.59657700	-0.55732400	1.42526400
C	-4.16040100	-0.78298200	4.48724100
H	-2.07755200	-0.45065200	4.92376200
H	-6.16929400	-1.06527500	3.76643400
H	-4.42164400	-1.00926700	5.52485900
C	2.09857300	-4.14873000	0.95712600
H	1.82431500	-5.21012600	0.93347300
N	1.15418700	-3.33794500	0.21623500
H	2.10517000	-3.81624500	2.01076100
S	0.02797800	-4.12457000	-0.73135800
O	-0.26408100	-3.29999000	-1.86209400
O	0.46391900	-5.47672800	-0.92423500
C	-1.35855500	-4.15140800	0.33188000
H	-1.10383400	-4.70002000	1.24811700
H	-1.64305200	-3.11795500	0.57769700
H	-2.18130700	-4.66299300	-0.18554300
C	2.15462400	-0.00061300	-1.00633900
C	2.91136300	-0.21699000	-2.12173200
H	2.60031100	-0.98279600	-2.82964500
C	6.29499800	-0.83384200	-1.55102800
H	7.27441100	-1.00217100	-1.08360500
H	6.26956000	-1.34299400	-2.51981900
H	6.15834600	0.25059000	-1.70715600
H	3.63310000	0.53149500	-2.46747000
O	2.29259500	1.06890000	-0.25064600
Si	2.05852800	2.72233100	-0.33913700
C	3.58078900	3.31283400	0.55563700
C	1.94665300	3.23337400	-2.13002000
C	0.46205400	2.98952600	0.58381300

H	3.63162800	2.62778900	1.43288200
C	4.82291800	3.05927200	-0.27611500
C	3.55293700	4.73087300	1.08504100
H	2.77810500	2.70453300	-2.64288600
C	0.65012500	2.76959700	-2.76797000
C	2.15493100	4.71752100	-2.36037800
H	-0.25858600	2.34079700	0.03545800
C	-0.10087300	4.39632000	0.56183400
C	0.53709400	2.45771800	2.00089000
H	5.74507700	3.19642200	0.31625400
H	4.85340900	2.03315500	-0.68534400
H	4.89098500	3.75268800	-1.13319800
H	4.49173900	4.97810100	1.61158200
H	3.43911600	5.47923600	0.28129200
H	2.73364800	4.89764800	1.80302900
H	-0.22037500	3.29774400	-2.33908600
H	0.64182700	2.97184400	-3.85333100
H	0.46611700	1.68679500	-2.64409100
H	3.14619400	5.06473500	-2.02778900
H	2.07325800	4.96619300	-3.43331500
H	1.40314400	5.33391000	-1.83859900
H	-1.04234000	4.45203300	1.13905000
H	0.58671900	5.13367100	1.01135100
H	-0.33222400	4.74957000	-0.45615500
H	1.18454900	3.08415100	2.64106900
H	-0.46292100	2.44977300	2.47500200
H	0.93313200	1.42722000	2.04681000

2-2b-ts

E_{sol} = -3169.858508 Hartree

Thermal correction to Free Energy = 0.766403 Hartree

Sum of electronic and thermal Free Energies = -3169.092105 Hartree

Number of Imaginary Frequencies: 1

C	6.22297800	-0.36919700	1.65652200
C	5.08387400	-0.91187800	2.23207000
C	4.05317200	-1.41042600	1.44103300
C	4.19439500	-1.37499100	0.07064100
C	5.32561100	-0.78800500	-0.48171600
C	6.36087800	-0.28278300	0.27727700
H	7.01899700	0.01823000	2.29703100
H	4.99106600	-0.94034700	3.32037700
H	3.13817600	-1.80064300	1.90199600
C	3.27914800	-1.82187000	-1.05249500
C	3.97139200	-1.16095900	-2.21565000

N	5.19048900	-0.77810800	-1.86546000
C	3.18129900	-3.32997500	-1.21931400
H	2.72791700	-3.54907600	-2.20142300
H	4.17017800	-3.81275600	-1.18729900
C	0.83959100	-1.92721000	-0.36928100
C	1.90363500	-1.25736500	-0.86625900
H	3.80459500	-1.44035300	-3.25741000
Au	-1.00235400	-0.93755500	-0.24952100
P	-3.04387300	0.24070900	-0.20120600
C	-3.47044700	1.03029400	-1.76802600
C	-4.73310600	1.57413600	-1.99312600
C	-2.50418900	1.10951800	-2.76715700
C	-5.01540600	2.19888200	-3.19371000
H	-5.50530100	1.51320600	-1.21837300
C	-2.78998500	1.73843600	-3.96754800
H	-1.51378500	0.66746000	-2.59650900
C	-4.04367000	2.28478200	-4.17921600
H	-6.00810500	2.62498800	-3.36315500
H	-2.02503100	1.79625700	-4.74645200
H	-4.27154700	2.77926500	-5.12738500
C	-4.45210000	-0.81301300	0.22264300
C	-4.41033700	-2.15116600	-0.15907000
C	-5.57137500	-0.32579400	0.89396400
C	-5.47972100	-2.98625400	0.11390100
H	-3.52147400	-2.54331900	-0.66667600
C	-6.63634200	-1.16621200	1.16712200
H	-5.61094000	0.72184900	1.21125000
C	-6.59221400	-2.49478700	0.77740100
H	-5.43715200	-4.03682400	-0.18595400
H	-7.51095200	-0.77676200	1.69471600
H	-7.43315200	-3.15739700	0.99955300
C	-3.06926300	1.55059600	1.04036100
C	-3.19251700	2.89719600	0.71958200
C	-2.88080600	1.17862800	2.37229000
C	-3.14645000	3.85720400	1.71983900
H	-3.32226500	3.20927500	-0.32121000
C	-2.84857200	2.13781800	3.36702000
H	-2.76315500	0.11886900	2.62978100
C	-2.98418300	3.48021700	3.04118500
H	-3.24477600	4.91424200	1.45792100
H	-2.71198300	1.83557100	4.40884100
H	-2.95186900	4.23930200	3.82746000
C	2.32159900	-3.90409300	-0.12772300
H	2.19748700	-4.98224700	-0.28432400

N	1.00532400	-3.28539200	-0.12959900
H	2.81946800	-3.77319800	0.85472900
S	-0.11571800	-4.04248600	0.83344200
O	-1.42223100	-3.72548700	0.34498100
O	0.29877800	-5.40787400	0.92465400
C	0.08972500	-3.28910100	2.40332800
H	1.11736100	-3.45577400	2.75495500
H	-0.12225900	-2.21264900	2.32734800
H	-0.61564700	-3.75603800	3.10282800
C	6.12600600	-0.15324800	-2.73802300
H	6.18433400	0.92922500	-2.53139900
H	7.12471400	-0.59160400	-2.60317800
H	5.80992200	-0.30011500	-3.77629800
C	1.96393900	0.17539400	-1.15396200
C	2.54179600	0.52850300	-2.35564800
H	2.23043700	-0.03623100	-3.23346200
H	7.24419600	0.17055400	-0.17914000
O	1.66392300	0.97258200	-0.17979300
H	2.86552100	1.55477900	-2.55273500
Si	1.93992900	2.54284200	0.39340600
C	0.79118800	2.44412100	1.85515600
C	3.75654500	2.60407700	0.82674600
C	1.41110800	3.75916500	-0.91498900
H	-0.18096100	2.16073800	1.39128200
C	1.17990700	1.30553600	2.77927700
C	0.56258000	3.72693800	2.62919900
H	3.97635800	1.58471400	1.21421900
C	4.65737200	2.83719100	-0.37118400
C	4.08902000	3.58699900	1.93336300
H	1.99712200	3.49572200	-1.82118500
C	1.72229100	5.20576700	-0.58751100
C	-0.05641800	3.57547800	-1.25040900
H	2.12878900	1.50517400	3.30958000
H	0.40923300	1.14775500	3.55607200
H	1.30112300	0.34994700	2.23813800
H	-0.09143000	3.54576500	3.50002800
H	1.49480600	4.16219700	3.02642000
H	0.07290500	4.50618500	2.02249800
H	4.49332700	3.82924600	-0.82855600
H	5.72148300	2.79895400	-0.07404000
H	4.52269800	2.08372900	-1.16388800
H	3.57963700	3.34922000	2.87989900
H	5.17299700	3.58377800	2.14379800
H	3.82338900	4.62627100	1.66961000

H	1.42027600	5.87266400	-1.41359100
H	1.18462500	5.55507100	0.31008500
H	2.79581600	5.38120900	-0.41251000
H	-0.70308600	3.89049500	-0.41164600
H	-0.35474800	4.17519600	-2.12791200
H	-0.30895700	2.52382200	-1.47798400

2-3a

E_{sol} = -3169.903250 Hartree

Thermal correction to Free Energy = 0.768585 Hartree

Sum of electronic and thermal Free Energies = -3169.134665 Hartree

Number of Imaginary Frequencies: 0

C	0.75902200	-3.90633200	3.62276800
C	0.13036300	-4.47388300	2.52409800
C	0.61659300	-4.23095200	1.24493000
C	1.73030600	-3.42990100	1.09107200
C	2.33588100	-2.83514600	2.19832600
C	1.86929400	-3.08863900	3.48235500
H	0.37841400	-4.11411000	4.62714800
H	-0.73637100	-5.12395200	2.66274000
H	0.12499100	-4.69800500	0.38547900
H	2.35401600	-2.65221300	4.35861300
C	2.48249800	-3.00785400	-0.14790200
C	3.66909500	-2.22020600	0.42491600
N	3.35824100	-2.01182500	1.82461300
C	2.80699500	-4.11273200	-1.13279900
H	3.66593800	-3.80602700	-1.75350700
H	3.06197800	-5.06015700	-0.64088600
C	1.55188100	-2.11719400	-0.93723600
C	1.34586500	-0.77885400	-0.61333300
H	4.59699300	-2.82298400	0.31052400
Au	-0.51304800	0.14090200	-0.32470700
P	-2.71647500	0.73933600	0.30040800
C	-2.93414000	2.17976900	1.36775100
C	-3.10986400	2.05188700	2.74171000
C	-2.82709300	3.45232500	0.80981400
C	-3.17850000	3.18037000	3.54177500
H	-3.19805400	1.06104200	3.19889400
C	-2.89846000	4.57507800	1.61291500
H	-2.68791400	3.56831000	-0.27120100
C	-3.07289800	4.44128000	2.98154000
H	-3.32092000	3.06834400	4.62010600
H	-2.81754500	5.56816900	1.16220000
H	-3.12710400	5.32990800	3.61631000

C	-3.81486600	1.02288100	-1.10530400
C	-3.41366900	0.54607600	-2.35085700
C	-5.03912300	1.68016600	-0.98818100
C	-4.23191100	0.70010500	-3.45682200
H	-2.43603000	0.05893500	-2.45472800
C	-5.85367400	1.83104800	-2.09653600
H	-5.35925600	2.08134800	-0.02062600
C	-5.45357900	1.33905800	-3.32897100
H	-3.90434900	0.32653500	-4.43062600
H	-6.81287000	2.34607800	-1.99665300
H	-6.09882300	1.46586300	-4.20221200
C	-3.42054100	-0.64418000	1.23427000
C	-2.55412000	-1.48788300	1.92933800
C	-4.79224300	-0.87440900	1.30480400
C	-3.05299900	-2.53494000	2.68554600
H	-1.47009500	-1.31518100	1.88216500
C	-5.28493000	-1.93006000	2.05166200
H	-5.49132000	-0.22807600	0.76589400
C	-4.41793100	-2.75995000	2.74404600
H	-2.36116400	-3.18157400	3.23326400
H	-6.36310400	-2.10541800	2.09315300
H	-4.81110000	-3.59216500	3.33384300
C	1.56750800	-4.22114300	-1.98671100
H	1.78256100	-4.42806300	-3.04270200
N	0.97589200	-2.88950600	-1.86651000
H	0.85654000	-4.98746200	-1.63454500
S	-0.35444600	-2.51813400	-2.84857100
O	-0.32476000	-1.12105600	-3.12299700
O	-0.29826200	-3.47678000	-3.90124700
C	-1.68064800	-2.91533200	-1.78434500
H	-1.66379500	-3.99515600	-1.58687800
H	-1.59717400	-2.34375000	-0.84744200
H	-2.61614200	-2.65428200	-2.29853000
C	2.50751200	-0.17106400	-0.20061300
C	3.83005800	-0.87692000	-0.25063400
H	4.18240000	-1.00166300	-1.28943600
C	4.44237600	-1.77246200	2.71551400
H	4.08548500	-1.29912900	3.64159400
H	4.99195400	-2.69802100	2.98579300
H	5.15801800	-1.07581100	2.25647300
H	4.59566900	-0.29048300	0.27866100
O	2.47911800	1.05117200	0.24466500
Si	3.17003100	2.54096800	-0.17930500
C	4.49755200	2.21346100	-1.44985900

C	1.71831100	3.49493100	-0.85380600
C	3.77737100	3.15561600	1.46739400
H	5.10117600	1.37818000	-1.04011000
C	3.91502200	1.74913100	-2.77273100
C	5.45959200	3.36820100	-1.65853400
H	1.24885700	2.79278700	-1.58033600
C	0.68891400	3.78732600	0.22087500
C	2.06936000	4.76189600	-1.60815400
H	2.90897800	2.99717800	2.14379700
C	4.12527200	4.62927800	1.52376900
C	4.91330100	2.29984600	1.99135300
H	4.70728600	1.40104000	-3.45767600
H	3.19247100	0.92008100	-2.67071800
H	3.38513100	2.56482500	-3.29343200
H	6.20234100	3.12200700	-2.43732000
H	4.95495000	4.29214200	-1.98830900
H	6.02487600	3.61195400	-0.74477200
H	1.06585700	4.51629800	0.96025800
H	-0.22383300	4.22876400	-0.21647100
H	0.37724700	2.88774000	0.78105200
H	2.71147800	4.57829100	-2.48360600
H	1.15836200	5.26206500	-1.98116300
H	2.59008100	5.49711200	-0.97076900
H	4.41569900	4.92631900	2.54648200
H	4.97470400	4.89027000	0.87016200
H	3.28150200	5.27473800	1.23187900
H	5.80653000	2.35424400	1.34288300
H	5.23256700	2.62648000	2.99635000
H	4.63032900	1.23641500	2.07666000

2-3b

E_{sol} = -3169.913200 Hartree

Thermal correction to Free Energy = 0.769456 Hartree

Sum of electronic and thermal Free Energies = -3169.143744 Hartree

Number of Imaginary Frequencies: 0

C	5.86984500	-2.53469100	2.79224900
C	4.60082000	-3.05996100	2.61577100
C	3.84070500	-2.67791900	1.51395600
C	4.36980100	-1.79173200	0.60273200
C	5.64954700	-1.26308600	0.79545900
C	6.41089100	-1.62192600	1.89710900
H	6.45657100	-2.82729300	3.66859900
H	4.19117100	-3.76030100	3.34803100
H	2.81770400	-3.05845500	1.39318500

C	3.80545700	-1.20273600	-0.66994500
C	4.74519000	-0.00954100	-0.85877800
N	5.97422800	-0.40303800	-0.22599200
C	3.76262900	-2.18680200	-1.81688900
H	3.55723000	-1.63777900	-2.75286700
H	4.71860400	-2.71820700	-1.94348500
C	1.25141900	-1.30757200	-0.75027500
C	2.44289300	-0.59644000	-0.51843200
H	4.91810100	0.21723300	-1.92591400
Au	-0.65731100	-0.56338000	-0.26823000
P	-2.90534300	-0.10654800	0.33848700
C	-3.18969900	-0.15423900	2.12135100
C	-4.46828900	-0.31192200	2.65546900
C	-2.09302300	-0.11241400	2.97704700
C	-4.64103400	-0.39868800	4.02476000
H	-5.33691100	-0.37824200	1.99107200
C	-2.26978100	-0.20362900	4.34690500
H	-1.08537000	-0.01886500	2.55479800
C	-3.54355600	-0.34368200	4.87004500
H	-5.64626200	-0.51965400	4.43716900
H	-1.40187700	-0.17325800	5.01088800
H	-3.68491200	-0.42152100	5.95148000
C	-3.61798500	1.40696100	-0.33919700
C	-3.26923200	1.74044400	-1.64765500
C	-4.52942100	2.20072300	0.34900700
C	-3.84839400	2.83269900	-2.26788800
H	-2.54204500	1.12233900	-2.19036400
C	-5.10045600	3.29876400	-0.27421900
H	-4.80016900	1.96581100	1.38288100
C	-4.76844700	3.61052900	-1.58137200
H	-3.57466100	3.08139300	-3.29706500
H	-5.81685400	3.91706700	0.27276100
H	-5.22524700	4.47542800	-2.06982200
C	-3.97839800	-1.43362900	-0.27307100
C	-3.74217700	-2.71606000	0.21975800
C	-4.99078600	-1.23666600	-1.20321000
C	-4.51241800	-3.78147500	-0.20233000
H	-2.94855600	-2.87575800	0.96055200
C	-5.75569000	-2.31109000	-1.63066400
H	-5.19597500	-0.23741200	-1.59900700
C	-5.52010300	-3.58022900	-1.13368100
H	-4.32539800	-4.78151000	0.19881000
H	-6.55201100	-2.14733100	-2.36198900
H	-6.12850000	-4.42288100	-1.47302300

C	2.68219500	-3.19376800	-1.57788500
H	2.52238200	-3.80285900	-2.47518300
N	1.41256700	-2.54318700	-1.24415200
H	2.95210200	-3.88876300	-0.76123600
S	0.04930300	-3.57389500	-1.42321300
O	-1.02641800	-2.80830800	-1.96378000
O	0.53331200	-4.72199800	-2.11721300
C	-0.28829900	-4.01913400	0.23241600
H	0.57941200	-4.55665100	0.63728900
H	-0.50575400	-3.12244800	0.82903200
H	-1.16019900	-4.68764800	0.21979800
C	6.97858100	0.58495300	-0.04483200
H	6.74101200	1.32413200	0.75131200
H	7.93903000	0.11444800	0.21131300
H	7.12469100	1.13258200	-0.98701700
C	2.57361100	0.74338200	-0.20960800
C	4.00301300	1.14818100	-0.19189100
H	4.16638300	2.11816500	-0.68428400
H	7.40274000	-1.19522700	2.06943100
H	4.31468300	1.27824200	0.86444000
O	1.61450400	1.55140500	0.06519300
Si	1.34207700	3.24560200	-0.13168100
C	2.35039900	4.26402200	1.07521800
C	1.68958700	3.53473800	-1.93887700
C	-0.46900300	3.22070400	0.28312800
H	2.30903100	3.70617100	2.03570100
C	3.81177000	4.49568900	0.73707300
C	1.68071800	5.61077000	1.31401000
H	2.73277500	3.19122900	-2.11015600
C	0.78347100	2.67297500	-2.80093400
C	1.62844800	4.98849300	-2.36502200
H	-0.81978500	2.32968800	-0.28576500
C	-1.30139100	4.39895500	-0.17759800
C	-0.71267500	2.91847200	1.74870700
H	4.24569100	5.24325300	1.42334900
H	4.43385800	3.59589900	0.83178400
H	3.95250300	4.89144200	-0.28372800
H	2.26788000	6.20293500	2.03647700
H	1.61471600	6.21979300	0.39526100
H	0.66484900	5.52988400	1.72614900
H	-0.27448700	2.98347900	-2.72175500
H	1.05585400	2.75018900	-3.86736100
H	0.82670800	1.60172200	-2.53438300
H	2.35127300	5.62052200	-1.82526300

H	1.85166300	5.09214200	-3.44072900
H	0.62966100	5.42981800	-2.20859400
H	-2.36115500	4.25176300	0.09487900
H	-0.98995300	5.34990200	0.28419300
H	-1.26954400	4.54519600	-1.26899400
H	-0.46547900	3.77574100	2.39787900
H	-1.77705300	2.68489000	1.93586600
H	-0.12351300	2.05890100	2.11135500

2-4a

E_{sol} = -1353.733847 Hartree

Thermal correction to Free Energy = 0.271142 Hartree

Sum of electronic and thermal Free Energies = -1353.462705 Hartree

Number of Imaginary Frequencies: 0

C	3.12978200	-2.52552100	1.20323600
C	1.78179300	-2.74304200	1.44321600
C	0.82853300	-1.89918600	0.87324700
C	1.25185700	-0.85758100	0.08055200
C	2.61580700	-0.64027900	-0.15656000
C	3.57213400	-1.47147800	0.40998000
H	3.87124700	-3.18774700	1.66311500
H	1.46582300	-3.56979600	2.08557500
H	-0.23963900	-2.05347300	1.07345500
H	4.64173300	-1.30189700	0.25382600
C	0.50822700	0.17034200	-0.74358000
C	1.57932700	1.24630400	-0.85400700
N	2.78645000	0.44773300	-0.98144400
C	0.02418700	-0.45170900	-2.05358600
H	-0.16836900	0.34469200	-2.79464400
H	0.73860000	-1.16855000	-2.48289000
C	-0.78145600	0.66003000	-0.15622900
C	-0.89667700	1.73591400	0.65134800
H	1.43974300	1.86844300	-1.75841400
C	-1.27505400	-1.10013500	-1.64504500
H	-2.00188800	-1.19182200	-2.46329500
N	-1.76370700	-0.15682300	-0.64454500
H	-1.12564400	-2.10435700	-1.20159300
S	-3.29769600	-0.29609200	-0.02492000
O	-3.81262800	1.01643800	0.19868200
O	-3.96025300	-1.20543400	-0.90269200
C	-3.03286600	-1.06750000	1.52408000
H	-2.60081200	-2.06545600	1.36665900
H	-2.36720100	-0.44457100	2.13889300
H	-4.00768300	-1.16250500	2.02258000

C	0.25593300	2.56305200	0.93334400
C	1.59584600	2.10827800	0.40394900
H	2.22830900	3.00081200	0.27543200
C	4.04149800	1.12039900	-1.01120500
H	4.36927500	1.51032000	-0.02337500
H	4.82528400	0.44000900	-1.37998100
H	3.98554100	1.96434200	-1.71517500
H	2.05923800	1.51888600	1.22117600
O	0.16777900	3.58079600	1.58599100
H	-1.86204200	2.08202100	1.02700600

2-4b

E_{sol} = -1353.732579 Hartree

Thermal correction to Free Energy = 0.270286 Hartree

Sum of electronic and thermal Free Energies = -1353.462293 Hartree

Number of Imaginary Frequencies: 0

C	3.18328700	2.75418900	-0.88198400
C	1.83880500	2.83893600	-1.21093400
C	0.96110200	1.83504300	-0.80122500
C	1.44337800	0.77822600	-0.06256900
C	2.80463600	0.69532000	0.25535700
C	3.69253900	1.68073200	-0.15776300
H	3.87022800	3.53784000	-1.21958100
H	1.47162900	3.68054500	-1.80502200
H	-0.09716400	1.86973300	-1.09363200
C	0.74534400	-0.42239900	0.53474600
C	1.95602100	-1.34924900	0.75635800
N	3.05966100	-0.44441500	0.98059200
C	-0.07151100	-0.07397700	1.77144300
H	-0.31069200	-1.00506400	2.31772100
H	0.48383600	0.58346200	2.46056200
C	-1.46046700	-1.03720300	-0.42446400
C	-0.12322300	-1.17869000	-0.40676800
H	1.81755500	-2.00248500	1.63907600
C	-1.35408200	0.61825000	1.37826700
H	-1.99360200	0.77799400	2.25865500
N	-2.10239100	-0.19489000	0.43108500
H	-1.14340700	1.61597300	0.94148000
S	-3.68196900	0.22685700	0.12035000
O	-4.27254000	-0.88234300	-0.55725700
O	-4.20811200	0.71018800	1.35700200
C	-3.53939400	1.56883500	-0.99610400
H	-2.97080800	2.38370000	-0.52565900
H	-3.04502000	1.22999900	-1.91671700

H	-4.55300100	1.92287800	-1.23054000
C	4.37404900	-0.98667300	1.01599400
H	4.76713700	-1.27410800	0.01580100
H	5.07800100	-0.26348300	1.45784100
H	4.38262300	-1.88258900	1.65582600
C	0.62744200	-2.22530700	-1.08745200
C	2.03619400	-2.18221200	-0.52422400
H	2.44071600	-3.19719700	-0.39266900
H	4.76203600	1.61587600	0.06421600
H	2.68044300	-1.68287700	-1.27471500
O	0.22943300	-2.99120500	-1.92955400
H	-2.10485000	-1.64081500	-1.07358100

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E_{sol} = -2681.167443 Hartree

Thermal correction to Free Energy = 0.574150 Hartree

Sum of electronic and thermal Free Energies = -2680.593293 Hartree

Number of Imaginary Frequencies: 0

C	5.79767300	1.79065900	1.06809900
C	5.95965900	0.57280700	1.73887000
C	5.52460100	-0.61382200	1.18466800
C	4.91223100	-0.58878200	-0.07007100
C	4.76310700	0.65452100	-0.72674800
C	5.20092100	1.85039600	-0.17563300
H	6.15497900	2.71207200	1.53642600
H	6.44377300	0.56613800	2.71930900
H	5.66200100	-1.55947400	1.72017000
C	4.32144800	-1.57427700	-0.91440100
C	3.84960800	-0.89867200	-2.00469300
N	4.11015000	0.43135000	-1.89466900
C	4.19570600	-3.02553800	-0.64321700
H	3.87599900	-3.55905000	-1.55411400
H	5.17667400	-3.45301500	-0.36364400
C	1.38526500	-1.82983200	0.44565900
C	1.68647300	-0.63794000	0.65606700
H	3.33696800	-1.27777000	-2.88792600
Au	-0.72706500	-1.04185100	0.15312400
P	-2.66356400	0.24961400	-0.02407200
C	-3.08030600	0.98733500	1.56704200
C	-4.35216000	0.91314600	2.12287600
C	-2.05999200	1.63185200	2.26495300
C	-4.59654000	1.48199200	3.36256400
H	-5.16120700	0.40349700	1.59006600
C	-2.31348000	2.20923200	3.49388500

H	-1.05141400	1.68653500	1.83279800
C	-3.58345000	2.13020300	4.04581500
H	-5.59727700	1.41666300	3.79769500
H	-1.50962500	2.71962000	4.03107300
H	-3.78242800	2.57778100	5.02337600
C	-2.40031300	1.63325000	-1.15640700
C	-1.83371000	1.34818700	-2.39821800
C	-2.75619300	2.94192800	-0.84883000
C	-1.64431000	2.35565800	-3.32586700
H	-1.54739600	0.31742600	-2.64202400
C	-2.55448600	3.94913700	-1.77921500
H	-3.20181500	3.18150300	0.12155900
C	-2.00449800	3.65884400	-3.01634200
H	-1.20684300	2.12152100	-4.29982800
H	-2.83671500	4.97591700	-1.53073400
H	-1.85156600	4.45676000	-3.74817100
C	-4.13455200	-0.60012600	-0.61572700
C	-4.23314300	-1.97599900	-0.43132700
C	-5.17788400	0.09160000	-1.22602100
C	-5.36733300	-2.65295500	-0.84307400
H	-3.40652900	-2.52195200	0.03943800
C	-6.30761700	-0.59127500	-1.63874700
H	-5.10844700	1.17360400	-1.38073800
C	-6.40295600	-1.96089500	-1.44784400
H	-5.43746500	-3.73393500	-0.69809300
H	-7.12381000	-0.04617400	-2.12042000
H	-7.29570400	-2.49662200	-1.78162600
C	3.24557600	-3.37791200	0.47984700
H	3.29848400	-4.45929800	0.67972300
N	1.85508300	-3.05434200	0.15945000
H	3.50984100	-2.85223100	1.41472700
S	0.75470600	-4.30781500	0.09680100
O	-0.45147200	-3.73755900	-0.42484000
O	1.42240300	-5.37136900	-0.58055000
C	0.48887100	-4.75101800	1.76515000
H	1.43517100	-5.06893300	2.22135700
H	0.06892400	-3.89257900	2.30568300
H	-0.22487800	-5.58464700	1.78580300
C	3.77168200	1.42887500	-2.84741500
H	3.17159700	2.23106400	-2.38484400
H	4.66982000	1.88779800	-3.29139900
H	3.18107400	0.97583300	-3.65220100
C	1.93068100	0.70895600	0.89798200
H	2.51504800	0.94376400	1.79783800

C	1.47152500	1.68668900	0.08090700
H	0.87829000	1.37313500	-0.79291800
C	1.62468900	3.10647400	0.24236100
C	2.37759100	3.69682900	1.26696300
C	0.99320300	3.93968900	-0.68892100
C	2.48480000	5.06835200	1.34755800
H	2.89043100	3.07482800	2.00653800
C	1.10106400	5.31293000	-0.60186800
H	0.40878500	3.48021900	-1.49527500
C	1.84654500	5.88160200	0.41864100
H	3.07544700	5.51844500	2.14961900
H	0.59680000	5.94633700	-1.33627400
H	1.93421500	6.96884400	0.49417700
H	5.07105900	2.80316800	-0.69794200

3-1a-ts

E_{sol} = -2681.150390 Hartree

Thermal correction to Free Energy = 0.579776 Hartree

Sum of electronic and thermal Free Energies = -2680.570614 Hartree

Number of Imaginary Frequencies: 1

C	-6.94825000	-0.73699100	-1.11666900
C	-6.37501800	-2.00448900	-1.20417800
C	-5.30877200	-2.37316000	-0.40429000
C	-4.80585400	-1.45284900	0.50600100
C	-5.44157100	-0.20505700	0.61070000
C	-6.49347300	0.18811200	-0.19563200
H	-7.78162100	-0.47600300	-1.77317500
H	-6.78191800	-2.72454500	-1.91939600
H	-4.89083000	-3.38085100	-0.47644700
H	-6.95538700	1.17448800	-0.10044900
C	-3.71831600	-1.46170500	1.47148000
C	-3.87126800	-0.23959200	2.16031000
N	-4.84479900	0.48665400	1.64138800
C	-3.19030800	-2.67349200	2.17495500
H	-2.55296400	-2.33621100	3.00819600
H	-4.00070100	-3.27752500	2.61116800
C	-1.93390000	-1.29477500	0.49681400
C	-1.37786300	-0.14925400	0.16530300
H	-3.27761900	0.14612300	2.98875400
Au	0.75433400	-0.11459200	0.15582900
P	3.09612200	0.11783300	0.08169700
C	3.59553400	1.50278400	-0.96702100
C	4.72957000	1.46358400	-1.77161200
C	2.81011400	2.65275600	-0.94903400

C	5.07219900	2.56296300	-2.54002000
H	5.35475600	0.56496700	-1.80112400
C	3.15971100	3.75034500	-1.71298700
H	1.90784500	2.68553500	-0.32448000
C	4.29024600	3.70496200	-2.51217900
H	5.96379300	2.52339400	-3.17192600
H	2.53574200	4.64789100	-1.69282500
H	4.56183600	4.56922300	-3.12480900
C	3.85306400	0.42743500	1.69009800
C	3.29199800	-0.18777600	2.80686200
C	4.97865400	1.23235700	1.84450100
C	3.85358800	-0.00886700	4.05767200
H	2.40114600	-0.81639400	2.68784600
C	5.53352300	1.41301000	3.09946100
H	5.42960200	1.72371200	0.97602400
C	4.97327500	0.79443500	4.20489100
H	3.40708900	-0.49510800	4.92897400
H	6.41565900	2.04815200	3.21433800
H	5.41311600	0.94297500	5.19519900
C	3.94092100	-1.32587000	-0.59835800
C	3.34647700	-1.95789100	-1.68835500
C	5.14415000	-1.81054700	-0.09694800
C	3.95598800	-3.04883700	-2.27874800
H	2.38647400	-1.59289100	-2.07138900
C	5.74383800	-2.91221800	-0.68472100
H	5.62195000	-1.32582900	0.76059500
C	5.15364200	-3.52923100	-1.77466500
H	3.48290300	-3.53748200	-3.13463800
H	6.68755100	-3.29220500	-0.28341400
H	5.62998300	-4.39958300	-2.23416700
C	-2.38106000	-3.52248700	1.22995000
H	-1.66081800	-4.15613600	1.76726200
N	-1.68626400	-2.59650900	0.35713900
H	-3.01546900	-4.19277600	0.62417300
S	-1.12174900	-3.21627300	-1.12805500
O	-0.04184800	-2.38390800	-1.54679100
O	-0.92645400	-4.60574900	-0.86594500
C	-5.17573100	1.82122900	2.01971600
H	-4.57948100	2.10880600	2.89210000
H	-4.96277600	2.51796400	1.19432600
H	-6.24287400	1.88883100	2.27270500
C	-2.12129700	1.04650100	-0.08680600
H	-3.18105900	0.92788300	-0.35942900
C	-1.59470900	2.28843500	-0.08933600

H	-0.53474600	2.38717300	0.19715700
C	-2.26715000	3.52693400	-0.40822500
C	-1.61520400	4.73352400	-0.13137500
C	-3.53512400	3.59094500	-1.00278300
C	-2.20830900	5.95058700	-0.40749800
H	-0.61764100	4.70121800	0.32086700
C	-4.12510800	4.80744600	-1.27782600
H	-4.06602800	2.67103900	-1.26954000
C	-3.46833300	5.99416800	-0.98118900
H	-1.67748400	6.87832200	-0.17681900
H	-5.11289400	4.83382700	-1.74632000
H	-3.94010800	6.95402800	-1.20701400
C	-2.44876300	-2.99244500	-2.24145800
H	-2.07213900	-3.23442600	-3.24395200
H	-3.26904400	-3.67195500	-1.98577800
H	-2.77487400	-1.94365500	-2.21822000

3-1b-ts

E_{sol} = -2681.157768 Hartree

Thermal correction to Free Energy = 0.577736 Hartree

Sum of electronic and thermal Free Energies = -2680.580032 Hartree

Number of Imaginary Frequencies: 1

C	5.79576200	0.67232200	2.37979100
C	5.26092700	-0.50405500	2.90633900
C	4.65002000	-1.44343800	2.09624000
C	4.59322600	-1.20141700	0.73019000
C	5.16565300	-0.02521400	0.22142200
C	5.75714000	0.93542500	1.02280200
H	6.25872900	1.39879100	3.05239700
H	5.32314800	-0.68104500	3.98318300
H	4.21809200	-2.35394000	2.52337100
C	3.98185100	-1.88455300	-0.38685300
C	4.33991300	-1.12685300	-1.50497800
N	4.98946600	-0.02559700	-1.14361300
C	3.65179600	-3.33811300	-0.46973500
H	3.60653100	-3.64183400	-1.52855900
H	4.47965600	-3.91001400	-0.01489900
C	1.04451900	-1.84755300	-0.32031600
C	1.97200600	-0.94100600	-0.24346100
H	4.12149300	-1.32258500	-2.55459700
Au	-0.79797600	-0.76286900	-0.15173000
P	-2.70638100	0.57179600	0.11046700
C	-2.28432800	2.30333500	0.40956700
C	-3.07822800	3.13050300	1.19910000

C	-1.12875600	2.81763600	-0.17488800
C	-2.72148100	4.45379100	1.39365000
H	-3.98535100	2.73796200	1.67041700
C	-0.77830700	4.14218800	0.02006800
H	-0.49419700	2.16684800	-0.79098300
C	-1.57326500	4.95964800	0.80646600
H	-3.34910500	5.09708600	2.01665300
H	0.13193300	4.53890000	-0.44215400
H	-1.29164200	6.00362800	0.96776500
C	-3.79701400	0.55053200	-1.32616900
C	-3.81386700	-0.59102200	-2.12208900
C	-4.61979300	1.62647700	-1.64630200
C	-4.65123900	-0.65866200	-3.22144500
H	-3.15685700	-1.43438100	-1.87468100
C	-5.44954400	1.55652000	-2.75098800
H	-4.61048300	2.53016200	-1.02774100
C	-5.46491600	0.41665400	-3.53807500
H	-4.65960000	-1.55771000	-3.84364000
H	-6.09042500	2.40609400	-3.00163600
H	-6.11850700	0.36691300	-4.41334000
C	-3.72525100	0.08653700	1.52218900
C	-3.09203600	-0.05718000	2.75582700
C	-5.09205600	-0.14634400	1.42288700
C	-3.81924700	-0.41267700	3.87509600
H	-2.01306800	0.12191000	2.83858100
C	-5.81400400	-0.51382600	2.54674600
H	-5.60376900	-0.04158100	0.46109400
C	-5.18269400	-0.64410900	3.77109100
H	-3.31527800	-0.51620200	4.83979100
H	-6.88801200	-0.69886400	2.46078200
H	-5.75754100	-0.93263100	4.65551800
C	2.37823900	-3.77156400	0.20078800
H	2.30429300	-4.86621400	0.14779100
N	1.22486100	-3.20604700	-0.47333400
H	2.36834400	-3.47048700	1.26913600
S	-0.14752700	-4.14408600	-0.51612500
O	-1.08682300	-3.44883900	-1.34086300
O	0.29092200	-5.45869700	-0.86209000
C	-0.75048500	-4.16575100	1.12588600
H	-0.00165400	-4.61721400	1.79005600
H	-0.97967100	-3.13771200	1.44318800
H	-1.66871900	-4.76705200	1.14755900
C	5.49492700	0.97540500	-2.02553800
H	5.18223800	1.97742200	-1.69574800

H	6.59427000	0.94487600	-2.05118600
H	5.10818900	0.79890600	-3.03526800
C	2.20845100	0.41314000	0.07933800
H	2.31818300	0.66614200	1.14413900
C	2.37655600	1.36326100	-0.86335100
H	2.28947400	1.05178700	-1.91536100
C	2.62498000	2.76790400	-0.65137200
C	2.63144400	3.61348100	-1.76646800
C	2.86175600	3.32574700	0.61124500
C	2.84898200	4.97067300	-1.62811600
H	2.45416600	3.18105000	-2.75765700
C	3.07655600	4.68174300	0.74513800
H	2.88386600	2.68775200	1.50023900
C	3.06823300	5.50886600	-0.37017600
H	2.84855300	5.61643200	-2.51038500
H	3.25854000	5.10569100	1.73644400
H	3.24148200	6.58226400	-0.25576400
H	6.17729200	1.85499200	0.60615700

3-2a

E_{sol} = -2681.183402 Hartree

Thermal correction to Free Energy = 0.579822 Hartree

Sum of electronic and thermal Free Energies = -2680.603580 Hartree

Number of Imaginary Frequencies: 0

C	5.30926200	-0.21254400	3.25121900
C	4.18468700	-1.00552100	3.44593900
C	3.48964800	-1.54778200	2.37303700
C	3.94315700	-1.27752100	1.09972300
C	5.06683400	-0.47976800	0.93209600
C	5.77605600	0.07175600	1.97728200
H	5.82945400	0.20474200	4.11625400
H	3.83854500	-1.19933000	4.46404900
H	2.59479300	-2.15579000	2.53553600
H	6.64972400	0.70705000	1.81391000
C	3.47115700	-1.71931900	-0.25519300
C	4.36037100	-0.91440600	-1.11977400
N	5.29228300	-0.32370900	-0.43793000
C	3.77049600	-3.20965600	-0.54070300
H	3.99872700	-3.34348100	-1.61012900
H	4.61784000	-3.58249100	0.04921800
C	1.94833900	-1.61523800	-0.47712900
C	1.25103100	-0.49285000	-0.27499600
H	4.38377600	-0.92177300	-2.21110300
Au	-0.78570800	-0.03842200	-0.11005400

P	-3.04020500	0.61164500	0.14354800
C	-3.23054300	2.13846400	1.08809200
C	-4.26148700	2.34457400	1.99905100
C	-2.28654300	3.14204300	0.88355300
C	-4.34220800	3.54020900	2.69370600
H	-5.01128000	1.56506000	2.17107500
C	-2.37707400	4.33770400	1.57191800
H	-1.46771100	2.97754200	0.17236300
C	-3.40157900	4.53433800	2.48402300
H	-5.15183900	3.69403600	3.41228400
H	-1.63122800	5.11942200	1.40389200
H	-3.46636600	5.47395900	3.03926100
C	-3.88908800	0.89558900	-1.42423600
C	-3.53275400	0.09508200	-2.50708400
C	-4.87166900	1.86717000	-1.58289300
C	-4.15911900	0.25810300	-3.72921300
H	-2.74887200	-0.66397300	-2.38567800
C	-5.48973200	2.03145300	-2.81066300
H	-5.15908200	2.50469500	-0.74015900
C	-5.13503700	1.22940500	-3.88256800
H	-3.87333300	-0.37371800	-4.57453300
H	-6.25881100	2.79972200	-2.93045700
H	-5.62260500	1.36655000	-4.85187300
C	-4.01958900	-0.63267700	1.01299200
C	-3.40593000	-1.31975900	2.05818400
C	-5.33334700	-0.93852000	0.67386000
C	-4.09665400	-2.29207500	2.75763100
H	-2.36655500	-1.08632100	2.32237200
C	-6.01929700	-1.91890600	1.37176600
H	-5.82751900	-0.41015800	-0.14824500
C	-5.40379400	-2.59483900	2.41119500
H	-3.60645300	-2.82500600	3.57711600
H	-7.04999600	-2.15810200	1.09563500
H	-5.94750300	-3.37204700	2.95546600
C	2.46523100	-3.88518800	-0.23106200
H	2.35779000	-4.85581300	-0.72946100
N	1.52702900	-2.92578700	-0.76213300
H	2.33248300	-4.02421200	0.86272100
S	-0.01466900	-3.41797500	-1.04350000
O	-0.65129100	-2.41633700	-1.83931500
O	0.09730400	-4.75694500	-1.53073600
C	-0.76445300	-3.49081800	0.53814900
H	-0.29181400	-4.29604000	1.11667600
H	-0.64794700	-2.52762000	1.05638800

H	-1.83178800	-3.71496300	0.40576400
C	2.02734900	0.71021200	-0.10253300
H	1.99178900	1.18403400	0.89286500
C	2.73603600	1.30729400	-1.08441500
H	2.63723600	0.90184400	-2.10195000
C	3.64217500	2.42833800	-0.94462600
C	4.06678900	2.91412600	0.29833700
C	4.19797400	3.00087300	-2.09353900
C	5.00161400	3.92745700	0.38157600
H	3.67303200	2.47422500	1.22097900
C	5.13716700	4.01046000	-2.00860300
H	3.88095700	2.63012600	-3.07495500
C	5.54760700	4.47759900	-0.76986700
H	5.32049300	4.28842300	1.36385200
H	5.55856100	4.43979500	-2.92222200
H	6.29479900	5.27275000	-0.69955800
C	6.39054100	0.41537800	-0.98208300
H	6.41065600	1.42964700	-0.55867200
H	7.33152900	-0.09530300	-0.73373100
H	6.28217100	0.47211300	-2.06996500

3-2b

E_{sol} = -2681.190110 Hartree

Thermal correction to Free Energy = 0.578192 Hartree

Sum of electronic and thermal Free Energies = -2680.611918 Hartree

Number of Imaginary Frequencies: 0

C	-6.79212100	1.28228500	-0.97096300
C	-6.39883600	0.55322300	-2.08496200
C	-5.42910300	-0.43675400	-1.99035400
C	-4.87548400	-0.68783300	-0.75502100
C	-5.30358700	0.03660300	0.34884600
C	-6.24663700	1.03830300	0.28107800
H	-7.55204700	2.06041100	-1.07736100
H	-6.85535400	0.76949900	-3.05385200
H	-5.10404500	-0.99034300	-2.87604800
C	-3.75394000	-1.57434100	-0.32452800
C	-3.80494600	-1.39240600	1.14379800
N	-4.60459400	-0.42312800	1.47113000
C	-3.75361300	-3.01012100	-0.82510400
H	-4.34311100	-3.63202200	-0.13302500
H	-4.25276300	-3.05800800	-1.80563700
C	-1.25984700	-1.56710000	-0.09882100
C	-2.38376100	-0.86045300	-0.42007600
H	-3.17589300	-1.88912900	1.88403000

Au	0.62343100	-0.66722000	-0.05451000
P	2.73177000	0.39909900	-0.13126700
C	2.65544800	2.03118300	-0.89817400
C	3.73347300	2.62304600	-1.55096900
C	1.44681100	2.71607000	-0.81650000
C	3.59731700	3.88676800	-2.09982800
H	4.68842800	2.09268400	-1.63327300
C	1.31563500	3.98062600	-1.36026900
H	0.59230800	2.23629900	-0.32617800
C	2.39323900	4.56664300	-2.00336200
H	4.44623400	4.34742800	-2.61235400
H	0.35753800	4.50687400	-1.28874000
H	2.29333100	5.56284200	-2.44346800
C	3.46277500	0.63928600	1.50335300
C	3.25250900	-0.35560900	2.45560100
C	4.23125900	1.75035300	1.83359300
C	3.81743400	-0.24756800	3.71329500
H	2.63434200	-1.22689100	2.20340600
C	4.78736000	1.85793200	3.09697500
H	4.40073800	2.54374500	1.09853500
C	4.58385200	0.86063700	4.03538500
H	3.64875500	-1.03427400	4.45366800
H	5.38825700	2.73596300	3.34972400
H	5.02354600	0.94976300	5.03265900
C	3.96292500	-0.52516400	-1.07799000
C	3.53076200	-1.21242000	-2.21098300
C	5.30722900	-0.57252300	-0.72221700
C	4.43001700	-1.92929100	-2.97935800
H	2.47018900	-1.18395600	-2.49216300
C	6.20297500	-1.29577200	-1.49226000
H	5.66158900	-0.04365400	0.16861100
C	5.76695000	-1.97415800	-2.61796000
H	4.08109400	-2.46591700	-3.86558500
H	7.25742100	-1.33096700	-1.20484000
H	6.47705800	-2.54869300	-3.21863500
C	-2.34956800	-3.52781300	-0.95838400
H	-2.32782900	-4.62157800	-0.86318600
N	-1.50554000	-2.93499300	0.06961100
H	-1.93433200	-3.25556300	-1.94929300
S	-0.29300900	-3.90308900	0.66067800
O	0.35769100	-3.15093900	1.68923400
O	-0.91191800	-5.15688300	0.96124900
C	0.82704300	-4.15534000	-0.66099300
H	0.31546700	-4.66464500	-1.48839200

H	1.23808400	-3.19075500	-0.99431800
H	1.64267800	-4.79147800	-0.29331700
C	-4.73270500	0.16166900	2.77045200
H	-4.43022100	1.21817300	2.73271500
H	-5.77779000	0.10129400	3.10267000
H	-4.09350600	-0.37775500	3.47595500
C	-2.43837800	0.58945200	-0.54579500
H	-2.97875300	0.98702900	-1.41673200
C	-1.97772900	1.44000100	0.38198700
H	-1.47737200	1.01023300	1.26465700
C	-2.06540900	2.88917200	0.36295300
C	-1.30369100	3.61990600	1.27982200
C	-2.89341400	3.59581100	-0.51559800
C	-1.34344000	5.00125400	1.30435800
H	-0.65669200	3.07822900	1.97949000
C	-2.93612700	4.97578600	-0.48575400
H	-3.53221500	3.05487900	-1.22202100
C	-2.15855400	5.68676900	0.41816400
H	-0.73194500	5.54988600	2.02575700
H	-3.59475400	5.50980100	-1.17639700
H	-2.19847800	6.77905700	0.43717900
H	-6.55942900	1.60561600	1.16049700

3-2a-ts

E_{sol} = -2681.172116 Hartree

Thermal correction to Free Energy = 0.579111 Hartree

Sum of electronic and thermal Free Energies = -2680.593005 Hartree

Number of Imaginary Frequencies: 1

C	4.73661800	-0.27403400	3.74491200
C	3.55367300	-1.00013400	3.74327600
C	3.01282900	-1.47493300	2.55449000
C	3.67063200	-1.19910600	1.37629700
C	4.84592900	-0.45262600	1.39534400
C	5.40748500	0.01865000	2.56706300
H	5.14319500	0.08892000	4.69272700
H	3.04069800	-1.19782700	4.68749800
H	2.07795000	-2.04559400	2.55577700
H	6.33272600	0.60004900	2.56764800
C	3.40581600	-1.60592900	-0.05076500
C	4.35184500	-0.70201000	-0.76641600
N	5.28539400	-0.27525500	0.10031900
C	3.74865900	-3.07604300	-0.32330700
H	4.03370600	-3.19647000	-1.38146800
H	4.56904100	-3.44401800	0.30666100

C	1.93102900	-1.52323600	-0.46496800
C	1.26726400	-0.34815500	-0.44087800
H	4.67377900	-0.91285700	-1.78961500
Au	-0.77276000	0.08063300	-0.22875500
P	-3.04679100	0.59498200	0.12729100
C	-3.34433300	2.36015900	0.37213500
C	-4.28652500	2.83989700	1.27680500
C	-2.59875900	3.26076100	-0.38516000
C	-4.48081400	4.20372000	1.41586000
H	-4.87701300	2.14288700	1.88059200
C	-2.80163300	4.62195700	-0.24703000
H	-1.84643500	2.88542900	-1.08969900
C	-3.74111800	5.09369100	0.65567400
H	-5.22120100	4.57438200	2.13004500
H	-2.21299200	5.32298300	-0.84460400
H	-3.89469600	6.17009800	0.77151500
C	-4.14221800	0.09122900	-1.21625700
C	-3.80869000	-1.04452800	-1.94965200
C	-5.30134900	0.79458300	-1.53000900
C	-4.62950700	-1.47519000	-2.97685600
H	-2.88442600	-1.59109400	-1.71944100
C	-6.11444200	0.36430500	-2.56384800
H	-5.57394000	1.69081800	-0.96306900
C	-5.77996300	-0.76830500	-3.28701700
H	-4.35996900	-2.36582000	-3.55105900
H	-7.02096000	0.92489800	-2.80771300
H	-6.42167000	-1.10238500	-4.10682200
C	-3.69254200	-0.19921700	1.61644700
C	-2.88696600	-0.18113300	2.75358100
C	-4.94827600	-0.79409900	1.67886100
C	-3.33817800	-0.73088000	3.93874600
H	-1.89167000	0.27810300	2.70644100
C	-5.39105700	-1.35461000	2.86601100
H	-5.59332300	-0.81842200	0.79445000
C	-4.59103300	-1.32189900	3.99495600
H	-2.70106100	-0.70567800	4.82714500
H	-6.37847700	-1.82206600	2.90626100
H	-4.94527700	-1.76452400	4.92992400
C	2.44052000	-3.77928500	-0.07809400
H	2.35359200	-4.73859400	-0.60137000
N	1.49335100	-2.81936800	-0.60189800
H	2.26550400	-3.94524800	1.00262800
S	0.09449100	-3.32595900	-1.32565800
O	-0.35096800	-2.27142400	-2.17825300

O	0.37159200	-4.62401900	-1.85360000
C	-1.01365700	-3.51476200	0.01063700
H	-0.61275100	-4.26089000	0.70987800
H	-1.15805100	-2.55028200	0.52005900
H	-1.97314100	-3.87119000	-0.38844700
C	2.08553900	0.79051200	-0.43802500
H	1.86519200	1.59483200	0.28301000
C	3.15952900	0.96063700	-1.31108500
H	3.04602800	0.50533100	-2.30167300
C	4.03562300	2.12570600	-1.24935700
C	4.26565900	2.79634900	-0.04590600
C	4.72263400	2.54974700	-2.38692200
C	5.13416400	3.87062900	0.00821900
H	3.77252200	2.45502800	0.87138900
C	5.60314200	3.61374100	-2.32834400
H	4.55597700	2.02674000	-3.33541700
C	5.81227000	4.27881700	-1.13011700
H	5.29992500	4.38716600	0.95793300
H	6.13318000	3.93149200	-3.23075700
H	6.50897900	5.12000500	-1.08254900
C	6.52394800	0.33591400	-0.25196000
H	6.60973700	1.35448100	0.15645100
H	7.36054600	-0.26828500	0.13384900
H	6.60411000	0.38882000	-1.34351400

3-2b-ts

E_{sol} = -2681.165221 Hartree

Thermal correction to Free Energy = 0.582666 Hartree

Sum of electronic and thermal Free Energies = -2680.582555 Hartree

Number of Imaginary Frequencies: 1

C	6.42835800	-0.36909200	2.11050900
C	5.25711300	-0.92207800	2.60439800
C	4.16731200	-1.15283700	1.76981200
C	4.27153200	-0.81638100	0.44008100
C	5.44955800	-0.24230900	-0.02801600
C	6.54717700	-0.01143300	0.77400500
H	7.27115200	-0.19915500	2.78485500
H	5.18935100	-1.18295200	3.66345800
H	3.23932500	-1.57086100	2.17422100
C	3.33012100	-0.97211600	-0.72741700
C	4.05346600	-0.14847200	-1.76698800
N	5.29803600	0.05713600	-1.37908300
C	3.27953000	-2.44233100	-1.16455100
H	2.83296900	-2.49451300	-2.17246100

H	4.28840500	-2.87964600	-1.21868100
C	0.83796600	-1.35991900	-0.33616200
C	1.90507900	-0.50120500	-0.62270000
H	3.83324500	-0.18203700	-2.83712400
Au	-1.08175900	-0.52922300	-0.19351400
P	-3.14468400	0.59532000	-0.00535600
C	-3.08233700	1.86391400	1.27615200
C	-4.06563100	2.03005800	2.24351300
C	-1.96868800	2.70231500	1.27907100
C	-3.93187200	3.02293500	3.20078400
H	-4.94555100	1.37882900	2.25734500
C	-1.84637500	3.69918100	2.22746900
H	-1.18361100	2.56618000	0.52403700
C	-2.82778500	3.85717000	3.19341400
H	-4.70608700	3.14431700	3.96356700
H	-0.97038700	4.35340100	2.21869300
H	-2.72755100	4.63778000	3.95262500
C	-3.60545700	1.46795100	-1.51768700
C	-3.33108400	0.85151500	-2.73656400
C	-4.21125100	2.72106000	-1.50301300
C	-3.66537400	1.47638300	-3.92417600
H	-2.84392200	-0.13102000	-2.75066800
C	-4.53634100	3.34578300	-2.69551500
H	-4.42789800	3.21716800	-0.55116600
C	-4.26591700	2.72564500	-3.90399300
H	-3.44648400	0.98561000	-4.87610700
H	-5.00751700	4.33192900	-2.67822800
H	-4.51938800	3.22532300	-4.84267200
C	-4.53375800	-0.48118700	0.40015000
C	-4.27884400	-1.65208100	1.10924000
C	-5.84268500	-0.16152200	0.05027500
C	-5.32139700	-2.48416600	1.47611100
H	-3.24526200	-1.91777500	1.36752400
C	-6.88149500	-1.00065500	0.41363600
H	-6.05327800	0.75376000	-0.51333000
C	-6.62180500	-2.15901400	1.12803500
H	-5.11441800	-3.40322700	2.03055500
H	-7.90709500	-0.74638700	0.13279100
H	-7.44404200	-2.82197500	1.41031000
C	2.44977100	-3.24634900	-0.21292000
H	2.33040400	-4.26215500	-0.61068600
N	1.12783800	-2.65019600	-0.07382500
H	2.92649600	-3.34528300	0.77909600
S	-0.09236700	-3.67884400	0.48726700

O	-1.28250300	-3.43927900	-0.26645000
O	0.49580400	-4.97901900	0.51400800
C	-0.32982700	-3.12969000	2.12858600
H	0.61470400	-3.22220500	2.68010200
H	-0.67789300	-2.08712300	2.12862900
H	-1.08950100	-3.77737900	2.58619000
C	6.35253100	0.56547100	-2.19462800
H	6.81736500	1.44181800	-1.72074000
H	7.12381800	-0.20622700	-2.34091100
H	5.94856100	0.86277500	-3.16810600
C	1.69470400	0.79037600	-1.10976900
H	0.69723600	1.01819700	-1.51930500
C	2.73176700	1.69690300	-1.32060000
H	2.56895100	2.39738800	-2.15306800
C	3.62634200	2.24063600	-0.30863700
C	3.41762200	2.06886500	1.06330800
C	4.70226600	3.03844900	-0.70828900
C	4.26333800	2.64876800	1.98825700
H	2.56788400	1.46654000	1.40337400
C	5.54774700	3.61944500	0.21879100
H	4.86624500	3.20517600	-1.77937700
C	5.33828400	3.42239400	1.57452500
H	4.07446100	2.50190400	3.05621600
H	6.37963900	4.24281500	-0.12286300
H	6.00158100	3.88496100	2.31029900
H	7.46056800	0.44455500	0.38446700

3-3a

E_{sol} = -2681.201514 Hartree

Thermal correction to Free Energy = 0.582832 Hartree

Sum of electronic and thermal Free Energies = -2680.618682 Hartree

Number of Imaginary Frequencies: 0

C	2.66690800	-0.79784800	4.40022200
C	2.02170900	-1.90714100	3.87095800
C	2.17852500	-2.22126300	2.52729200
C	2.98049600	-1.41704400	1.74454200
C	3.57886200	-0.27337100	2.26556200
C	3.45293300	0.02964100	3.61584000
H	2.55254800	-0.56606900	5.46298200
H	1.40175300	-2.53876300	4.51152000
H	1.68199300	-3.10537400	2.11032100
H	3.94661700	0.90308600	4.04841100
C	3.36379700	-1.53850500	0.29352000
C	4.25669400	-0.29785000	0.06401000

N	4.25927200	0.43778200	1.31304200
C	3.96235700	-2.87332800	-0.13032200
H	4.62991100	-2.71205000	-0.99252900
H	4.54581700	-3.34509300	0.67033600
C	2.09603900	-1.47087800	-0.51257800
C	1.40607500	-0.24200400	-0.65629400
H	5.28399600	-0.64052800	-0.18438400
Au	-0.63054900	0.10276500	-0.33356300
P	-2.89909900	0.58685900	0.07158700
C	-3.19721100	2.35958200	0.24427000
C	-4.01752800	2.89348400	1.23251600
C	-2.57757600	3.21170100	-0.66802800
C	-4.21472200	4.26289600	1.30275500
H	-4.50956700	2.23691700	1.95701200
C	-2.78727100	4.57644100	-0.60024800
H	-1.92226400	2.79542200	-1.44312600
C	-3.60478600	5.10378200	0.38768200
H	-4.85769700	4.67617100	2.08430400
H	-2.30028300	5.23683300	-1.32247100
H	-3.76272800	6.18389500	0.44728000
C	-4.01198200	0.04875100	-1.24422200
C	-3.68466900	-1.09022700	-1.97442600
C	-5.18650400	0.73615000	-1.53799100
C	-4.52476900	-1.54178200	-2.97650800
H	-2.74988600	-1.62445500	-1.76019900
C	-6.02054200	0.28487600	-2.54571400
H	-5.45487200	1.63452700	-0.97194300
C	-5.69079900	-0.85157500	-3.26517200
H	-4.25911500	-2.43486000	-3.54855800
H	-6.93939000	0.83208300	-2.77261200
H	-6.34866000	-1.20183800	-4.06504400
C	-3.52246000	-0.15884400	1.59286300
C	-2.68304300	-0.15268900	2.70511600
C	-4.79839300	-0.70126900	1.70156100
C	-3.12095600	-0.66521600	3.91207500
H	-1.67189100	0.26412000	2.62004500
C	-5.22700800	-1.22569900	2.90959000
H	-5.46976500	-0.71559700	0.83679500
C	-4.39285300	-1.20607500	4.01412200
H	-2.45755100	-0.65050500	4.78101700
H	-6.23038100	-1.65320900	2.98654500
H	-4.73608900	-1.61923000	4.96659700
C	2.77855600	-3.70408000	-0.55365200
H	2.97852200	-4.35165400	-1.41599500

N	1.79848200	-2.68432700	-0.92657100
H	2.36350800	-4.32763000	0.25680600
S	0.40712300	-3.16683400	-1.81295000
O	-0.03244300	-2.03644700	-2.55582900
O	0.80679900	-4.37312100	-2.45343600
C	-0.69465600	-3.53739900	-0.51522000
H	-0.26348600	-4.33443800	0.10437700
H	-0.89312200	-2.63326800	0.07962600
H	-1.62649200	-3.89889100	-0.97153700
C	2.26394800	0.77470700	-0.89756500
H	1.88176000	1.79998600	-0.98053200
C	3.73238400	0.56352800	-1.10495700
H	3.88668000	-0.04649700	-2.01835000
C	4.51368800	1.83276700	-1.27125700
C	4.19974800	2.97759000	-0.54512900
C	5.61544200	1.86284800	-2.11883100
C	4.97247900	4.12001900	-0.66088800
H	3.35179100	2.96987600	0.14777300
C	6.39059700	3.00383900	-2.23418200
H	5.86763600	0.96815800	-2.70026100
C	6.07116500	4.13640100	-1.50366000
H	4.71433100	5.01013100	-0.07956200
H	7.25238100	3.01026200	-2.90779000
H	6.68033400	5.03976100	-1.59543900
C	5.48316400	1.06769400	1.71024100
H	5.28250700	1.92060800	2.37620900
H	6.16467800	0.36818400	2.23688900
H	6.00624900	1.46470300	0.83184600

3-3b

E_{sol} = -2681.213781 Hartree

Thermal correction to Free Energy = 0.585434 Hartree

Sum of electronic and thermal Free Energies = -2680.628347 Hartree

Number of Imaginary Frequencies: 0

C	5.62033600	-0.84676600	2.80730900
C	4.40365700	-1.50311300	2.90042700
C	3.61364400	-1.65730700	1.76246900
C	4.05943300	-1.16228000	0.55889200
C	5.26896300	-0.46257800	0.48692600
C	6.07117100	-0.30792700	1.61007000
H	6.23492000	-0.72701900	3.70451800
H	4.06165900	-1.89237500	3.86216400
H	2.63548100	-2.15057500	1.83954200
C	3.44707500	-1.16762800	-0.81937800

C	4.27613000	-0.08957100	-1.54231800
N	5.47424900	0.01314700	-0.76908200
C	3.42291300	-2.53197300	-1.47946300
H	3.14888400	-2.40806300	-2.54225700
H	4.40633500	-3.02595800	-1.44645700
C	0.89826200	-1.45940800	-0.62151500
C	2.04908000	-0.64001200	-0.86208600
H	4.52041000	-0.39605300	-2.57633900
Au	-0.93709700	-0.51097500	-0.28582900
P	-2.95053700	0.65822300	0.11070000
C	-2.81893900	1.92147700	1.39227900
C	-3.78875200	2.10560800	2.37047100
C	-1.69011100	2.73795600	1.38190000
C	-3.62672000	3.09479500	3.32598600
H	-4.68057000	1.47131900	2.39318900
C	-1.53945200	3.73192800	2.32997900
H	-0.91776600	2.58907900	0.61688700
C	-2.50702800	3.90777400	3.30642000
H	-4.39038200	3.23043700	4.09682000
H	-0.65178800	4.37005200	2.31221200
H	-2.38347300	4.68600000	4.06468300
C	-3.52261100	1.50996900	-1.37291200
C	-3.36014800	0.85621200	-2.59244700
C	-4.12892500	2.76192600	-1.33847400
C	-3.81073400	1.44043100	-3.76158500
H	-2.87724500	-0.12852700	-2.62064800
C	-4.57167000	3.34547400	-2.51380400
H	-4.25955400	3.28552100	-0.38581100
C	-4.41418100	2.68784400	-3.72260700
H	-3.68224800	0.91969800	-4.71397800
H	-5.04657400	4.32954100	-2.48291500
H	-4.76336600	3.15519000	-4.64719900
C	-4.30848100	-0.42352100	0.60387600
C	-4.01948500	-1.55914900	1.35508400
C	-5.62996700	-0.13725100	0.27394500
C	-5.03891600	-2.39225500	1.77875600
H	-2.97688900	-1.79234200	1.60847900
C	-6.64621700	-0.97645800	0.69560300
H	-5.86944800	0.75149600	-0.31981400
C	-6.35209100	-2.10182200	1.44746800
H	-4.80482000	-3.28326500	2.36746600
H	-7.68207500	-0.74775700	0.43074900
H	-7.15668500	-2.76513700	1.77579900
C	2.42311100	-3.42657800	-0.80416700

H	2.23948500	-4.32491100	-1.40679800
N	1.13429400	-2.75530900	-0.60317600
H	2.78718100	-3.77162500	0.18066300
S	-0.18537800	-3.82641500	-0.22903800
O	-1.34503200	-3.31628500	-0.88222800
O	0.30326200	-5.13311200	-0.51663600
C	-0.31442500	-3.60194400	1.49582300
H	0.60973800	-3.95168800	1.97454800
H	-0.49524000	-2.54030000	1.71661200
H	-1.16071500	-4.20960600	1.84358700
C	6.53870700	0.89169700	-1.08980400
H	6.54792400	1.81230400	-0.47177600
H	7.51491100	0.39252000	-0.95809300
H	6.46149800	1.19367300	-2.14302100
C	2.01129300	0.64175500	-1.26185800
H	1.09077400	1.23076100	-1.35935700
C	3.35019700	1.17714200	-1.61777600
H	3.31041000	1.53060100	-2.66615100
C	3.75863700	2.35754700	-0.77929800
C	3.63613000	2.33874800	0.60686300
C	4.30020100	3.48553700	-1.38714500
C	4.06725000	3.41299500	1.36593900
H	3.20414300	1.46248800	1.10428600
C	4.72928900	4.56104000	-0.62999100
H	4.39467500	3.51019100	-2.47849600
C	4.61920400	4.52467700	0.75057100
H	3.97194100	3.37970900	2.45485700
H	5.15708300	5.43812500	-1.12336900
H	4.96074500	5.37176500	1.35197900
H	7.01473300	0.24139100	1.56221200

3-4a

E_{sol} = -1509.502276 Hartree

Thermal correction to Free Energy = 0.339367 Hartree

Sum of electronic and thermal Free Energies = -1509.162909 Hartree

Number of Imaginary Frequencies: 0

C	0.47515400	3.93475100	-1.18070600
C	-0.76792100	3.41239200	-1.50168400
C	-1.18544700	2.20663200	-0.93404500
C	-0.34297300	1.54912500	-0.06865700
C	0.91446400	2.07871900	0.24164200
C	1.34019600	3.28046000	-0.30879000
H	0.79537000	4.87911200	-1.63442300
H	-1.42031800	3.94096400	-2.20222600

H	-2.16859400	1.79144100	-1.18703400
H	2.32705100	3.69415300	-0.08151700
C	-0.51926200	0.31370000	0.79636100
C	0.94873100	-0.05578100	1.05901800
N	1.55205400	1.26816500	1.13343900
C	-1.34814100	0.64150600	2.03818600
H	-1.13847500	-0.10168300	2.82834400
H	-1.15096500	1.64627500	2.43929500
C	-1.34371500	-0.74926300	0.13772100
C	-0.79972500	-1.61069000	-0.73620900
H	1.08090100	-0.55660500	2.04234600
C	-2.76842600	0.48168800	1.55158100
H	-3.47822700	0.21394500	2.34613000
N	-2.63474300	-0.62055600	0.60719600
H	-3.14315900	1.39687100	1.04895800
S	-3.96509500	-1.23809800	-0.14890900
O	-3.66707500	-2.58987900	-0.50429200
O	-5.06151900	-0.92645200	0.71169000
C	-4.11154900	-0.30391500	-1.62244500
H	-4.31309200	0.74723600	-1.37305000
H	-3.18724100	-0.39659500	-2.21080600
H	-4.95348300	-0.71385900	-2.19729500
C	0.63208200	-1.59004300	-0.87949400
H	1.06181100	-2.25828900	-1.63788800
C	1.48445000	-0.93062400	-0.06651000
C	2.92887500	-1.15732800	-0.19381100
C	3.55396600	-1.10818700	-1.44401200
C	3.71518700	-1.47173600	0.91945700
C	4.91027400	-1.35853100	-1.57409300
H	2.95735000	-0.84510300	-2.32557700
C	5.07031100	-1.71770300	0.78897700
H	3.24856500	-1.54130800	1.90900100
C	5.67686000	-1.65880700	-0.45850400
H	5.37828100	-1.30508800	-2.56290500
H	5.66311700	-1.96810200	1.67553900
H	6.75018700	-1.84781400	-0.55974500
C	2.89236200	1.51560300	1.52287500
H	3.64067200	1.40185400	0.71022600
H	2.97385300	2.54734900	1.90815200
H	3.17309300	0.83983800	2.34331000
H	-1.38212500	-2.36946200	-1.26105900

3-4b

E_{sol} = -1509.508790 Hartree

Thermal correction to Free Energy = 0.339665 Hartree
Sum of electronic and thermal Free Energies = -1509.169125 Hartree
Number of Imaginary Frequencies: 0

C	0.34628500	4.03941500	-1.15958100
C	-0.84578400	3.39567000	-1.45524800
C	-1.11914800	2.15160400	-0.88707900
C	-0.20693400	1.58609400	-0.02498500
C	1.00598300	2.23008600	0.24402100
C	1.29625700	3.46781900	-0.31975200
H	0.56146300	5.01191900	-1.61618600
H	-1.56130600	3.85431300	-2.14381100
H	-2.04084100	1.61648400	-1.14950300
C	-0.23969000	0.27953800	0.73716200
C	1.25634000	0.12425800	1.10300300
N	1.76197700	1.47878800	1.09525100
C	-1.23084400	0.25660300	1.89017300
H	-1.02691100	-0.63060900	2.51769400
H	-1.13518700	1.14654500	2.53459600
C	-1.75181700	-1.41508600	-0.26845100
C	-0.52395800	-0.88602400	-0.15727700
H	1.41162400	-0.31208800	2.11249900
C	-2.64521000	0.19357800	1.36958300
H	-3.36034300	0.09163300	2.19915600
N	-2.81775400	-0.95217100	0.48927800
H	-2.89245400	1.13777100	0.84122900
S	-4.33751000	-1.20223800	-0.10873500
O	-4.33634300	-2.50784200	-0.68991700
O	-5.23760800	-0.86640400	0.94858400
C	-4.52883200	-0.02761100	-1.40043000
H	-4.45456300	0.99114000	-0.99385100
H	-3.76089900	-0.19733400	-2.16839500
H	-5.52576600	-0.16786600	-1.84244300
C	3.11833500	1.79495900	1.35872700
H	3.79279700	1.67045500	0.48420100
H	3.19851700	2.84195700	1.69766000
H	3.49609800	1.16019900	2.17367200
C	0.72868400	-1.37919100	-0.64033800
H	0.82562600	-2.17382800	-1.38849100
C	1.76766100	-0.82178500	0.02226500
C	3.16393300	-1.18321600	-0.17980400
C	3.65322400	-1.43372100	-1.46722900
C	4.04501300	-1.32923100	0.89834100
C	4.96826900	-1.81521200	-1.66817200
H	2.98438600	-1.30160500	-2.32518600

C	5.35919500	-1.71219200	0.69449600
H	3.68259800	-1.16713700	1.91992300
C	5.82955500	-1.95351700	-0.58875400
H	5.32931800	-1.99704100	-2.68577900
H	6.02753000	-1.83040000	1.55353700
H	6.87138600	-2.24890100	-0.74723500
H	2.24739200	3.97392200	-0.12896300
H	-1.96737000	-2.30309900	-0.86962500

4-1

E_{sol} = -2603.779477 Hartree

Thermal correction to Free Energy = 0.546369 Hartree

Sum of electronic and thermal Free Energies = -2603.233108 Hartree

Number of Imaginary Frequencies: 0

C	6.08919800	-2.22057500	-0.57840900
C	6.33363200	-0.98183000	-1.18052100
C	5.79053900	0.18016300	-0.67277200
C	4.98145100	0.10748700	0.46180900
C	4.75098000	-1.15553700	1.05262100
C	5.29563500	-2.32741100	0.54627000
H	6.53533000	-3.12200400	-1.00789400
H	6.97265000	-0.93776700	-2.06736000
H	5.99893700	1.14372000	-1.15010700
C	4.26562500	1.06388000	1.23958600
C	3.64946900	0.35499400	2.23205200
N	3.93675600	-0.97032700	2.12252300
C	4.16802500	2.51981400	0.98260500
H	3.71249500	3.03513400	1.84466400
H	5.17601200	2.95812600	0.85995800
C	1.53697700	1.37064900	-0.45880500
C	1.77169000	0.17684900	-0.68950700
H	3.01393200	0.70294900	3.04594200
Au	-0.59717600	0.57399400	-0.18578000
P	-2.71275100	-0.37570500	0.09217800
C	-4.00768200	0.82167000	0.44757500
C	-5.24780500	0.42503500	0.94424700
C	-3.75956600	2.16844700	0.20280900
C	-6.22702100	1.37122000	1.18210400
H	-5.45202200	-0.63216400	1.14556300
C	-4.74468600	3.11052700	0.44186000
H	-2.77665700	2.47965900	-0.17266800
C	-5.97670300	2.71158100	0.93098400
H	-7.19929700	1.05797600	1.57127200
H	-4.54336900	4.16775700	0.25097100

H	-6.75406000	3.45581100	1.12479600
C	-3.22432000	-1.30217800	-1.36818900
C	-2.40570600	-2.35211300	-1.78376400
C	-4.36004900	-0.98424800	-2.10199100
C	-2.73397400	-3.08640600	-2.90585300
H	-1.49961600	-2.59905400	-1.21397600
C	-4.67650200	-1.71698600	-3.23469400
H	-5.00773900	-0.15882000	-1.79105200
C	-3.87040200	-2.76780400	-3.63421200
H	-2.09207000	-3.91313300	-3.22098100
H	-5.57120100	-1.46222500	-3.80923200
H	-4.12569500	-3.34505900	-4.52709000
C	-2.71785300	-1.56381200	1.45073500
C	-1.93431500	-1.27576600	2.56545300
C	-3.49367400	-2.71881000	1.43450200
C	-1.93592600	-2.12489600	3.65636700
H	-1.31480400	-0.37003900	2.57288600
C	-3.48434200	-3.56963700	2.52645300
H	-4.11054300	-2.95849100	0.56210600
C	-2.71058900	-3.27318800	3.63605000
H	-1.32037200	-1.89094000	4.52904600
H	-4.09382200	-4.47730000	2.50911000
H	-2.70620400	-3.95015900	4.49456700
C	3.39040400	2.88976300	-0.26098100
H	3.48687700	3.96961400	-0.44794100
N	1.96013600	2.59760000	-0.12498800
H	3.76620500	2.35728100	-1.15419300
S	0.88126500	3.86347400	-0.33148500
O	-0.39189200	3.36201700	0.09089800
O	1.47972500	4.98560200	0.31168900
C	0.84302600	4.12185500	-2.05798300
H	1.84275700	4.40659700	-2.41056000
H	0.50498800	3.20333500	-2.55613900
H	0.13695600	4.93633800	-2.26492200
C	3.48128200	-1.99817800	2.99007100
H	2.91513300	-2.76671700	2.43573900
H	4.32066200	-2.49540800	3.50241400
H	2.82102700	-1.56541000	3.75098700
C	1.98833500	-1.18229100	-1.00531900
C	1.55084800	-2.20111800	-0.14668200
C	2.69720600	-1.51358300	-2.16573600
C	1.81261300	-3.51932700	-0.45447400
H	0.99732400	-1.93256300	0.76083900
C	2.96904300	-2.83645000	-2.45139600

H	3.04318300	-0.71499100	-2.82751500
C	2.52427200	-3.83802400	-1.60326400
H	1.46304300	-4.31168000	0.21219600
H	3.53332800	-3.08917800	-3.35244000
H	2.73398500	-4.88464200	-1.83989000
H	5.10484600	-3.29650700	1.01762400

4-1a-ts

E_{sol} = -2603.763084 Hartree

Thermal correction to Free Energy = 0.545082 Hartree

Sum of electronic and thermal Free Energies = -2603.218002 Hartree

Number of Imaginary Frequencies: 1

C	7.03753700	-0.14884800	1.92777500
C	6.34367000	-1.35549500	1.85315500
C	5.43108800	-1.60359300	0.84242800
C	5.21139300	-0.62007800	-0.11503600
C	5.94603300	0.57369100	-0.02920000
C	6.85196400	0.83998800	0.98029400
H	7.74532900	0.01571900	2.74375200
H	6.52536400	-2.12324800	2.61002600
H	4.90083700	-2.56035800	0.81378300
H	7.39946600	1.78465200	1.02583200
C	4.31807800	-0.48778700	-1.25225600
C	4.64232600	0.76701500	-1.79815500
N	5.57563000	1.37603300	-1.08140800
C	3.83335600	-1.61339400	-2.11060000
H	3.26585300	-1.18709100	-2.95324800
H	4.67107400	-2.18434200	-2.54123400
C	2.38055700	-0.40732800	-0.46878100
C	1.70018200	0.69053000	-0.30087600
H	4.22775800	1.24761400	-2.68437700
Au	-0.41513600	0.50665500	-0.26563400
P	-2.75784600	0.36182300	-0.07818700
C	-3.54171900	1.96781600	0.17136400
C	-4.68871500	2.12371700	0.94495900
C	-2.98250400	3.07750500	-0.45764800
C	-5.26631900	3.37391100	1.08161900
H	-5.13827500	1.26035600	1.44627400
C	-3.56708800	4.32351900	-0.32326600
H	-2.07450600	2.95826800	-1.06169500
C	-4.70771100	4.47257000	0.44942800
H	-6.16520100	3.49049700	1.69243700
H	-3.12190800	5.18959700	-0.81984200
H	-5.16549200	5.45929600	0.56304800

C	-3.56834500	-0.36502400	-1.51883000
C	-3.02702200	-1.53430700	-2.04983700
C	-4.70562800	0.18801100	-2.09661900
C	-3.62370900	-2.14637300	-3.13597400
H	-2.13066600	-1.97428600	-1.59614400
C	-5.29358100	-0.42452000	-3.19094900
H	-5.14219700	1.10547900	-1.68977100
C	-4.75698100	-1.59005100	-3.70925800
H	-3.19566500	-3.06602900	-3.54389900
H	-6.18601300	0.01742100	-3.64197800
H	-5.22433300	-2.07063000	-4.57298000
C	-3.27033300	-0.65821700	1.32207700
C	-2.50904600	-0.60088600	2.48706600
C	-4.39617800	-1.47417400	1.27960000
C	-2.87551100	-1.33874300	3.59690600
H	-1.61456500	0.03392800	2.52140900
C	-4.75439600	-2.21683800	2.39139500
H	-5.00216300	-1.53267400	0.36941900
C	-3.99711300	-2.15034700	3.54863800
H	-2.27287100	-1.28673700	4.50762400
H	-5.63891400	-2.85840200	2.35035500
H	-4.28119300	-2.74299500	4.42282100
C	2.95506100	-2.54957500	-1.30902000
H	2.21617300	-3.05276700	-1.95289800
N	2.28946400	-1.71953600	-0.32944400
H	3.52978300	-3.33111100	-0.79097000
S	1.66485000	-2.45346600	1.07339800
O	0.24111700	-2.48386000	0.95809200
O	2.39130800	-3.67870100	1.19440800
C	2.10783500	-1.35902800	2.35938400
H	3.19428800	-1.20401400	2.37253900
H	1.56639000	-0.41073600	2.26362300
H	1.79842200	-1.86061400	3.28597900
C	6.10407600	2.67668800	-1.33078100
H	5.50663200	3.16834700	-2.10648200
H	6.06825200	3.28438200	-0.41588500
H	7.14898700	2.60859600	-1.66813900
C	2.26871400	2.01212100	-0.09445000
C	3.19228200	2.23911300	0.93001300
C	1.87027200	3.09388800	-0.88254700
C	3.70579200	3.50302200	1.14988000
H	3.50660100	1.39913900	1.56147600
C	2.40717400	4.35199800	-0.67725400
H	1.13324600	2.92896700	-1.67696700

C	3.31958700	4.56393200	0.34418900
H	4.42560400	3.66098800	1.95889000
H	2.09585100	5.18404400	-1.31522200
H	3.72871300	5.56309400	0.51735100

4-1b-ts

E_{sol} = -2603.766657 Hartree

Thermal correction to Free Energy = 0.546929 Hartree

Sum of electronic and thermal Free Energies = -2603.219728 Hartree

Number of Imaginary Frequencies: 1

C	-6.01493300	1.20139100	-1.97155100
C	-5.53714700	0.09812300	-2.68094300
C	-4.90817900	-0.95259800	-2.04022700
C	-4.76492000	-0.89749200	-0.65912500
C	-5.26805900	0.21809200	0.03156000
C	-5.88994700	1.28105200	-0.59726200
H	-6.50191100	2.01659900	-2.51320800
H	-5.66418600	0.06836500	-3.76623100
H	-4.53031700	-1.80681100	-2.61059300
C	-4.12761300	-1.74192100	0.31738100
C	-4.37367600	-1.11878800	1.54267700
N	-5.01120200	0.03677600	1.36938400
C	-3.84509000	-3.20180800	0.18965000
H	-3.77569700	-3.64709100	1.19600000
H	-4.70803700	-3.68066700	-0.30538200
C	-1.15673300	-1.83772100	0.17353200
C	-2.00379600	-0.86482100	0.24827800
H	-4.10423100	-1.45698300	2.54305600
Au	0.75972500	-0.85321400	0.08799900
P	2.76462700	0.35069100	-0.06696400
C	2.52276200	1.98446400	-0.79958800
C	3.52677300	2.61140200	-1.53323400
C	1.29878600	2.62487100	-0.62370800
C	3.30905900	3.86613100	-2.07400200
H	4.48938000	2.11140500	-1.68578500
C	1.08687300	3.87946100	-1.16596800
H	0.50110700	2.12879500	-0.05480900
C	2.09086800	4.50006100	-1.89116800
H	4.10085700	4.35251700	-2.64992300
H	0.12045800	4.37374500	-1.02626800
H	1.91920600	5.48829400	-2.32719000
C	3.56592700	0.60210700	1.52837800
C	3.39097800	-0.37500100	2.50448100
C	4.35719300	1.71333500	1.80266700

C	4.01009300	-0.24981900	3.73485500
H	2.75776200	-1.24498700	2.29296400
C	4.96681400	1.83816300	3.03889800
H	4.49726400	2.49335200	1.04705300
C	4.79560200	0.85895400	4.00335000
H	3.86874900	-1.02243600	4.49547200
H	5.58269500	2.71612700	3.25148200
H	5.27711100	0.96390000	4.97958400
C	3.98563200	-0.45160000	-1.12622400
C	3.58413300	-0.79858100	-2.41567300
C	5.28286100	-0.73276000	-0.71444900
C	4.47316800	-1.40067400	-3.28475100
H	2.55979400	-0.58199200	-2.74328000
C	6.16642800	-1.34877500	-1.58676100
H	5.61360300	-0.47085900	0.29557200
C	5.76711200	-1.67829700	-2.87005300
H	4.15191500	-1.66127500	-4.29664100
H	7.18454100	-1.56942900	-1.25537000
H	6.46908500	-2.16148700	-3.55474700
C	-2.61005400	-3.58680400	-0.57716100
H	-2.58915500	-4.67906900	-0.69051600
N	-1.41457400	-3.18591200	0.13984200
H	-2.60489100	-3.12803400	-1.58797200
S	-0.10658400	-4.20909500	0.08494900
O	0.85746100	-3.66579600	0.99258400
O	-0.63349700	-5.52303200	0.27681900
C	0.51707100	-4.08792900	-1.54574300
H	-0.23779400	-4.44996200	-2.25630500
H	0.78347100	-3.04242500	-1.76439000
H	1.41598200	-4.71440700	-1.61497200
C	-5.42231000	0.93280200	2.39874100
H	-5.08251600	1.95560800	2.17798300
H	-6.51917400	0.94126900	2.48535900
H	-4.99186200	0.61257800	3.35376800
H	-6.26386600	2.14252100	-0.03825300
C	-2.18537400	0.54039500	0.09066400
C	-2.23948200	1.09971400	-1.19501900
C	-2.32774400	1.37737400	1.20216600
C	-2.43146200	2.45548100	-1.35808800
H	-2.12857800	0.44062800	-2.06118300
C	-2.51259200	2.73642600	1.03229000
H	-2.28235700	0.94124700	2.20525300
C	-2.57792200	3.27372600	-0.24501700
H	-2.47078600	2.88349000	-2.36290400

H	-2.61097800	3.38569100	1.90606300
H	-2.73862800	4.34765300	-0.37571000

4-2a

E_{sol} = -2603.796168 Hartree
Thermal correction to Free Energy = 0.551978 Hartree
Sum of electronic and thermal Free Energies = -2603.244190 Hartree
Number of Imaginary Frequencies: 0

C	7.12257200	-0.54440300	1.47802800
C	6.29024000	-1.65402100	1.51862400
C	5.13948700	-1.72578400	0.74520500
C	4.82978300	-0.65880200	-0.07511900
C	5.69307300	0.43033300	-0.10720700
C	6.83668200	0.53157300	0.65308900
H	8.01818600	-0.51686600	2.10292800
H	6.54568700	-2.49162000	2.17205100
H	4.50818500	-2.61770600	0.79515800
H	7.48874500	1.40675900	0.60736900
C	3.71461600	-0.39125600	-1.04499500
C	4.06575200	0.96120300	-1.51339000
N	5.18676900	1.36408400	-1.01945200
C	3.70246000	-1.36949500	-2.23842500
H	3.16350700	-0.89520300	-3.07435200
H	4.71171000	-1.63918100	-2.57717800
C	2.26496000	-0.57848200	-0.56262400
C	1.41697100	0.36854800	-0.14525700
H	3.53790000	1.55145100	-2.26499800
Au	-0.66443800	0.24500400	-0.03677800
P	-3.03228400	0.18624300	0.00667800
C	-3.83480300	1.79818500	-0.12854400
C	-4.95277600	2.14622100	0.62149400
C	-3.30752500	2.71412000	-1.03583300
C	-5.53358500	3.39288600	0.46200700
H	-5.37746900	1.43723700	1.33972700
C	-3.89740500	3.95343900	-1.19953300
H	-2.42002600	2.44740300	-1.62336200
C	-5.00978100	4.29521600	-0.44745100
H	-6.41051300	3.66036900	1.05829700
H	-3.47790300	4.66509100	-1.91611300
H	-5.47125600	5.27932200	-0.56908800
C	-3.71686100	-0.81477400	-1.33035200
C	-3.00526600	-1.95303300	-1.70179100
C	-4.91604600	-0.51476800	-1.96968400
C	-3.49463900	-2.78848300	-2.68933500

H	-2.05714500	-2.18736000	-1.20416700
C	-5.39578400	-1.35073100	-2.96476400
H	-5.48386600	0.37933800	-1.68979000
C	-4.68857900	-2.48640100	-3.32357300
H	-2.93090300	-3.68216300	-2.97124400
H	-6.33685400	-1.11011300	-3.46653500
H	-5.07101700	-3.14184100	-4.11074800
C	-3.68292700	-0.53807400	1.52917300
C	-3.14784000	-0.09332000	2.73686400
C	-4.68827700	-1.49935700	1.53987400
C	-3.62337200	-0.58960800	3.93570200
H	-2.34769100	0.65695100	2.73400300
C	-5.15182000	-2.00345600	2.74378200
H	-5.11593500	-1.86224900	0.59966700
C	-4.62550200	-1.54826000	3.94005300
H	-3.20140300	-0.23052200	4.87847300
H	-5.93869000	-2.76246200	2.74409100
H	-4.99514000	-1.94806100	4.88851600
C	2.92881700	-2.55044800	-1.70990100
H	2.41085000	-3.08651700	-2.52000200
N	1.98537900	-1.93213500	-0.80121100
H	3.57691700	-3.27827400	-1.19369300
S	1.19415500	-2.91939200	0.27144800
O	-0.21825300	-2.83595400	0.05101600
O	1.83327300	-4.19595500	0.13773600
C	1.51589200	-2.26955800	1.86536200
H	2.59460600	-2.19936100	2.05098500
H	1.03213100	-1.29371400	1.99032300
H	1.07029300	-2.98723100	2.56723300
C	5.84796200	2.59550800	-1.32749700
H	5.20961200	3.19780600	-1.98101000
H	6.04798100	3.14409700	-0.39781100
H	6.80137800	2.38300900	-1.83008700
C	2.00375300	1.65800400	0.21367800
C	2.94883600	1.75556000	1.24177400
C	1.64296600	2.83785500	-0.45173800
C	3.54185800	2.96644800	1.55837700
H	3.21346300	0.85081700	1.80252100
C	2.24321700	4.04365300	-0.14256800
H	0.88656200	2.78671000	-1.24383100
C	3.19880200	4.11464700	0.86234400
H	4.28159500	3.01351500	2.36369600
H	1.95883500	4.94686200	-0.69090700
H	3.66541000	5.07133400	1.11153600

4-2b

E_{sol} = -2603.801460 Hartree

Thermal correction to Free Energy = 0.548418 Hartree

Sum of electronic and thermal Free Energies = -2603.253042 Hartree

Number of Imaginary Frequencies: 0

C	-6.75956100	2.04409400	-0.90435800
C	-6.39619000	1.30152500	-2.01891300
C	-5.47174300	0.26944100	-1.92485100
C	-4.92757000	-0.00482300	-0.69055900
C	-5.32257100	0.73746600	0.41178300
C	-6.22541500	1.77505100	0.34742100
H	-7.48689500	2.85265300	-1.00931100
H	-6.84263800	1.53787800	-2.98766500
H	-5.17828700	-0.30204500	-2.81042600
C	-3.88074800	-0.97568200	-0.25344700
C	-3.92182000	-0.78391300	1.21329200
N	-4.65429700	0.23792600	1.53728100
C	-4.02531100	-2.41076200	-0.74458800
H	-4.63849100	-2.97747300	-0.02617700
H	-4.56604000	-2.41680700	-1.70380600
C	-1.40013300	-1.24139000	-0.04067800
C	-2.44174500	-0.42071100	-0.35195400
H	-3.33406900	-1.32479900	1.95704400
Au	0.53065700	-0.45308400	0.07061100
P	2.68479600	0.51839600	0.09691400
C	2.76679700	2.05610600	-0.84651600
C	3.94835800	2.51499400	-1.42287100
C	1.59990000	2.80413400	-0.98464000
C	3.96164500	3.71378400	-2.11457700
H	4.86974500	1.93063400	-1.32737100
C	1.61927100	4.00297000	-1.67475200
H	0.66422100	2.43684500	-0.54372000
C	2.79948900	4.45886200	-2.23847300
H	4.89253900	4.06999200	-2.56396000
H	0.69706700	4.58243900	-1.77977900
H	2.81324700	5.40324600	-2.78915200
C	3.25861000	0.91383600	1.76317600
C	2.90305600	0.04135100	2.79067500
C	4.02972600	2.03410200	2.05539700
C	3.32025900	0.28174500	4.08719600
H	2.28644700	-0.83828000	2.56677200
C	4.43717100	2.27508600	3.35680200
H	4.31531500	2.73307500	1.26337800

C	4.08437900	1.40170800	4.37219300
H	3.03563000	-0.40871600	4.88518400
H	5.03795400	3.16130400	3.57904100
H	4.40435800	1.59853600	5.39894400
C	3.95825200	-0.54745100	-0.61556500
C	3.64775300	-1.23689200	-1.78664200
C	5.21419400	-0.70782800	-0.04150400
C	4.58238200	-2.06891900	-2.37487000
H	2.65712800	-1.11594800	-2.24371600
C	6.14448700	-1.54824500	-0.63095600
H	5.47283900	-0.17467700	0.87883600
C	5.83084600	-2.22863300	-1.79467500
H	4.33074100	-2.60592800	-3.29333700
H	7.12848900	-1.67212400	-0.17002300
H	6.56587800	-2.89484300	-2.25433100
C	-2.68385800	-3.05756400	-0.93557200
H	-2.76931500	-4.15030600	-0.87431200
N	-1.75956500	-2.58569600	0.08406300
H	-2.27263400	-2.79306000	-1.93056000
S	-0.61086600	-3.68091000	0.57647200
O	0.12020200	-3.05426600	1.63455800
O	-1.31520400	-4.90359200	0.80833700
C	0.44786300	-3.91466200	-0.79572200
H	-0.12449600	-4.32816200	-1.63641800
H	0.91135300	-2.95774800	-1.07677400
H	1.22969100	-4.62668200	-0.50231100
C	-4.75084300	0.82881300	2.83585300
H	-4.40732800	1.87255800	2.79233900
H	-5.79536000	0.81044700	3.17507100
H	-4.12773900	0.26628200	3.53809100
H	-6.51706400	2.35133600	1.22842700
C	-2.27048200	1.04452500	-0.44370700
C	-2.39844400	1.70830900	-1.66250700
C	-1.99257400	1.80094000	0.69562800
C	-2.24186100	3.08101200	-1.74220500
H	-2.61326800	1.12804900	-2.56624400
C	-1.84764100	3.17694500	0.62047800
H	-1.88451500	1.28910700	1.66025300
C	-1.97396300	3.82003200	-0.60008800
H	-2.33353200	3.58274300	-2.70975800
H	-1.62936700	3.75145100	1.52533200
H	-1.86395000	4.90663800	-0.66222900

4-3a

E_{sol} = -1432.107602 Hartree
Thermal correction to Free Energy = 0.306360 Hartree
Sum of electronic and thermal Free Energies = -1431.801242 Hartree
Number of Imaginary Frequencies: 0

C	-4.94162200	-1.25029600	0.53245900
C	-4.61462400	-2.43047900	-0.14782700
C	-3.31666100	-2.69357300	-0.53568100
C	-2.32516400	-1.75391500	-0.24285400
C	-2.67932500	-0.56020300	0.42910700
C	-3.98361800	-0.29981600	0.83288800
H	-5.98080600	-1.07312300	0.82745200
H	-5.40501900	-3.15453300	-0.36910200
H	-3.06674300	-3.62254500	-1.06005800
H	-4.24776800	0.62412800	1.35633900
C	-0.92699700	-1.69013700	-0.45515300
C	-0.49836100	-0.48924000	0.06046000
N	-1.56067600	0.19548400	0.60587200
C	0.00352300	-2.68435700	-1.03249400
H	0.06298500	-3.56839300	-0.36775100
H	-0.34197300	-3.06072300	-2.01198100
C	0.88978300	-0.06813500	0.01916400
C	1.37660100	1.18832700	-0.02818500
C	1.37486300	-2.07079000	-1.19769900
H	2.14002600	-2.85641500	-1.29008800
N	1.69797200	-1.24037200	-0.04080000
H	1.41041800	-1.44719000	-2.11580600
S	3.26742100	-1.26508800	0.45164000
O	3.36889800	-0.37396900	1.56404500
O	3.60615400	-2.64722000	0.59541500
C	4.23520100	-0.64558600	-0.87670100
H	4.10341600	-1.28747300	-1.75883200
H	3.95623700	0.38818400	-1.12139400
H	5.28913300	-0.67761600	-0.56622100
C	-1.49855400	1.23660400	1.58406600
H	-0.46454000	1.37626800	1.92144000
H	-1.87244900	2.19901900	1.19443100
H	-2.10297700	0.95488300	2.46156700
C	0.62265700	2.41646200	-0.23885500
C	0.99689100	3.58442300	0.43277800
C	-0.43172200	2.48882700	-1.15599400
C	0.31648100	4.77178400	0.22855200
H	1.83231700	3.54594800	1.14141200
C	-1.10684700	3.67902400	-1.36288900
H	-0.71178900	1.59554300	-1.72661600

C	-0.74407900	4.82305300	-0.66516900
H	0.61808500	5.67160900	0.77493000
H	-1.92483500	3.71730800	-2.08959200
H	-1.28061100	5.76229300	-0.83150900
H	2.45611900	1.32609800	0.09412100

4-3b

E_{sol} = -1432.115732 Hartree

Thermal correction to Free Energy = 0.305839 Hartree

Sum of electronic and thermal Free Energies = -1431.809893 Hartree

Number of Imaginary Frequencies: 0

C	5.15536100	-1.50538900	0.44541100
C	4.63669100	-2.60228000	-0.25390600
C	3.31344600	-2.63786000	-0.64473400
C	2.48788300	-1.55457600	-0.33252500
C	3.03383600	-0.45434600	0.37085800
C	4.36497900	-0.41712400	0.76779600
H	6.21079500	-1.50550700	0.73705100
H	5.29609800	-3.44272900	-0.49375800
H	2.91744900	-3.49978600	-1.19359000
C	1.12645700	-1.24524600	-0.56858200
C	0.88689000	-0.00801900	-0.01327900
N	2.04839700	0.46273800	0.56281700
C	0.06977800	-2.10490300	-1.14317100
H	-0.30926900	-1.73180500	-2.11362900
H	0.47945200	-3.10936200	-1.34239700
C	-1.58800900	0.19494600	-0.17785100
C	-0.35224400	0.74248300	-0.05600200
C	-1.10834000	-2.26195300	-0.19358400
H	-1.71217100	-3.13696500	-0.47675700
N	-1.99281100	-1.11566400	-0.24516700
H	-0.73879300	-2.42740000	0.83823000
S	-3.60655600	-1.41428200	0.06322300
O	-4.32348500	-0.22145900	-0.26099600
O	-3.92874000	-2.64957200	-0.57671100
C	-3.66115400	-1.64989500	1.79784600
H	-3.03431200	-2.50879600	2.07544400
H	-3.30831700	-0.73938800	2.30110300
H	-4.70307000	-1.85303600	2.08243800
C	2.19530800	1.57469400	1.44406200
H	2.83689500	1.28739300	2.29221200
H	2.64804000	2.45095500	0.94843700
H	1.22176600	1.87374700	1.85164800
H	4.78057300	0.44146000	1.30469800

C	-0.29851800	2.21762100	-0.17830500
C	0.66406600	2.82119600	-0.99216600
C	-1.20838800	3.04196600	0.48787400
C	0.71100000	4.19704800	-1.13704300
H	1.38370700	2.19247200	-1.52945500
C	-1.16808900	4.41786500	0.33202200
H	-1.95159700	2.59053100	1.15602700
C	-0.20638100	5.00341700	-0.47832800
H	1.47080000	4.64683300	-1.78489500
H	-1.89089700	5.04345600	0.86570700
H	-0.16754100	6.09127600	-0.59170100
H	-2.42344800	0.88602500	-0.31860500

5-1

E_{sol} = -3,092.042207 Hartree

Thermal correction to Free Energy = 0.506957 Hartree

Sum of electronic and thermal Free Energies = -3,091.53525 Hartree

Number of Imaginary Frequencies = 0

C	-7.29108900	0.97883300	2.53006400
C	-7.25531500	1.82764500	1.41902200
C	-6.43389200	1.56417900	0.34253500
C	-5.62205300	0.42864500	0.36957100
C	-5.69855000	-0.42800400	1.49356500
C	-6.51507800	-0.16101100	2.58414200
H	-7.94936900	1.21988100	3.36930700
H	-7.89465300	2.71530100	1.40558100
H	-6.42496000	2.23671700	-0.52223500
C	-4.67147000	-0.14927300	-0.52324300
C	-4.24731900	-1.30223800	0.07677200
N	-4.86001700	-1.47372800	1.27716500
C	-4.26481600	0.35662400	-1.85806600
H	-3.57544000	-0.35434200	-2.34346800
H	-5.15151100	0.41017100	-2.51657800
C	-1.79325400	1.39109300	-0.41079700
C	-1.92460500	0.99988700	0.74972900
H	-3.53196400	-2.04342400	-0.27606500
Au	0.44932800	0.94361700	0.11700600
P	2.70263600	0.59974200	0.64949600
C	3.55196800	2.17691200	0.90923000
C	4.93045100	2.31217800	0.76075800
C	2.80001400	3.27457200	1.31607700
C	5.53967500	3.52676100	1.01985800
H	5.53572800	1.46330900	0.42617100
C	3.41357100	4.48731800	1.57752700

H	1.71263300	3.17171400	1.42426300
C	4.78426100	4.61388900	1.42845600
H	6.62167800	3.62542800	0.89672900
H	2.81194700	5.34386500	1.89375300
H	5.27077500	5.57276800	1.62713800
C	2.98907200	-0.34083500	2.16364100
C	1.91384500	-0.74762800	2.94504300
C	4.28951400	-0.62859800	2.57583600
C	2.13820300	-1.43284200	4.12768300
H	0.88818100	-0.55374100	2.60927600
C	4.50642000	-1.31635700	3.75439500
H	5.14478900	-0.32267000	1.96339800
C	3.43088700	-1.71574900	4.53261100
H	1.28831100	-1.75684500	4.73437500
H	5.52835200	-1.54405700	4.06893400
H	3.60557800	-2.26021000	5.46462900
C	3.62437700	-0.22648200	-0.66050900
C	3.92737400	0.49434100	-1.81390200
C	3.91969300	-1.58402500	-0.60157200
C	4.54287300	-0.13091500	-2.88110700
H	3.67736800	1.55938300	-1.87884100
C	4.53010700	-2.20492800	-1.67760400
H	3.65701600	-2.16948900	0.28416200
C	4.84628200	-1.48172000	-2.81388100
H	4.78190000	0.44335000	-3.78040900
H	4.75517200	-3.27314200	-1.62442700
H	5.32697900	-1.97629600	-3.66243500
C	-2.06787700	0.31579700	2.01743300
H	-3.16343200	0.33514900	2.22725800
H	-1.60705500	0.90880600	2.82722000
O	-1.54274100	-0.95892600	2.06802800
H	-1.55602500	-1.33228600	1.18045100
C	-3.64332600	1.74027300	-1.89902800
H	-3.75383000	2.15586700	-2.90990300
N	-2.20213800	1.73269000	-1.63528700
H	-4.13963600	2.42855500	-1.18822800
S	-1.25874700	2.86263000	-2.45135400
O	0.09763100	2.50174100	-2.17523100
O	-1.75619000	2.89811300	-3.78581100
C	-1.61810300	4.37297900	-1.65135700
H	-2.68473900	4.60489300	-1.76512000
H	-1.35094100	4.30017200	-0.58874500
H	-1.01961300	5.15940900	-2.12880900
C	-4.58060500	-2.50891000	2.20977100

H	-4.10584400	-2.11161700	3.12250800
H	-5.50047300	-3.04070700	2.49911200
H	-3.89401200	-3.23246500	1.75455200
H	-6.55000700	-0.83133300	3.44799400
Sb	0.20275300	-2.85089300	-1.08130900
F	-0.62524100	-4.19706900	-0.13872200
F	1.62931200	-3.94080000	-1.46875900
F	-0.67979400	-3.37152200	-2.60746400
F	-1.23576500	-1.74077300	-0.65611700
F	0.97273900	-1.46398200	-2.01457400
F	1.02188700	-2.30309400	0.47629800

5-1a-ts

E_{sol} = -3092.033898 Hartree

Thermal correction to Free Energy = 0.507161 Hartree

Sum of electronic and thermal Free Energies = -3,091.526737 Hartree

Number of Imaginary Frequencies = 1

C	-6.21911200	1.53784300	-2.52263000
C	-5.76052200	0.41009700	-3.20387000
C	-5.20384600	-0.66029100	-2.52771500
C	-5.12079200	-0.59421000	-1.14499200
C	-5.62114700	0.53425000	-0.47975800
C	-6.15781000	1.62184700	-1.14325800
H	-6.63791100	2.37235600	-3.09053400
H	-5.83456800	0.38020900	-4.29407800
H	-4.82891000	-1.53266800	-3.07166700
H	-6.51427400	2.50584500	-0.60903500
C	-4.56203800	-1.46835400	-0.13697000
C	-4.84066800	-0.81471600	1.07880500
N	-5.43146600	0.35009700	0.86969400
C	-4.44301700	-2.95418700	-0.24542600
H	-4.77495300	-3.42158900	0.69483800
H	-5.09736300	-3.33538900	-1.04403500
C	-2.46390800	-1.14996400	-0.03056900
C	-1.85123600	-0.04820300	-0.34662800
H	-4.61870700	-1.14688600	2.09383200
Au	0.26058200	-0.33992200	-0.41125800
P	2.52974200	-0.97735900	-0.38294300
C	3.61538900	-0.35595500	-1.68506400
C	4.55049600	-1.17150500	-2.31709200
C	3.53176600	0.99129200	-2.03127200
C	5.39646100	-0.64207500	-3.27650600
H	4.62426300	-2.23198200	-2.05522400
C	4.38508000	1.51390400	-2.98622600

H	2.79769900	1.63917600	-1.54081400
C	5.31674600	0.69945400	-3.61003300
H	6.12874300	-1.28812200	-3.76795100
H	4.31634100	2.57276000	-3.24928500
H	5.98636700	1.11563200	-4.36784200
C	3.37611600	-0.63367100	1.17224800
C	2.60663100	-0.36293200	2.29926500
C	4.76364600	-0.67420900	1.28120100
C	3.21401600	-0.14710300	3.52335400
H	1.51459000	-0.30638900	2.20635400
C	5.36690900	-0.45558100	2.50642200
H	5.37983100	-0.88016900	0.39903400
C	4.59403600	-0.19382600	3.62678900
H	2.60245000	0.07184100	4.40268300
H	6.45684800	-0.48586900	2.58645100
H	5.07661300	-0.01471300	4.59174100
C	2.55253300	-2.78022500	-0.55204700
C	1.84377700	-3.33445500	-1.61835500
C	3.14858800	-3.62407800	0.37821000
C	1.74534700	-4.70615300	-1.75668900
H	1.35794600	-2.67730000	-2.35014900
C	3.03497400	-4.99926700	0.24344800
H	3.70311900	-3.21008800	1.22606100
C	2.33601300	-5.54256200	-0.82034800
H	1.19341900	-5.12809200	-2.60087100
H	3.50380300	-5.65340000	0.98363600
H	2.24759200	-6.62776200	-0.92183100
C	-2.44746500	1.31202800	-0.54407300
H	-3.25069200	1.24277500	-1.30181900
H	-1.68860900	1.99025100	-0.97153600
O	-3.00101000	1.85579800	0.60349800
H	-2.26155800	2.17705500	1.12488700
C	-2.99932100	-3.34788500	-0.50454300
H	-2.78044500	-4.38655000	-0.22343400
N	-2.17805700	-2.43463700	0.25076500
H	-2.72863600	-3.21212400	-1.56505200
S	-1.81223100	-2.86666300	1.86219100
O	-1.85567100	-1.67343700	2.64729100
O	-2.63073000	-3.99572100	2.19042800
C	-0.15546500	-3.38579800	1.68907600
H	-0.09734100	-4.18985600	0.94266100
H	0.44356900	-2.51834800	1.37883600
H	0.18714300	-3.75240600	2.66593700
C	-5.73703300	1.32488900	1.86270600

H	-5.45291500	0.93785000	2.84673800
H	-5.17544900	2.24816500	1.66522700
H	-6.81461900	1.54386200	1.86092000
Sb	0.80469500	3.55234000	0.43122400
F	0.61047800	2.71655600	-1.20878200
F	1.92252300	4.77560700	-0.36329000
F	-0.67690300	4.57277000	0.04808300
F	-0.32263400	2.32941500	1.26252600
F	1.00580500	4.40311700	2.04858600
F	2.22248600	2.43828100	0.80883600

5-1b-ts

E_{sol} = -3092.026545 Hartree

Thermal correction to Free Energy = 0.504512 Hartree

Sum of electronic and thermal Free Energies = -3,091.522033 Hartree

Number of Imaginary Frequencies = 1

C	-7.01981700	1.06146900	2.66488400
C	-6.90007300	1.98868800	1.62768300
C	-6.10675400	1.73541800	0.52655100
C	-5.41756900	0.52662100	0.45773200
C	-5.58149100	-0.40280900	1.50278900
C	-6.36256900	-0.15259100	2.61946500
H	-7.64870500	1.29777700	3.52743700
H	-7.44721100	2.93299100	1.69101500
H	-6.02945800	2.47361300	-0.27741700
C	-4.51480100	-0.07066200	-0.48842300
C	-4.25022400	-1.33957100	0.01145700
N	-4.85953800	-1.52440800	1.18738600
C	-4.30346000	0.33050600	-1.90636200
H	-3.71874400	-0.44412700	-2.43059300
H	-5.28483400	0.36884700	-2.41121900
C	-1.78396300	1.17170700	-0.68888900
C	-2.35769200	0.55095400	0.27441900
H	-3.62455300	-2.12189900	-0.41661200
Au	0.32043800	1.00729000	-0.10583100
P	2.51828400	0.83845400	0.68084300
C	3.32945000	2.45404000	0.73234300
C	4.70122800	2.60648400	0.54840300
C	2.55280700	3.57362000	1.01926700
C	5.28202500	3.85823500	0.65454600
H	5.32612300	1.73771900	0.31703500
C	3.13834000	4.82193500	1.13180700
H	1.46964700	3.45942500	1.15581800
C	4.50402800	4.96523200	0.94847100

H	6.35962800	3.96787500	0.50551400
H	2.51926000	5.69411400	1.35911700
H	4.96639200	5.95283800	1.02986900
C	2.66368200	0.19639800	2.36506200
C	1.57277300	-0.40755400	2.98029600
C	3.87152500	0.29231000	3.05347300
C	1.68912800	-0.91226300	4.26479900
H	0.62671800	-0.50850700	2.43658200
C	3.98245000	-0.21117800	4.33590900
H	4.74129800	0.76130000	2.58116400
C	2.89104800	-0.81246300	4.94314600
H	0.82774700	-1.39169600	4.73719000
H	4.93412500	-0.13342500	4.86818900
H	2.98085000	-1.20952600	5.95808200
C	3.58474600	-0.19611700	-0.34095800
C	3.89801900	0.23923700	-1.62759600
C	4.00841200	-1.45060100	0.08015100
C	4.64663800	-0.56124400	-2.46799800
H	3.55103000	1.21891200	-1.97591000
C	4.75107300	-2.25129800	-0.77119300
H	3.75033600	-1.81780100	1.07734200
C	5.07416900	-1.80905900	-2.04114400
H	4.89233400	-0.20961900	-3.47339900
H	5.07447100	-3.23956200	-0.43451800
H	5.65836700	-2.44539900	-2.71159500
C	-2.24492800	-0.00514300	1.61296500
H	-3.19375700	0.14074800	2.16497100
H	-1.51274300	0.64253300	2.14671800
O	-1.91071100	-1.34035900	1.69789600
H	-1.34315400	-1.55800900	0.95179200
C	-3.64577500	1.66956500	-2.13267800
H	-3.79281900	1.97384400	-3.17599600
N	-2.21505700	1.59974600	-1.90647400
H	-4.09453500	2.44406600	-1.47798300
S	-1.28696300	2.77379000	-2.65122600
O	0.07752300	2.36885800	-2.51134300
O	-1.86299500	2.96048000	-3.94451500
C	-1.53603500	4.21406400	-1.69292800
H	-2.59917100	4.48839600	-1.69981700
H	-1.19304300	4.03282700	-0.66503300
H	-0.94690200	5.02558800	-2.13876800
C	-4.70471300	-2.65816400	2.03481000
H	-4.13460200	-2.40103000	2.94059700
H	-5.68896000	-3.04883900	2.33182800

H	-4.16177800	-3.44166900	1.49567300
H	-6.45951400	-0.88408900	3.42613200
Sb	0.53956600	-3.15833100	-0.93325300
F	-0.28982700	-4.47472300	0.04862100
F	2.10218500	-4.12173700	-0.94228600
F	-0.03360200	-3.95374100	-2.48807900
F	-1.03764600	-2.17112000	-0.85386300
F	1.32114400	-1.81229800	-1.91313600
F	1.02690200	-2.32754600	0.64364000

5-2a

E_{sol} = -3092.058716 Hartree

Thermal correction to Free Energy = 0.509411 Hartree

Sum of electronic and thermal Free Energies = -3,091.549305 Hartree

Number of Imaginary Frequencies = 0

C	-6.50665900	-0.16972900	-3.08224400
C	-5.55971900	-1.16847500	-3.26314500
C	-4.72710100	-1.56812400	-2.22613100
C	-4.86197100	-0.94346700	-1.00603500
C	-5.81487400	0.05032200	-0.85072800
C	-6.65517100	0.46690100	-1.85890300
H	-7.14295800	0.12827700	-3.91891400
H	-5.46367900	-1.64320900	-4.24303500
H	-3.96974900	-2.34223000	-2.38226700
H	-7.39366900	1.25849900	-1.71311200
C	-4.15829200	-1.13395100	0.30416600
C	-4.78660400	-0.06568800	1.10318300
N	-5.73570300	0.52797000	0.46481600
C	-4.46004200	-2.50065700	0.96188000
H	-4.58176100	-2.37632300	2.05095300
H	-5.37564500	-2.95929900	0.56325400
C	-2.61244900	-1.10907900	0.25204200
C	-1.81479800	-0.24179700	-0.37603700
H	-4.55393400	0.19092100	2.13931300
Au	0.23831300	-0.52433900	-0.41715700
P	2.56147500	-0.99570700	-0.42174800
C	3.50064100	-0.25898400	-1.77909100
C	4.34373500	-0.99420200	-2.60489000
C	3.35980400	1.11288700	-1.98599900
C	5.03624400	-0.36395900	-3.62572700
H	4.46506500	-2.07140900	-2.45182200
C	4.06148300	1.73659500	-3.00011300
H	2.69762800	1.69862500	-1.33889800
C	4.89804400	0.99912700	-3.82339000

H	5.69636700	-0.94869500	-4.27272000
H	3.94865600	2.81345500	-3.15208000
H	5.44637900	1.49354000	-4.63037500
C	3.46417800	-0.51930700	1.06918800
C	2.78842000	-0.49632000	2.28646500
C	4.81995500	-0.20662600	1.03306400
C	3.46442100	-0.17829700	3.45106700
H	1.71339600	-0.71353300	2.31861900
C	5.49051400	0.11695800	2.19975000
H	5.36072700	-0.21565200	0.08093800
C	4.81459900	0.12931500	3.40862800
H	2.92566500	-0.15597600	4.40195400
H	6.55449200	0.36660000	2.16197100
H	5.34488300	0.38969500	4.32884700
C	2.82219900	-2.78045200	-0.57110300
C	2.02091300	-3.47885500	-1.47491100
C	3.75438000	-3.48055000	0.18819600
C	2.16129800	-4.84603600	-1.62621000
H	1.27469800	-2.93676200	-2.06870600
C	3.88200400	-4.85252700	0.04328700
H	4.39027600	-2.95429000	0.90667600
C	3.08990900	-5.53674700	-0.86262300
H	1.53092100	-5.37989600	-2.34220600
H	4.61386200	-5.39278500	0.64973800
H	3.19240700	-6.62003000	-0.97212800
C	-2.41391400	1.00642200	-0.95251800
H	-3.00601400	0.74654500	-1.85540600
H	-1.62121500	1.68970900	-1.30120500
O	-3.28616200	1.68187200	-0.09139700
H	-2.71674000	2.12146800	0.54608900
C	-3.19872400	-3.28831700	0.69730100
H	-3.07437700	-4.13937400	1.37935800
N	-2.13951000	-2.31594000	0.83922600
H	-3.16990100	-3.66880500	-0.33858200
S	-1.45823700	-2.25173700	2.37640100
O	-1.02792200	-0.91052200	2.62772500
O	-2.32150300	-2.90544000	3.32381800
C	-0.06160000	-3.27210000	2.13253200
H	-0.38815400	-4.27850500	1.84027400
H	0.56072500	-2.83684200	1.33799800
H	0.49638900	-3.32730800	3.07629100
C	-6.51016700	1.62749600	0.94453700
H	-6.28934000	1.79314900	2.00293900
H	-6.25837000	2.52964400	0.36897400

H	-7.57932700	1.40975800	0.82200400
Sb	0.62064000	3.57946100	0.38762500
F	0.46973600	2.81397000	-1.28659800
F	2.03040100	4.58333500	-0.23431800
F	-0.57321400	4.88232200	-0.12521900
F	-0.79609900	2.55820900	1.01377300
F	0.76948800	4.35402400	2.04858400
F	1.79189500	2.25286600	0.90079400

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E_{sol} = -3092.074708 Hartree
Thermal correction to Free Energy = 0.510612 Hartree
Sum of electronic and thermal Free Energies = -3,091.564096 Hartree
Number of Imaginary Frequencies = 0

C	7.12446500	-1.20072200	2.50772500
C	6.25876200	-2.23368000	2.17875800
C	5.23054100	-2.04757200	1.26263600
C	5.09332400	-0.81076600	0.67056100
C	5.96440000	0.20704000	1.03152800
C	6.98933500	0.05635200	1.93715200
H	7.91869300	-1.37283000	3.23812000
H	6.38116000	-3.20848800	2.65806000
H	4.53596300	-2.86128700	1.03572100
C	4.11238600	-0.26908200	-0.33649900
C	4.54114200	1.15327400	-0.37686800
N	5.59375700	1.36928900	0.33659700
C	4.30043800	-0.83167500	-1.75158200
H	3.92382300	-0.10052300	-2.48707000
H	5.36702300	-0.99917800	-1.96282100
C	1.71469100	-1.06764100	-0.64457000
C	2.65226400	-0.39140900	0.05751300
H	4.12142000	1.93248800	-1.01450000
Au	-0.31598600	-0.90504700	-0.10791700
P	-2.56981100	-0.78710100	0.58029300
C	-3.39187200	-2.39785900	0.44078700
C	-4.74655000	-2.53834700	0.15115900
C	-2.62593700	-3.53885300	0.67031600
C	-5.31797300	-3.79781500	0.08814900
H	-5.36373200	-1.65414900	-0.03773500
C	-3.20215100	-4.79560000	0.61682300
H	-1.55777100	-3.43375400	0.89929800
C	-4.54924200	-4.92626300	0.32096300
H	-6.38094300	-3.89735800	-0.14763600
H	-2.59051400	-5.68303300	0.80075300

H	-5.00450500	-5.91897300	0.26685000
C	-2.81781800	-0.32776700	2.31126000
C	-1.71508500	-0.02424900	3.09999700
C	-4.09089500	-0.30929700	2.88014600
C	-1.87733700	0.29636100	4.43765100
H	-0.71409200	-0.04173200	2.65454200
C	-4.25051600	0.01461200	4.21454800
H	-4.96918200	-0.54771800	2.26899500
C	-3.14424200	0.31643800	4.99412600
H	-1.00281700	0.53476600	5.04919000
H	-5.25172500	0.02946700	4.65314300
H	-3.27365300	0.56972600	6.04988900
C	-3.59585900	0.33860900	-0.38642600
C	-3.84869000	0.01149900	-1.71782800
C	-4.02647100	1.56303900	0.10800100
C	-4.54934300	0.88198700	-2.52977800
H	-3.48799200	-0.93997500	-2.12620700
C	-4.72318900	2.43492600	-0.71270100
H	-3.80767100	1.85318900	1.13989800
C	-4.98939600	2.09637700	-2.02696400
H	-4.74594600	0.61225200	-3.57111700
H	-5.05363600	3.39865400	-0.31621100
H	-5.53661800	2.79024900	-2.67083200
C	2.34109600	0.39968500	1.28092900
H	2.88398500	-0.00642200	2.15851000
H	1.25946600	0.33182000	1.51011800
O	2.76344600	1.72938300	1.18026200
H	2.16006000	2.15087400	0.55734000
C	3.52899200	-2.10594200	-1.91040300
H	3.70207400	-2.51918600	-2.91125900
N	2.12261900	-1.81256800	-1.75686000
H	3.86374500	-2.86156400	-1.16725300
S	1.09788400	-2.98012200	-2.33624200
O	-0.18303100	-2.38248000	-2.56079400
O	1.78728900	-3.61062700	-3.42112300
C	0.94504500	-4.14030900	-1.03049600
H	1.92295700	-4.60023900	-0.83284000
H	0.57443200	-3.62875000	-0.13120900
H	0.23023900	-4.91374800	-1.33993300
C	6.24911000	2.62733500	0.51200700
H	6.12760300	2.96122500	1.55186000
H	7.31942600	2.52157700	0.29199500
H	5.80755400	3.36631600	-0.16338600
H	7.65679200	0.87844700	2.20452300

Sb	-0.56373500	3.29471500	-0.63686900
F	0.30643500	4.48198500	0.47027500
F	-2.13881800	4.21592000	-0.42867700
F	-0.11786300	4.32789100	-2.09145800
F	1.05364400	2.38377100	-0.82711000
F	-1.35756600	2.07111800	-1.75447500
F	-0.94339000	2.24944900	0.83542400

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E_{sol} = -1315.608984 Hartree
Thermal correction to Free Energy = 0.266412 Hartree
Sum of electronic and thermal Free Energies = -1,315.342572 Hartree
Number of Imaginary Frequencies = 0

C	3.06121000	2.67225200	-0.57911000
C	1.72065100	3.00928700	-0.47063300
C	0.79434100	2.05075900	-0.05975200
C	1.22937000	0.78153100	0.25401400
C	2.58384600	0.45381400	0.14120700
C	3.51586200	1.39172400	-0.28557300
H	3.78084600	3.42596300	-0.91706600
H	1.38728600	4.02094600	-0.71770900
H	-0.27050700	2.30794000	-0.00655200
H	4.57318100	1.13385600	-0.39515500
C	0.48035100	-0.44357300	0.72524800
C	1.55566800	-1.55549500	0.60815800
N	2.79665800	-0.84146800	0.51633600
C	-0.14068100	-0.29365900	2.11267300
H	-0.25700800	-1.29321600	2.56798900
H	0.45653900	0.33083700	2.79270600
C	-0.71647900	-0.74160900	-0.13127400
C	-0.56850200	-1.33428200	-1.31513600
H	1.56287900	-2.20691700	1.50356200
C	0.81539600	-1.81105800	-1.59639700
H	1.49656400	-1.00514300	-1.95638800
H	0.81135200	-2.58594800	-2.37954400
O	1.35957100	-2.42602900	-0.44988100
C	-1.50365600	0.29496700	1.83225100
H	-2.25300200	0.04278700	2.59560700
N	-1.84986100	-0.33448800	0.56622600
H	-1.46805400	1.40062900	1.74503900
S	-3.25721200	0.07514800	-0.18221200
O	-3.57558600	-0.97553200	-1.09625400
O	-4.15523200	0.43218600	0.86983000
C	-2.87428700	1.51251900	-1.11285500

H	-2.61276800	2.33438900	-0.43189400
H	-2.04456500	1.29537400	-1.80086000
H	-3.76756300	1.78783000	-1.69110600
C	3.97219100	-1.54863500	0.14992200
H	3.94673900	-2.55356800	0.59606000
H	4.09182000	-1.66759200	-0.94752000
H	4.86834600	-1.03561700	0.53596700
H	-1.39598900	-1.57948700	-1.98168200

5-3b

E_{sol} = -1315.611088 Hartree
Thermal correction to Free Energy = 0.265910 Hartree
Sum of electronic and thermal Free Energies = -1,315.345178 Hartree
Number of Imaginary Frequencies = 0

C	3.33055600	2.68198500	-0.37031900
C	1.98982100	2.92707600	-0.62370300
C	1.04835100	1.91678100	-0.43149700
C	1.46796200	0.68651900	0.02416800
C	2.82587100	0.44655400	0.26205500
C	3.77448000	1.43780100	0.06633100
H	4.06461800	3.47817300	-0.53589300
H	1.67261900	3.90828000	-0.98871300
H	-0.00967100	2.09460600	-0.66609800
C	0.70601500	-0.57814600	0.35092500
C	1.85911900	-1.58280000	0.32089200
N	3.01019800	-0.84574300	0.70153900
C	-0.09306500	-0.51310700	1.64086600
H	-0.30209500	-1.54171600	1.98840800
H	0.46334600	0.00206900	2.44054400
C	-1.49086500	-1.08156400	-0.66651100
C	-0.16190400	-1.10986100	-0.73128200
H	1.72128600	-2.46801500	0.97853300
C	0.70703200	-1.89051600	-1.65831000
H	0.85893900	-1.39771200	-2.63974100
H	0.29658800	-2.90175800	-1.86504400
O	1.95704800	-1.97315000	-1.02862300
C	-1.39470600	0.21023100	1.40507000
H	-1.99707900	0.25144500	2.32427400
N	-2.17102100	-0.48822300	0.39561800
H	-1.18711600	1.25724300	1.09565000
S	-3.65994200	0.14077600	0.05434400
O	-4.31462700	-0.80578500	-0.79356900
O	-4.22597700	0.51779400	1.31094300
C	-3.35158600	1.59291900	-0.88222400

H	-2.81697000	2.33100200	-0.26858400
H	-2.76663700	1.33617400	-1.77695900
H	-4.32005300	2.01244600	-1.18783800
C	4.28979900	-1.46541200	0.62016900
H	4.68735600	-1.52400800	-0.41357400
H	5.01968300	-0.91619400	1.23640500
H	4.22276300	-2.48725600	1.02233600
H	4.83979100	1.25099100	0.23167200
H	-2.13537500	-1.58206100	-1.39475100