Supporting Information

Mechanistic study on ligand-controlled copper-catalyzed regiodivergent silacarboxylation of allenes with carbon dioxide and silylborane

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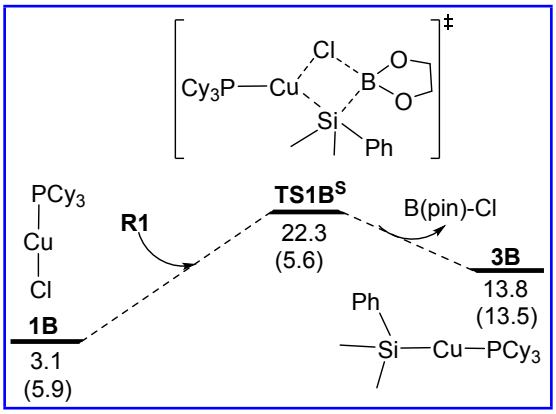

Fig. S1. Free energy diagrams for the disfavored transmetalation of **1B** with **R1** catalyzed by **Cu/L$_B$**.

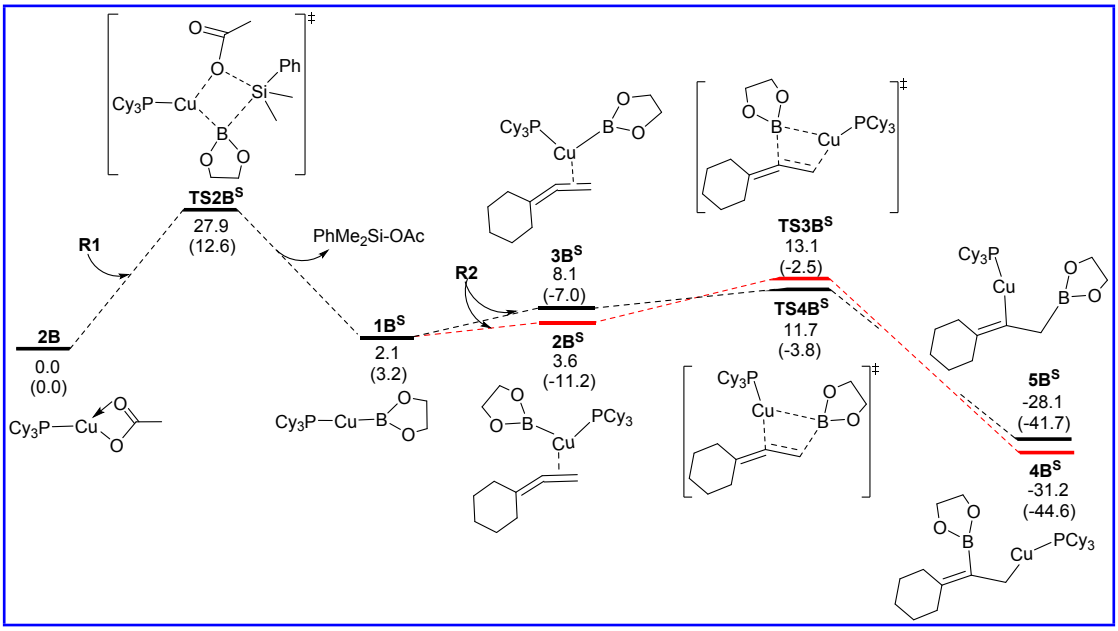

Fig. S2. Free energy diagrams for the disfavored pathways that **2B** reacted with **R1** catalyzed by **Cu/L$_B$**.

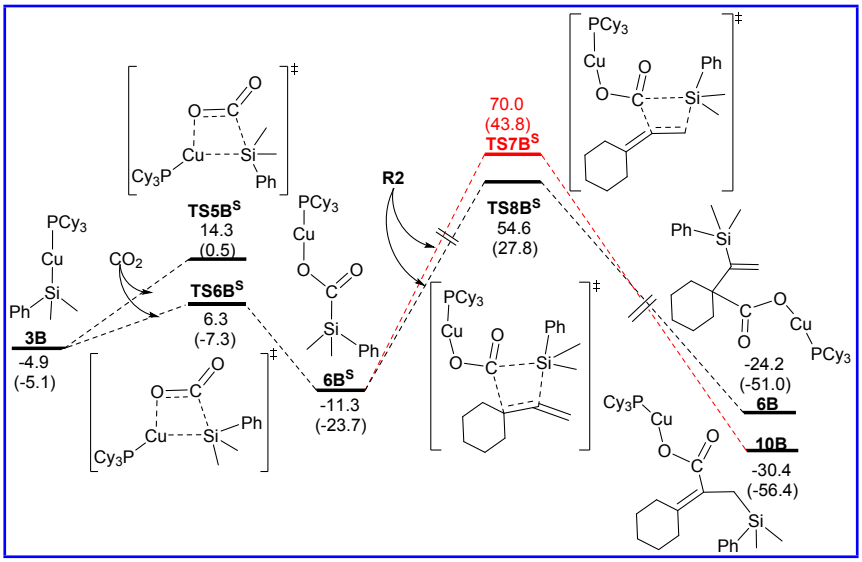

Fig. S3. Free energy diagrams for the disfavored pathways that **3B** reacts with CO_2 firstly catalyzed by **Cu/L$_B$**.

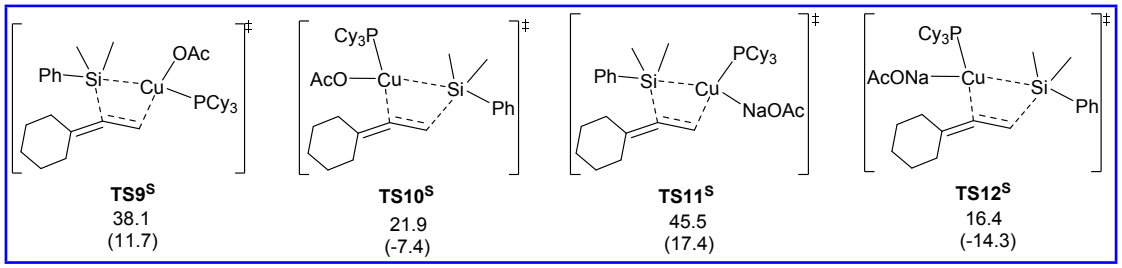

Fig. S4. Other transition state forms for the regioselectivity-determining step with the additive NaOAc catalyzed by **Cu/L$_B$**.

Cartesian Coordinates and Sum of Electronic and Thermal Free Energies for All of the Calculated Structures

L_A

Sum of electronic and thermal Free Energies= -1385.157490

C	-2.43865000	-0.42126600	1.74045400
C	-3.16641500	-0.81595800	-0.89109000
C	-4.30577900	-0.74673700	0.15326700
C	-3.83134500	0.09586200	1.34146600
H	-2.56336000	-1.41231600	2.19871000
H	-3.19946600	0.08302500	-1.51439600
H	-5.22700100	-0.35512600	-0.29506800
H	-4.53523000	-1.76288100	0.50292600
H	-3.76003400	1.15295000	1.05235200
H	-4.53228600	0.04592700	2.18506600
P	-1.53835200	-0.80863000	0.10406700
C	-0.74285300	0.82792000	-0.33944100
C	0.66613600	0.93911100	-0.18771400
C	-1.45454700	1.92573800	-0.84667400
C	1.29233800	2.13309500	-0.57666600
C	-0.81510600	3.10937800	-1.21626100
H	-2.53229600	1.86928000	-0.95662400
C	0.56692400	3.20976900	-1.08739700
H	2.36893400	2.23473000	-0.49228300
H	-1.39570700	3.94233500	-1.60256200
H	1.08347000	4.11853900	-1.38354800
C	2.15341200	-1.57500800	-0.84254100
C	3.33719200	0.21200000	0.92853600
C	3.69190700	-1.63247200	-0.69555500
H	1.72135800	-2.56376500	-0.65727800
C	4.18810800	-0.24106800	-0.27589000
H	3.30437800	1.30289200	1.00090100
H	3.96604200	-2.36439600	0.07387400
H	4.16059900	-1.96870800	-1.62859300
H	5.25850200	-0.24848000	-0.03282100
H	4.05575100	0.45883200	-1.10997500
P	1.58511400	-0.47444700	0.62514300
C	-1.68603800	0.47088500	2.72831300
H	-0.70872700	0.05128800	2.98283200
H	-1.52494900	1.47232200	2.31709900
H	-2.26018100	0.57824100	3.65663300
C	-3.26904100	-2.03689300	-1.81333200
H	-4.23234800	-2.04854300	-2.33802300
H	-2.47783600	-2.03940200	-2.56956900
H	-3.18598500	-2.97061100	-1.24628800
C	1.71634900	-1.11627800	-2.23830000
H	0.62785700	-1.05860700	-2.32134300
H	2.11723300	-0.13027000	-2.49239300
H	2.07216000	-1.82950200	-2.99219100
C	3.87349400	-0.32554500	2.26672600
H	4.88853400	0.04642200	2.45182100
H	3.23965300	-0.01312000	3.10200900
H	3.91298300	-1.42010900	2.28318000

1A

Sum of electronic and thermal Free Energies= -1868.893299

Cu	-1.38098600	-0.03286400	0.00000800
C	1.14007800	0.12822400	-0.00003500
O	0.85337600	1.32621100	-0.00000800
O	0.26329000	-0.84598800	-0.00003200
C	2.58124600	-0.36227400	0.00001000
H	2.76183200	-0.98512000	0.88099200
H	2.76147800	-0.98664300	-0.87995500
H	3.26401900	0.48732700	-0.00080800

2A

Sum of electronic and thermal Free Energies= -3254.126445

Cu	0.15038100	1.26355100	-0.47411500
C	0.66328500	3.61676300	-0.01427900
O	0.71792700	2.89891300	1.02023600
O	0.38140000	3.13864300	-1.16585800
C	0.90986200	5.11344800	0.08084100
H	1.55304600	5.44429400	-0.73911700
H	-0.04263500	5.64550000	-0.02067000
H	1.35755800	5.37279700	1.04148400
C	-3.12125600	0.07085300	-1.29899800
C	-2.72313800	0.28438100	1.42810500
C	-4.06477300	0.80946500	0.87370400
C	-4.38183600	0.03034100	-0.41132200

H	-3.05628300	1.07683300	-1.73385800
H	-2.89400100	-0.71716300	1.84314900
H	-4.85794700	0.71213400	1.62425500
H	-3.97339500	1.87972500	0.64421000
H	-4.63295800	-1.00997300	-0.16274200
H	-5.24816800	0.44569700	-0.94050200
P	-1.65242000	0.06970100	-0.10686800
C	-1.01863400	-1.67294300	0.02644100
C	0.37843200	-1.90704500	-0.04871700
C	-1.88244500	-2.76711800	0.20380200
C	0.84694400	-3.22985500	0.02328500
C	-1.39912400	-4.07189500	0.27481600
H	-2.95192000	-2.59865000	0.28808100
C	-0.02669100	-4.30439900	0.17654600
H	1.91305400	-3.42707300	-0.03453000
H	-2.08884000	-4.90098900	0.40497600
H	0.36297700	-5.31713000	0.22822800
C	2.47100800	-0.26479300	1.38768900
C	3.00238800	-1.12013800	-1.21897800
C	3.95196000	-0.30353000	0.94108700
H	2.21484900	0.73848600	1.74231700
C	4.10610500	-1.36264300	-0.16372400
H	2.71278800	-2.05573500	-1.70837300
H	4.24006100	0.67836900	0.54781400
H	4.60975400	-0.50670000	1.79446900
H	5.10317100	-1.32780900	-0.61964100
H	3.99363400	-2.36302400	0.27261900
P	1.52509600	-0.45510400	-0.24509800
C	-3.08125000	-0.93666600	-2.44835500
H	-2.16547100	-0.83167100	-3.03885800
H	-3.13002600	-1.96925000	-2.09213100
H	-3.92994800	-0.77377400	-3.12251000
C	-2.08143000	1.16954400	2.50014600
H	-2.78774000	1.35403600	3.31838300
H	-1.19442100	0.69251400	2.92875300
H	-1.75610900	2.13086600	2.09180300
C	2.13874800	-1.27341000	2.49217700
H	1.07290500	-1.26408900	2.73904400
H	2.40256900	-2.29980800	2.21956300
H	2.69369400	-1.01672700	3.40207800
C	3.41994800	-0.11221700	-2.30124300
H	4.28734400	-0.48677800	-2.85744200
H	2.60913600	0.06562200	-3.01387700
H	3.68890900	0.85823400	-1.87130300

R1

Sum of electronic and thermal Free Energies= -854.835556

Si	0.13499200	1.17796200	0.25267000
C	0.13326000	2.60684000	-0.99294000
H	0.10069100	2.23974000	-2.02352000
H	-0.72088800	3.27661800	-0.84478200
H	1.04343400	3.20637400	-0.88516900
C	0.15212200	1.88905100	2.01498600
H	-0.73844200	2.50076400	2.19626900
H	0.16745400	1.08999400	2.76285400
H	1.03227800	2.52060200	2.18016700
C	-1.41983600	0.11327800	0.01719300
C	-1.43809100	-1.23728500	0.41566000
C	-2.60059800	0.64328300	-0.53448500
C	-2.58601200	-2.01919700	0.27856800
H	-0.53969600	-1.68559800	0.83310600
C	-3.75106600	-0.13449000	-0.67652700
H	-2.62721000	1.67942800	-0.86290700
C	-3.74635600	-1.46898100	-0.26835900
H	-2.57388000	-3.05900700	0.59445700
H	-4.64939200	0.29995400	-1.10702900
H	-4.64016900	-2.07682900	-0.37868000
B	1.76304700	-0.00463300	-0.02492900
O	2.04015500	-1.10084900	0.75976700
O	2.69570800	0.19540800	-1.01184400
C	3.23819700	-1.73016800	0.26221600
C	3.70816500	-0.82443200	-0.90196900
H	4.67209500	-0.34532500	-0.70177600
H	3.77870000	-1.35941500	-1.85393800
H	3.96975700	-1.79334100	1.07359800
H	2.99452100	-2.74613000	-0.06484100

TS1A

Sum of electronic and thermal Free Energies= -4108.906099

Cu	0.02397100	-0.24689000	-0.21959600
C	0.53387700	-2.08371100	2.58444200
O	-0.27236700	-1.54434700	3.31910800
O	0.84169600	-1.52683900	1.39482200
C	1.23757100	-3.37022400	2.95132300
H	0.88853900	-4.17006300	2.29126500
H	2.31482900	-3.26906800	2.80623700
H	1.00225200	-3.62267700	3.98513000
C	0.19588900	3.40167800	-0.73311800
C	-0.10594800	2.72355300	1.93431100
C	0.86169700	3.88305500	1.60703500

C	0.42157300	4.53317200	0.29086200
H	1.18381600	3.03445300	-1.03722000
H	-1.05363700	3.14316300	2.29479600
H	0.89147000	4.60102400	2.43499100
H	1.87701900	3.48276500	1.49252000
H	-0.50723600	5.10081100	0.43849100
H	1.16817500	5.24524800	-0.08142400
P	-0.47961000	1.93530900	0.25850700
C	-2.33075500	2.01068300	0.08094800
C	-3.05860300	0.85638100	-0.30498300
C	-3.02810200	3.21767900	0.26591200
C	-4.43704100	0.97458600	-0.55279800
C	-4.39840200	3.31141700	0.03414900
H	-2.49102600	4.10351300	0.58957700
C	-5.10416300	2.18657500	-0.39445300
H	-5.00273200	0.10284000	-0.86592500
H	-4.90993200	4.25857800	0.17957600
H	-6.17043500	2.24933200	-0.59204000
C	-2.85154400	-1.83476600	1.02656900
C	-3.02052500	-1.78783400	-1.75845300
C	-2.98242500	-3.20175400	0.31854300
H	-2.06091400	-1.86434800	1.77947200
C	-3.70039200	-2.97470400	-1.02431700
H	-3.76729000	-1.16538000	-2.26207100
H	-1.98010900	-3.60724500	0.13784400
H	-3.52003100	-3.91770200	0.95182400
H	-3.67827700	-3.87626600	-1.64726000
H	-4.75686400	-2.74381800	-0.84279800
P	-2.19059200	-0.77745600	-0.39172100
C	-0.56919500	3.81966700	-1.99054400
H	-0.69619700	2.98782300	-2.68981800
H	-1.56319900	4.20958300	-1.75547200
H	-0.01635300	4.60798600	-2.51440100
C	0.44610700	1.74740000	2.97576400
H	0.63321500	2.27516500	3.91871800
H	-0.23313200	0.91606700	3.17764100
H	1.39411700	1.31706900	2.63713700
C	-4.14062200	-1.37771500	1.71727600
H	-4.03564800	-0.37961900	2.15061800
H	-5.00357300	-1.35918500	1.04496000
H	-4.37325200	-2.07104000	2.53403100
C	-1.98401900	-2.24310100	-2.79701900
H	-2.46106500	-2.86952100	-3.56004600
H	-1.52984700	-1.38667800	-3.30480300
H	-1.17838600	-2.81741500	-2.32864700
B	1.42768400	-2.19273100	0.19591700
O	2.75497300	-2.69649700	0.39752600
O	0.60915500	-3.26535000	-0.30158500
C	2.81002200	-4.05842000	-0.01182200
C	1.45936900	-4.32889600	-0.71446200
H	1.56792900	-4.33040100	-1.80753900
H	1.01871700	-5.28887300	-0.41930800
H	3.66537800	-4.22208100	-0.67712100
H	2.94122500	-4.70094900	0.87060600
Si	2.10204000	-0.57619400	-1.44990600
C	3.32516200	0.67993200	-0.68433100
C	3.66006100	1.88369300	-1.33411700
C	3.92562700	0.43976400	0.56800800
C	4.53955900	2.80882400	-0.76314000
H	3.23391100	2.10700800	-2.30951000
C	4.80717900	1.35731200	1.14342200
H	3.70450500	-0.48447100	1.09427200
C	5.11444300	2.54918600	0.48185800
H	4.77890100	3.72805100	-1.29267200
H	5.25613500	1.14208300	2.11003300
H	5.79910700	3.26467500	0.92974900
C	3.14933800	-1.79214000	-2.49068900
H	2.52253800	-2.54495200	-2.98221700
H	3.66512000	-1.23145600	-3.27909800
H	3.90657400	-2.30286400	-1.89317000
C	1.19670100	0.32881700	-2.89785100
H	0.53600800	-0.38208600	-3.40592400
H	0.59597200	1.19793800	-2.62151600
H	1.93230500	0.65899200	-3.64280300

B(pin)-OAc

Sum of electronic and thermal Free Energies= -482.451730

O	0.84933600	-0.83895400	0.06797900
B	-0.43137400	-0.36174500	0.01633000
O	-0.79155700	0.90889400	-0.36935600
O	-1.48610300	-1.17488500	0.33453000
C	-2.22791800	0.94756700	-0.41611500
C	-2.68100200	-0.38927300	0.22965200
H	-3.10077000	-0.24457400	1.23144700
H	-3.41528900	-0.92369900	-0.37980100
H	-2.58455900	1.82587500	0.12941300
H	-2.54400200	1.03397600	-1.46128300
C	2.04041300	-0.14936400	-0.03510900
O	2.98166000	-0.68297700	-0.55613000

C	2.06489800	1.21881700	0.60335100
H	1.36063900	1.88601300	0.10066900
H	1.75984500	1.14899800	1.65241000
H	3.07597400	1.61904000	0.53864100

3A

Sum of electronic and thermal Free Energies= -3626.504054

Cu	0.13390800	-0.88771600	-0.11326000
C	1.06913000	2.34678200	-1.25262900
C	0.72933600	2.44936300	1.48659100
C	1.94132600	3.20660000	0.89850800
C	1.60575900	3.60638200	-0.54392000
H	1.92283700	1.67765500	-1.42310900
H	-0.05776000	3.17517400	1.72709700
H	2.19285600	4.07298000	1.52169500
H	2.81717100	2.54554500	0.89853800
H	0.84396700	4.39808700	-0.55112800
H	2.48124700	4.00570200	-1.07020300
P	0.08483900	1.39894000	0.05480600
C	-1.69623300	1.89918100	-0.14662300
C	-2.67465400	0.87760400	-0.23312800
C	-2.10443900	3.24037000	-0.24785900
C	-4.01399100	1.23666900	-0.46109200
C	-3.43881000	3.57927600	-0.46203200
H	-1.36729800	4.03320100	-0.16461000
C	-4.39698100	2.57090900	-0.57973100
H	-4.77379800	0.46516400	-0.54095800
H	-3.72844400	4.62316000	-0.54277400
H	-5.43914400	2.82276300	-0.75457600
C	-2.81247900	-1.47020200	1.64923100
C	-3.34695200	-1.90828900	-1.05644000
C	-3.60480100	-2.74750100	1.28184300
H	-1.93689100	-1.74016900	2.24914400
C	-4.35269500	-2.49450900	-0.03759400
H	-3.84996400	-1.24064500	-1.76350800
H	-2.90993600	-3.58548900	1.15305100
H	-4.28922000	-3.02500800	2.09214200
H	-4.81142200	-3.41347400	-0.42172600
H	-5.16977700	-1.78333400	0.13594700
P	-2.13130900	-0.89201500	-0.02803700
C	0.37502600	2.58612300	-2.59374500
H	0.04561600	1.64669700	-3.04951700
H	-0.50076600	3.23356200	-2.49276200
H	1.06793700	3.06674600	-3.29382300
C	1.06138100	1.63203400	2.73838700
H	1.44826300	2.28412700	3.53048500
H	0.17783900	1.11990600	3.13362700
H	1.82284400	0.87626800	2.52084800
C	-3.63789700	-0.44932300	2.43977600
H	-3.07420900	0.46906700	2.62738200
H	-4.55848900	-0.16660500	1.92154000
H	-3.91780800	-0.87607200	3.41000000
C	-2.60651700	-2.99311300	-1.85417300
H	-3.31961600	-3.58624900	-2.43864200
H	-1.87914000	-2.55601200	-2.54433600
H	-2.05591000	-3.67497400	-1.19818400
Si	1.99003100	-2.23235700	-0.32271900
C	3.56791200	-1.16773000	-0.05378800
C	4.18325800	-0.47566300	-1.11617400
C	4.10516400	-0.95225300	1.23100100
C	5.26450400	0.38571900	-0.91226900
H	3.81344600	-0.61693100	-2.13005700
C	5.18621300	-0.09382600	1.44777600
H	3.67261400	-1.47122700	2.08439800
C	5.77082300	0.58356500	0.37472400
H	5.71814400	0.89726100	-1.75851400
H	5.57802300	0.04202900	2.45349500
H	6.61385700	1.24987900	0.53817000
C	2.13998100	-3.69294300	0.91520000
H	2.05986500	-3.36911000	1.95918800
H	1.32557900	-4.40620500	0.73915700
H	3.08736100	-4.23556500	0.80627000
C	2.21423700	-3.06180600	-2.04033800
H	1.39003700	-3.76384200	-2.21520100
H	2.19427300	-2.33753600	-2.86277600
H	3.15349600	-3.62412800	-2.11371300

R2

Sum of electronic and thermal Free Energies= -311.90039

C	-2.21059600	0.00012400	-0.13058200
C	-1.37856800	1.27065400	-0.36247900
C	-0.10659400	1.28057600	0.50721600
C	-0.10676800	-1.28066900	0.50715100
C	-1.37877100	-1.27053800	-0.36250300
H	0.51271400	2.15408600	0.28426900
H	-1.08763100	1.32674800	-1.41987000
H	-1.97905300	2.16367700	-0.15120200
H	-2.59031200	0.00014500	0.90151700
H	-3.09049900	0.00020000	-0.78492500
H	0.51241500	-2.15425000	0.28413500

H	-0.40269800	-1.35561800	1.56484800
H	-1.08788800	-1.32668800	-1.41990500
H	-1.97938800	-2.16346300	-0.15119000
H	-0.40254500	1.35549900	1.56490900
C	0.68979200	-0.00009900	0.31513000
C	1.95258500	-0.00017400	-0.03447800
C	3.21553300	-0.00000800	-0.37634800
H	3.52590600	0.00006300	-1.41958900
H	4.00930400	0.00041000	0.36836300

TS2A

Sum of electronic and thermal Free Energies= -3938.361450

C	-2.04266100	-1.44434300	2.41766400
C	-0.82597200	-3.37206400	0.89340900
C	-0.36190000	-3.34368200	2.36206400
C	-1.49246900	-2.69058400	3.17127200
H	-1.58297500	-0.53511400	2.81688400
H	-1.71919100	-4.00965700	0.84695400
H	-0.13689900	-4.35457100	2.72215900
H	0.56294600	-2.75846100	2.44929900
H	-2.30622000	-3.41838200	3.28497500
H	-1.16702600	-2.41975100	4.18115900
P	-1.33727700	-1.58336200	0.65901200
C	-2.75668300	-1.58506300	-0.53102100
C	-3.38310100	-0.35838100	-0.87627300
C	-3.20113600	-2.77005500	-1.14057400
C	-4.46520800	-0.38236600	-1.76986900
C	-4.26053500	-2.76593200	-2.04791400
H	-2.72708700	-3.71644200	-0.90457600
C	-4.90632200	-1.56965200	-2.35399800
H	-4.97464000	0.54293200	-2.02091300
H	-4.58610100	-3.69772800	-2.50183000
H	-5.74259300	-1.55714400	-3.04720700
C	-2.05269600	2.26771300	-1.50765000
C	-4.30303000	2.27941400	0.13265400
C	-2.76059600	3.62502600	-1.29493100
H	-0.98355100	2.37482100	-1.29469100
C	-4.23925500	3.34561000	-0.98490300
H	-5.19165900	1.64965900	0.02062000
H	-2.30251200	4.15333300	-0.44995200
H	-2.64020000	4.27048700	-2.17346300
H	-4.76835100	4.26001500	-0.68920200
H	-4.73756600	2.97396400	-1.88852500
P	-2.74420100	1.19804500	-0.08062200
C	-3.56309700	-1.32440700	2.55098700
H	-3.94582900	-0.41630300	2.07934400
H	-4.07708800	-2.18063500	2.10128100
H	-3.83813900	-1.28909800	3.61209900
C	0.21760200	-3.88250300	-0.10079000
H	0.54079600	-4.89611500	0.16370800
H	-0.17861000	-3.91798900	-1.12122900
H	1.10191200	-3.23792100	-0.11560800
C	-2.20922400	1.74047700	-2.93909600
H	-1.79893400	0.73408200	-3.05613900
H	-3.25509900	1.69927200	-3.25566700
H	-1.68002600	2.40263500	-3.63517600
C	-4.32113000	2.90198200	1.53866900
H	-5.21053900	3.53005100	1.66943600
H	-4.33414900	2.13345800	2.31765100
H	-3.43956000	3.52691600	1.71703300
Cu	0.38515800	-0.13961800	0.33455800
C	3.80213200	-1.31509300	-0.00735900
C	4.52469100	-2.66734300	0.14419200
C	4.21279500	-1.40360900	-2.53700200
C	5.56434300	-2.87936000	-0.96684500
C	4.93056700	-2.75562400	-2.36059600
H	4.51789000	-0.49878900	0.15973400
H	3.78676300	-3.48066800	0.10902900
H	6.36104600	-2.12899800	-0.86369600
H	4.95968600	-0.59642300	-2.51617500
H	5.69330400	-2.87122100	-3.13999600
H	3.01113000	-1.19204900	0.73727900
H	5.00271200	-2.71825600	1.12956700
H	3.70625000	-1.35006500	-3.50493500
H	6.04281700	-3.85978400	-0.85583200
H	4.20512500	-3.56777000	-2.50468700
C	3.22788600	-1.15833800	-1.40275100
C	1.98043700	-0.84546900	-1.64946700
C	0.74228000	-0.56013400	-2.01093000
H	0.02369200	-1.34062900	-2.25138900
H	0.45429400	0.46197600	-2.25192500
Si	1.49211500	1.43172900	1.60208100
C	2.24523800	0.72596300	3.22386900
H	1.44142900	0.32335500	3.85269800
H	2.95363500	-0.09206200	3.04691400
H	2.76531800	1.49380200	3.81091000
C	0.34939100	2.84409200	2.23303200
H	-0.06857600	3.43255400	1.40789700
H	-0.49764600	2.42466200	2.78897900

H	0.88161600	3.53695300	2.89666700
C	2.93291200	2.35447900	0.72757500
C	4.28116100	2.22672300	1.11191100
C	2.66992000	3.19561000	-0.37149400
C	5.30892600	2.89285900	0.43677800
H	4.53831400	1.60146100	1.96380200
C	3.68488700	3.87165700	-1.04946400
H	1.64120700	3.32758100	-0.70540400
C	5.01488300	3.71944400	-0.64845900
H	6.33945800	2.77231800	0.76380400
H	3.44166000	4.51692700	-1.89073900
H	5.81051500	4.24100200	-1.17423800

4A

Sum of electronic and thermal Free Energies= -3938.370517

C	-2.17532400	-2.64625100	0.90039200
C	-1.59754100	-3.07177100	-1.75720000
C	-1.13802600	-4.19633700	-0.81017500
C	-2.02771500	-4.12300300	0.43796900
H	-1.42619100	-2.42307500	1.66442600
H	-2.62602300	-3.30540600	-2.06026100
H	-1.21054300	-5.17278400	-1.30350700
H	-0.08601600	-4.04931200	-0.53938900
H	-3.02276400	-4.51310200	0.18684500
H	-1.63803300	-4.74439300	1.25112300
P	-1.63092000	-1.60222700	-0.59014000
C	-3.08815600	-0.55285000	-1.06463300
C	-3.35143600	0.64404000	-0.34770200
C	-3.93720200	-0.91000600	-2.12393900
C	-4.49506700	1.38904100	-0.67622600
C	-5.04889900	-0.13540500	-2.45551900
H	-3.74265200	-1.80611100	-2.70255400
C	-5.34125200	1.00993400	-1.71762800
H	-4.72891500	2.28523400	-0.11036400
H	-5.68963500	-0.43653100	-3.27947800
H	-6.21592800	1.60907600	-1.95411600
C	-1.50710800	2.87095600	0.57153600
C	-3.30710200	1.77794500	2.40070800
C	-1.72511900	3.64275300	1.89274800
H	-0.43750900	2.72707000	0.38950900
C	-3.13774700	3.31569900	2.40286600
H	-4.34161400	1.50092000	2.17252100
H	-0.98334700	3.32633600	2.63649300
H	-1.58246600	4.71989700	1.74340900
H	-3.31344900	3.73035800	3.40299600
H	-3.87949600	3.77396000	1.73776400
P	-2.17352900	1.13340800	1.00527600
C	-3.56428800	-2.36408400	1.47813100
H	-3.65332800	-1.34425300	1.85968000
H	-4.35126100	-2.51291000	0.73154700
H	-3.76034400	-3.04822600	2.31245000
C	-0.73065400	-2.89474100	-3.00478300
H	-0.72591000	-3.81425300	-3.60139200
H	-1.09827100	-2.08539200	-3.64352400
H	0.30685100	-2.66621600	-2.73882300
C	-2.09399000	3.61057900	-0.63752300
H	-2.04636300	3.01646200	-1.55352100
H	-3.13847200	3.89889300	-0.48913100
H	-1.52189000	4.53005500	-0.81038200
C	-2.91308600	1.14411200	3.74472000
H	-3.56295500	1.51201500	4.54774300
H	-2.99674600	0.05339600	3.71784500
H	-1.87873300	1.38221600	4.01496900
Cu	0.37016300	-0.44147800	-0.43096900
C	3.02410500	2.14126500	0.05902900
C	4.50021500	2.22887400	-0.37851200
C	2.31706200	3.15467100	-2.16023600
C	4.72809000	3.36636100	-1.38384900
C	3.79361100	3.23468500	-2.59526300
H	2.77161600	3.05512400	0.62127900
H	4.78980200	1.27214200	-0.82957400
H	4.54440600	4.33255500	-0.89060400
H	2.03711600	4.11679700	-1.70187100
H	3.93192200	4.07862000	-3.28278000
H	2.87684100	1.29582100	0.73000800
H	5.13672400	2.36254400	0.50356000
H	1.66229300	3.00473500	-3.02331300
H	5.77438500	3.37940400	-1.71277900
H	4.04899800	2.32453100	-3.15438100
C	2.10058200	2.04922100	-1.13285600
C	1.18310300	1.11490900	-1.35522300
C	0.11884500	0.68677000	-2.11830400
H	0.27509700	0.03412600	-2.97796300
H	-0.82650600	1.22673500	-2.12090900
Si	1.73791800	-1.25458400	1.29879000
C	1.46448700	-3.09194700	1.81429800
H	0.44743500	-3.29771300	2.16535300
H	1.67721700	-3.77539300	0.98406700
H	2.15000000	-3.35676400	2.62898400

C	1.51739200	-0.29169800	2.94212100
H	1.76635000	0.77054100	2.84239300
H	0.46745700	-0.34778100	3.25269300
H	2.12300900	-0.70593400	3.75811700
C	3.62158300	-1.28650800	0.91897800
C	4.60048100	-0.86737400	1.83918700
C	4.08603000	-1.80960800	-0.30315300
C	5.96663900	-0.96348900	1.55785900
H	4.29525000	-0.45642100	2.79867500
C	5.44737800	-1.91733100	-0.59356500
H	3.36557400	-2.14147800	-1.04979700
C	6.39603500	-1.49109900	0.33932600
H	6.69594000	-0.62838200	2.29185400
H	5.76941100	-2.33009500	-1.54685200
H	7.45727300	-1.56819400	0.11749500

TS3A

Sum of electronic and thermal Free Energies= -3938.345626

C	-2.54747500	-2.67947200	1.12800100
C	-2.77959900	-2.61664100	-1.62132700
C	-2.94935600	-3.99176700	-0.93505300
C	-3.43628800	-3.77113000	0.50346300
H	-1.56418100	-3.12370000	1.32597500
H	-3.76976100	-2.24546000	-1.90813500
H	-3.63206600	-4.62850700	-1.50992300
H	-1.97975700	-4.50628300	-0.91622700
H	-4.48485100	-3.44651400	0.50575500
H	-3.39406800	-4.69526900	1.09284200
P	-2.16844600	-1.44922800	-0.25849300
C	-3.51451900	-0.17000200	-0.13031000
C	-3.18035800	1.17856000	0.14190900
C	-4.87038100	-0.52289000	-0.24652900
C	-4.21981000	2.10776300	0.32107700
C	-5.88604100	0.41789300	-0.08859000
H	-5.14704100	-1.55086200	-0.45412900
C	-5.55871300	1.74083500	0.20401100
H	-3.98247600	3.13828200	0.56069000
H	-6.92495500	0.11527100	-0.18347700
H	-6.33923700	2.48365400	0.34187700
C	-1.02805700	3.10876600	-0.81939300
C	-1.41679500	2.68889200	1.91166400
C	-0.61357700	4.25776000	0.13399300
H	-0.15306900	2.78069300	-1.38964200
C	-1.43585600	4.15825800	1.42912800
H	-2.33891100	2.44955800	2.45113500
H	0.45166700	4.16517800	0.37415300
H	-0.74083000	5.23224700	-0.35232600
H	-1.04832400	4.83201900	2.20341000
H	-2.46736000	4.47356300	1.23072800
P	-1.39069600	1.64165200	0.32654000
C	-3.07047300	-2.07500700	2.43125300
H	-2.38877000	-1.31228900	2.82174700
H	-4.05106000	-1.60943700	2.29480900
H	-3.17002300	-2.85270500	3.19702300
C	-1.90928200	-2.66220400	-2.87850500
H	-2.35921900	-3.33268600	-3.62049900
H	-1.80337600	-1.67313700	-3.33097600
H	-0.90521800	-3.03401700	-2.65587400
C	-2.12048500	3.49227200	-1.82402500
H	-2.45102800	2.62869700	-2.40876600
H	-3.00247500	3.92492900	-1.34419200
H	-1.72733800	4.23834700	-2.52437200
C	-0.22327000	2.36949100	2.82208300
H	-0.26379500	2.98180900	3.73081600
H	-0.22341800	1.31769900	3.12329900
H	0.73209400	2.56605600	2.32717200
Cu	-0.25066700	-0.28697000	-0.35883800
C	2.80910400	1.69327300	0.40715600
C	4.31520700	1.99322700	0.54290700
C	3.03801500	1.84762300	-2.13666000
C	4.83933500	2.82010500	-0.63770900
C	4.54629800	2.10520100	-1.96250100
H	2.26275900	2.63712200	0.58399800
H	4.86590500	1.04796800	0.59021500
H	4.35684500	3.80955000	-0.64262000
H	2.54565100	2.82607000	-2.28569600
H	4.92140500	2.69284200	-2.81031400
H	2.48149500	1.00984500	1.19946600
H	4.49986900	2.51627300	1.49007700
H	2.84381300	1.26852500	-3.04468900
H	5.91615800	2.99906900	-0.52744200
H	5.07979200	1.14615900	-1.97573700
C	2.40708600	1.14765800	-0.94228500
C	1.49242700	0.16784200	-1.15177300
C	0.63961800	-0.11561000	-2.24685100
H	0.63147000	-1.10402800	-2.70044700
H	0.38284900	0.69727000	-2.92482600
Si	1.61590200	-1.59280300	0.54390100
C	1.25380000	-3.25786900	-0.33322200

H	0.20479200	-3.55862300	-0.24916500
H	1.49492000	-3.19689000	-1.39996900
H	1.86992100	-4.05597300	0.09749300
C	1.11760800	-1.80996900	2.38957800
H	1.32717800	-0.90316800	2.96749900
H	0.04815100	-2.01544600	2.49203400
H	1.66575600	-2.63876200	2.85599100
C	3.52538800	-1.57866000	0.58720300
C	4.25517800	-1.51309200	1.78703800
C	4.26530200	-1.73297700	-0.60160800
C	5.65111400	-1.59566600	1.80507700
H	3.73307300	-1.39348100	2.73244500
C	5.65767000	-1.82646800	-0.59413100
H	3.74227000	-1.77816700	-1.55342600
C	6.35788600	-1.75511300	0.61307500
H	6.18437200	-1.53751800	2.75082900
H	6.19751600	-1.95256800	-1.52945600
H	7.44251800	-1.82347400	0.62297800

5A

Sum of electronic and thermal Free Energies= -3938.406687

C	2.33406700	-3.16874800	-0.54252300
C	3.28649400	-2.41820300	1.94123200
C	2.98718900	-3.91768700	1.72714300
C	3.14439100	-4.22678400	0.23292200
H	1.27179300	-3.41832400	-0.42636900
H	4.36930200	-2.26350400	1.85771400
H	3.64126500	-4.53700500	2.35207700
H	1.95528300	-4.12851200	2.03807000
H	4.20375400	-4.17243000	-0.05203600
H	2.80299300	-5.23927500	-0.01457400
P	2.48753300	-1.56590500	0.45701500
C	3.87164500	-0.59226000	-0.31621100
C	3.62680200	0.75234600	-0.68786500
C	5.13376600	-1.15275800	-0.57915000
C	4.64149800	1.46759600	-1.34739200
C	6.13104600	-0.42540700	-1.22501600
H	5.34095600	-2.17705200	-0.28423500
C	5.87903200	0.88934200	-1.62033900
H	4.46543200	2.49457800	-1.65219000
H	7.09541000	-0.88364300	-1.42523100
H	6.64535100	1.46406600	-2.13282200
C	2.27750000	2.85702800	0.99517500
C	1.63359800	2.70173300	-1.71892800
C	1.60985100	4.09658100	0.35460600
H	1.70889400	2.55303800	1.88063600
C	1.94305600	4.10481000	-1.14578400
H	2.31149500	2.46226300	-2.54477500
H	0.52363800	4.03502600	0.48638700
H	1.94026400	5.01604100	0.85241500
H	1.37989300	4.88048200	-1.67852400
H	3.00660800	4.33751100	-1.28194100
P	1.96520600	1.49611600	-0.29733600
C	2.63420800	-3.07359100	-2.03878400
H	2.00193200	-2.32580700	-2.52812000
H	3.67699300	-2.80526400	-2.23057700
H	2.44002300	-4.03733900	-2.52324100
C	2.80826700	-1.87416300	3.28992700
H	3.25877400	-2.43926200	4.11450000
H	3.08326400	-0.82252800	3.42072500
H	1.71965200	-1.94631200	3.38154900
C	3.72990400	3.09715600	1.42116100
H	4.19957400	2.18315900	1.79627600
H	4.35060700	3.47039000	0.60189200
H	3.75719500	3.84267300	2.22456000
C	0.18743600	2.55654400	-2.21753800
H	-0.02141800	3.29767300	-2.99804700
H	0.01131100	1.56316900	-2.64061400
H	-0.54040600	2.69215700	-1.41205500
Cu	0.70845600	-0.19646300	0.64468600
C	-3.80011800	1.82026800	-0.61389300
C	-5.01692100	2.49138400	0.05856600
C	-2.30510700	2.65823700	1.21617500
C	-4.59945400	3.70511300	0.89971300
C	-3.50788200	3.33077600	1.91156800
H	-3.38728200	2.53181900	-1.35107900
H	-5.51382000	1.75294100	0.70104300
H	-4.21540900	4.49144200	0.23235200
H	-1.84465100	3.41057600	0.55022600
H	-3.17700100	4.22123700	2.46253300
H	-4.14302300	0.95348600	-1.18425300
H	-5.74882000	2.79058500	-0.70286400
H	-1.54571900	2.39656300	1.95608200
H	-5.46959500	4.13272400	1.41407000
H	-3.92186700	2.63468800	2.65366600
C	-2.72219000	1.45345500	0.39152400
C	-2.18401300	0.20976500	0.54297300
C	-1.07809200	-0.14298900	1.49499300
H	-1.27233400	-1.12312400	1.94757300

H	-1.03251000	0.56202100	2.33619700
Si	-2.72673400	-1.23778600	-0.56314400
C	-1.90494200	-2.85261800	0.01046900
H	-0.82412400	-2.71617300	0.11563600
H	-2.29226100	-3.18084700	0.98037700
H	-2.09141900	-3.65520400	-0.71205600
C	-2.19465000	-0.97925000	-2.37165900
H	-2.64602400	-0.08708400	-2.81610700
H	-1.10596200	-0.85527800	-2.41619000
H	-2.44913800	-1.83809000	-3.00350400
C	-4.60391000	-1.54467600	-0.49063200
C	-5.32185700	-2.06834100	-1.58120000
C	-5.31803400	-1.31546100	0.70114000
C	-6.68672400	-2.35211200	-1.49014500
H	-4.81302400	-2.25568900	-2.52411700
C	-6.68120500	-1.59964400	0.80210000
H	-4.79894900	-0.89325900	1.55831600
C	-7.37024100	-2.11967900	-0.29573300
H	-7.21623800	-2.75230800	-2.35123400
H	-7.20699500	-1.41148800	1.73485800
H	-8.43218300	-2.33881900	-0.22161400

CO_2

Sum of electronic and thermal Free Energies= -188.590066

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16915600
O	0.00000000	0.00000000	-1.16915600

TS4A

Sum of electronic and thermal Free Energies= -4126.966724

C	1.50584500	-2.81016800	-1.42589900
C	2.22562500	-3.10221000	1.22455500
C	1.47150200	-4.28139500	0.57617700
C	1.76264400	-4.24848700	-0.93113000
H	0.41912700	-2.66795900	-1.48186400
H	3.29747000	-3.33566800	1.20919200
H	1.76778300	-5.23184600	1.03556100
H	0.39269300	-4.16804200	0.74624300
H	2.80936100	-4.52755600	-1.11357000
H	1.14558000	-4.96676000	-1.48424100
P	1.97032500	-1.67239900	0.01429000
C	3.70732700	-1.07804700	-0.27840500
C	4.00598900	0.29364400	-0.09960900
C	4.73368700	-1.95213500	-0.67729600
C	5.31485800	0.73965900	-0.35445200
C	6.02478300	-1.49280900	-0.92520100
H	4.52126000	-3.00925100	-0.80375800
C	6.31516100	-0.13685000	-0.76767900
H	5.56129800	1.78927100	-0.22939900
H	6.79746900	-2.18712900	-1.24272500
H	7.31707300	0.23589600	-0.96089800
C	3.07007100	2.00481900	2.19656900
C	3.10649100	3.09820300	-0.37024700
C	3.07337300	3.54819500	2.08448500
H	2.22562500	1.68529900	2.81689800
C	3.74802800	3.93760600	0.75898100
H	3.82575900	2.90078700	-1.17099300
H	2.04092000	3.91755000	2.08860800
H	3.57490200	4.00055500	2.94826400
H	3.64803700	5.01100400	0.55734500
H	4.82297900	3.72802900	0.82214100
P	2.64506300	1.44498900	0.42982800
C	2.08388900	-2.46076100	-2.79813900
H	1.82729800	-1.43582300	-3.07949200
H	3.17256500	-2.56021400	-2.82461800
H	1.66771200	-3.13088300	-3.55906700
C	1.81747000	-2.79160900	2.66586400
H	1.97495600	-3.66684500	3.30715200
H	2.40933800	-1.96855500	3.08019900
H	0.76246300	-2.51022800	2.73423700
C	4.35308200	1.43672300	2.81382700
H	4.34847300	0.34262100	2.82144400
H	5.25189400	1.75419600	2.27781800
H	4.44543100	1.77875000	3.85138000
C	1.87228100	3.77055100	-0.98800000
H	2.15767800	4.70841500	-1.47887300
H	1.39701900	3.12367000	-1.72998500
H	1.11799000	4.00755700	-0.23049500
Cu	0.72348900	0.19113000	0.35124000
Si	-3.02298800	-1.25594300	0.31840500
C	-2.94745600	-2.39648700	-1.19453500
H	-1.91578400	-2.73678900	-1.34127700
H	-3.56115400	-3.29125700	-1.03828200
H	-3.25958800	-1.91821400	-2.12532800
C	-2.24228700	-2.22539700	1.75058200
H	-1.17026100	-2.37222300	1.58832800
H	-2.37188900	-1.72771900	2.71655100
H	-2.71451200	-3.21173300	1.82355900
C	-4.82941900	-0.94022300	0.81634800
C	-5.91775900	-1.49676900	0.12202800

C	-5.11931300	-0.14890800	1.94517100
C	-7.23527400	-1.27634000	0.53190000
H	-5.74064500	-2.11049400	-0.75772600
C	-6.43204500	0.07587200	2.36166700
H	-4.30610600	0.30574600	2.50759200
C	-7.49562200	-0.48906200	1.65392900
H	-8.05700800	-1.71819400	-0.02579000
H	-6.62620300	0.69208900	3.23579100
H	-8.51924500	-0.31538300	1.97473300
C	-3.71706200	1.13285400	-1.79836600
C	-4.74819800	2.16576500	-1.28691400
C	-1.84500800	2.65059100	-1.10852900
C	-4.18382200	3.59425200	-1.29751200
C	-2.84707400	3.67972800	-0.54493600
H	-3.52550900	1.31918500	-2.86286000
H	-5.04427100	1.89784100	-0.26540800
H	-4.02549900	3.91332400	-2.33834700
H	-1.66264000	2.90751300	-2.16313000
H	-2.43366100	4.69468900	-0.61742500
H	-4.15354300	0.13265100	-1.74175700
H	-5.65622600	2.11582300	-1.90176900
H	-0.88133300	2.71923200	-0.60131400
H	-4.91213300	4.29251000	-0.86588700
H	-3.01116500	3.47708700	0.52203900
C	-2.41413200	1.23792100	-1.02133100
C	-2.10969800	0.40831900	0.06580300
C	-1.09384600	0.72763600	1.05244800
H	-1.20968700	0.17205900	1.98607800
H	-1.01570500	1.79634000	1.27433800
C	-0.90980600	0.24003100	-2.47906300
O	-1.59876000	-0.12395300	-3.37875100
O	0.16847200	0.41300100	-1.97539700

TS5A

Sum of electronic and thermal Free Energies= -4126.955902

C	2.54744200	-2.53157400	-1.78725700
C	2.76908700	-3.05976100	0.91765200
C	2.48858500	-4.26098900	-0.01130600
C	3.06014300	-3.93205700	-1.39819500
H	1.48188100	-2.61376800	-2.03668100
H	3.84018400	-3.05312200	1.15574300
H	2.91503600	-5.17929900	0.40911300
H	1.40477800	-4.41767000	-0.08967900
H	4.15830700	-3.94371900	-1.36438600
H	2.76067300	-4.67357700	-2.14821100
P	2.46981000	-1.55208900	-0.17801400
C	4.03202700	-0.56543600	-0.01082400
C	3.97176800	0.80568000	0.34236200
C	5.28874900	-1.15050000	-0.24614500
C	5.16890900	1.53941300	0.41637700
C	6.46473500	-0.41013400	-0.15817300
H	5.34893300	-2.20153400	-0.51003500
C	6.40354500	0.94510100	0.16903100
H	5.13834100	2.59409900	0.67097700
H	7.42185400	-0.88613900	-0.35062600
H	7.31267000	1.53593600	0.23336400
C	2.27475300	2.15009300	2.47252800
C	2.50489900	3.34879800	-0.04400900
C	1.95191900	3.66175600	2.37224000
H	1.42327700	1.62168100	2.91510400
C	2.73688500	4.25325100	1.18944800
H	3.37403500	3.35739100	-0.70908600
H	0.87796300	3.79654100	2.19805800
H	2.18546800	4.17100200	3.31447400
H	2.43069600	5.28518000	0.98113000
H	3.80446100	4.28589200	1.44014900
P	2.32585800	1.60453300	0.65524900
C	3.24236400	-1.85517600	-2.96971800
H	2.75322200	-0.90790800	-3.21444400
H	4.30237600	-1.66357400	-2.77724000
H	3.17331400	-2.50032600	-3.85281600
C	1.97580400	-3.06393300	2.22591500
H	2.19762600	-3.96843300	2.80414100
H	2.23065100	-2.20187900	2.85151900
H	0.89796300	-3.03750200	2.04131900
C	3.51255100	1.84378200	3.32370500
H	3.76182400	0.77865000	3.30845000
H	4.39705300	2.39132500	2.98717100
H	3.32156800	2.12835500	4.36481200
C	1.26284000	3.74156400	-0.85954500
H	1.40379700	4.73347100	-1.30410600
H	1.06916500	3.02250700	-1.66024000
H	0.36571500	3.78437900	-0.23183100
Cu	0.83466700	0.02771400	-0.11164800
Si	-3.12297000	-1.42090700	0.15811300
C	-3.58864300	-2.76238600	-1.09666700
H	-2.75292800	-2.87950900	-1.79308300
H	-3.76263700	-3.72661400	-0.60452900
H	-4.48178300	-2.51771000	-1.67804200

C	-1.72260100	-2.14679000	1.21568600
H	-0.84781400	-2.34120200	0.58737600
H	-1.42703500	-1.48606600	2.03772800
H	-2.04579500	-3.09593700	1.65807900
C	-4.58109400	-1.09786800	1.34169800
C	-5.44677800	-2.13628600	1.73317700
C	-4.80266400	0.17197300	1.90677600
C	-6.48236600	-1.92136700	2.64505500
H	-5.31674400	-3.13294100	1.31694600
C	-5.83411200	0.39583300	2.82145400
H	-4.16394700	1.00197200	1.61415600
C	-6.67798200	-0.65238600	3.19330200
H	-7.13813700	-2.74199100	2.92510900
H	-5.98250700	1.38820300	3.24005500
H	-7.48414100	-0.48116600	3.90182600
C	-4.78546100	0.48059400	-1.84019700
C	-5.75175400	1.66850900	-1.63966500
C	-2.91893200	2.07446800	-2.34377700
C	-5.31900100	2.89901300	-2.44738000
C	-3.86396700	3.27711800	-2.14097800
H	-4.85401800	0.15207400	-2.89009400
H	-5.77940000	1.92189100	-0.57165400
H	-5.41381200	2.67865300	-3.52068700
H	-2.94921600	1.79236900	-3.40871400
H	-3.54482800	4.11438700	-2.77461400
H	-5.12606100	-0.35643300	-1.22736600
H	-6.76958100	1.36746000	-1.91738900
H	-1.88530000	2.36147500	-2.14638400
H	-5.98764300	3.74475300	-2.24288300
H	-3.78826800	3.62151800	-1.10005300
C	-3.34870000	0.86367400	-1.53451700
C	-2.54993500	0.19547100	-0.65948400
C	-1.15784200	0.65575300	-0.34357500
H	-0.98150000	0.50862900	0.74219200
H	-1.01284600	1.71521400	-0.54991000
C	-0.15304400	-0.27715000	-1.98330000
O	0.52539800	0.58038500	-2.54203800
O	-0.61395600	-1.38450700	-2.18154600

6A

Sum of electronic and thermal Free Energies= -4127.022258

C	3.70040000	-3.20900500	-0.39053100
C	3.92012300	-2.00167600	2.08770100
C	3.87659400	-3.54382100	2.06114700
C	4.43307900	-4.00736400	0.70707400
H	2.68881100	-3.62580200	-0.48223800
H	4.96860500	-1.69150000	2.18250200
H	4.43724700	-3.96140700	2.90556800
H	2.83736100	-3.88251500	2.16899600
H	5.51218400	-3.80599300	0.66047800
H	4.30674300	-5.08660300	0.55806900
P	3.35123700	-1.50731700	0.36009700
C	4.66368900	-0.33678800	-0.23929300
C	4.28133300	0.93978300	-0.72507500
C	6.02600500	-0.68194300	-0.23599900
C	5.27514100	1.79924600	-1.22299000
C	6.99835600	0.18687200	-0.72664500
H	6.33389400	-1.64732900	0.15455200
C	6.61884900	1.43112000	-1.23174000
H	4.99738200	2.77609200	-1.60675600
H	8.04416300	-0.10668500	-0.71801200
H	7.36630600	2.11561600	-1.62269600
C	2.31286700	2.80712000	0.60964500
C	2.24523600	2.55946600	-2.17378300
C	1.60585200	3.93077500	-0.18486700
H	1.63284900	2.40230500	1.36581200
C	2.21857300	3.99368100	-1.59446500
H	3.09144800	2.42726100	-2.85559400
H	0.53552000	3.70582600	-0.26227100
H	1.69056300	4.88977900	0.33972900
H	1.65667100	4.67221000	-2.24763500
H	3.23925000	4.39123800	-1.53108300
P	2.48616700	1.42725300	-0.68036000
C	4.34235400	-3.23844400	-1.77826800
H	3.75668500	-2.66135300	-2.50106500
H	5.35686800	-2.83068000	-1.77201600
H	4.39763700	-4.26963100	-2.14541000
C	3.10103200	-1.35761500	3.20945800
H	3.39257700	-1.77090800	4.18235600
H	3.26351100	-0.27580800	3.24806100
H	2.02746800	-1.51409000	3.06865900
C	3.59815400	3.26617200	1.30564700
H	4.11074700	2.43358300	1.79622800
H	4.30969100	3.72617900	0.61362500
H	3.35321200	4.00824800	2.07441900
C	0.95383200	2.19064200	-2.92045500
H	0.80456900	2.85851600	-3.77685100
H	0.98903100	1.16269700	-3.29354500
H	0.07372000	2.26871200	-2.27386600

Cu	1.47783600	-0.41784800	-0.00983800
Si	-3.87759000	-1.14877100	-0.91780200
C	-3.29461300	-0.32816200	-2.52377600
H	-2.19999600	-0.29771700	-2.51249500
H	-3.60413700	-0.89668500	-3.40812400
H	-3.66117300	0.69677700	-2.63546700
C	-3.24014100	-2.93135400	-0.92197000
H	-2.14622200	-2.93344600	-0.89655300
H	-3.61350200	-3.50879100	-0.06915100
H	-3.57167300	-3.44387200	-1.83220400
C	-5.78005600	-1.22321500	-0.87339700
C	-6.54813300	-1.25611100	-2.05204600
C	-6.47305900	-1.31670300	0.34880800
C	-7.93929200	-1.37848100	-2.01587300
H	-6.05714600	-1.18170800	-3.01980300
C	-7.86282300	-1.44171300	0.39449700
H	-5.91551000	-1.28009400	1.28204700
C	-8.60086300	-1.47252400	-0.79059600
H	-8.50615200	-1.39822600	-2.94330200
H	-8.37020800	-1.51182800	1.35339200
H	-9.68308100	-1.56682700	-0.75893300
C	-4.52293000	1.89410900	0.11091900
C	-5.59899000	2.47286900	1.05587800
C	-2.86351400	1.88526300	1.99259600
C	-4.97615800	3.28010000	2.20334500
C	-3.92399400	2.45595100	2.95727000
H	-4.00777900	2.73317600	-0.38354300
H	-6.18639500	1.64165800	1.46689400
H	-4.49815500	4.18141500	1.79213600
H	-2.33506600	2.73398100	1.52880700
H	-3.43674900	3.06830800	3.72617000
H	-5.00821200	1.31324800	-0.67613800
H	-6.29612700	3.09694000	0.48339700
H	-2.10064800	1.32383800	2.53321100
H	-5.75699500	3.62829600	2.89092700
H	-4.41574100	1.62501600	3.48144100
C	-3.49858400	1.07423800	0.87507800
C	-3.20215300	-0.21893100	0.59981800
C	-2.17674000	-0.97518700	1.45293100
H	-2.35441600	-2.05251400	1.38535900
H	-2.24792500	-0.70267400	2.50776400
C	-0.74798700	-0.71461300	0.98145500
O	-0.41406500	-1.14136900	-0.17829200
O	0.05626700	-0.08080800	1.71624900

TS6A

Sum of electronic and thermal Free Energies= -4126.877024

C	3.87274200	-2.82391900	-1.44580600
C	3.03111200	-2.84261000	1.18781500
C	3.07748500	-4.20094500	0.45808300
C	4.14941100	-4.10897900	-0.63783400
H	3.00057600	-3.01931900	-2.08348100
H	3.94202300	-2.75080200	1.79295900
H	3.27736100	-5.01343800	1.16635500
H	2.09949800	-4.40734900	0.00287300
H	5.14641100	-4.05702800	-0.17880900
H	4.14768300	-4.99035200	-1.29056500
P	3.16847200	-1.58087400	-0.20581200
C	4.54077100	-0.45315300	0.33679700
C	4.29453600	0.94149700	0.42299500
C	5.81742800	-0.93996500	0.66510100
C	5.35004400	1.79119000	0.79480700
C	6.85051600	-0.08187800	1.03563300
H	6.00961000	-2.00809400	0.63065800
C	6.61690700	1.29259200	1.09142900
H	5.18256500	2.86166800	0.86133300
H	7.83056900	-0.48308900	1.27743600
H	7.41451800	1.97342500	1.37493400
C	1.82269100	2.10794500	1.70134000
C	2.84877300	3.34247800	-0.58443500
C	1.45477900	3.59374300	1.47099200
H	0.91113600	1.50875000	1.79097000
C	2.56148300	4.25361800	0.63058700
H	3.88502200	3.44841100	-0.92147200
H	0.50215300	3.65441300	0.93198600
H	1.30837700	4.10939900	2.42734400
H	2.27584400	5.26279100	0.30930300
H	3.46694200	4.36150300	1.24091600
P	2.58817300	1.58157500	0.04646600
C	5.00812400	-2.34272500	-2.35016300
H	4.72799400	-1.43410300	-2.89270200
H	5.92066800	-2.12588100	-1.78845100
H	5.24749100	-3.11117300	-3.09405800
C	1.80692100	-2.63472900	2.08335800
H	1.69827500	-3.47099700	2.78420300
H	1.90040500	-1.71834100	2.67501900
H	0.88721800	-2.54176100	1.49825500
C	2.68306200	1.87787000	2.94779900
H	2.97367700	0.82793500	3.04937000

H	3.60190900	2.47183200	2.93970000
H	2.11362500	2.15413400	3.84277900
C	1.91899600	3.62156300	-1.77603600
H	2.05119800	4.65062900	-2.13019300
H	2.12676600	2.94490400	-2.61019500
H	0.86474600	3.49075400	-1.51002700
Cu	1.52621800	-0.21489800	-0.70229300
Si	-5.24779100	-1.17081200	-0.77455900
C	-6.41193000	-0.25589200	-1.96153800
H	-6.11977200	-0.44869600	-2.99968200
H	-7.44271800	-0.61015600	-1.84321800
H	-6.41266600	0.82788900	-1.81384100
C	-5.46969200	-3.02527400	-1.10674800
H	-5.14567000	-3.28707600	-2.12057800
H	-4.89789700	-3.63869700	-0.40415300
H	-6.52504800	-3.30414100	-1.01234700
C	-5.76577200	-0.79459500	1.01510300
C	-6.99249400	-0.18155800	1.32792800
C	-4.92977200	-1.15680800	2.08953000
C	-7.37402700	0.05294700	2.65132200
H	-7.66514300	0.12090300	0.52920400
C	-5.30466000	-0.92715900	3.41391100
H	-3.96449000	-1.61547200	1.88753200
C	-6.53059600	-0.32116900	3.69816400
H	-8.32788500	0.52885000	2.86411000
H	-4.63914400	-1.21580900	4.22330300
H	-6.82434700	-0.13892100	4.72847800
C	-2.29605500	1.07267000	-2.34261300
C	-3.38526900	2.02729600	-2.87027600
C	-3.03694600	1.60048700	0.02119600
C	-3.65400800	3.17535600	-1.88751100
C	-4.04904200	2.64220600	-0.50387500
H	-1.36096400	1.63755200	-2.24479800
H	-4.31272800	1.47091600	-3.05370800
H	-2.74199800	3.78345000	-1.79409500
H	-2.09139000	2.11341700	0.24812700
H	-4.13719600	3.46725600	0.21478800
H	-2.10308700	0.27123600	-3.05597000
H	-3.06167900	2.42866400	-3.83986800
H	-3.38836600	1.17404700	0.96466800
H	-4.43389700	3.84298600	-2.27512700
H	-5.04354600	2.18197400	-0.55995700
C	-2.70487700	0.49076300	-0.97201100
C	-3.41824900	-0.75670800	-0.99216300
C	-2.42684900	-1.78243300	-1.03725100
H	-2.56529400	-2.71588200	-1.60083700
H	-1.95919700	-1.96614500	-0.07521900
C	-0.89507600	-0.51819500	-0.83537800
O	-0.12442100	-0.45511800	-1.84519000
O	-0.48230800	-0.45703500	0.35715900

7A

Sum of electronic and thermal Free Energies= -4127.007058

C	1.66473000	-2.93194700	-1.44034100
C	2.36943200	-3.20994600	1.21785700
C	1.55949700	-4.36136100	0.58350100
C	1.85054100	-4.37298500	-0.92399600
H	0.58704600	-2.72751400	-1.47861300
H	3.42589800	-3.50501600	1.24969900
H	1.80224800	-5.31725500	1.06220300
H	0.48794500	-4.18457000	0.74652700
H	2.88096800	-4.70832700	-1.10441300
H	1.19503700	-5.06880000	-1.46162300
P	2.22296400	-1.80369500	-0.02939800
C	3.98331800	-1.31541400	-0.38580500
C	4.34857200	0.05500800	-0.35677900
C	4.95546800	-2.26886000	-0.73399600
C	5.65556700	0.41385600	-0.72873500
C	6.25158500	-1.89506300	-1.08201300
H	4.69432700	-3.32280400	-0.74245000
C	6.59977300	-0.54393900	-1.09178500
H	5.94343300	1.46034200	-0.73481800
H	6.98150000	-2.65254300	-1.35303700
H	7.60281700	-0.23755100	-1.37466500
C	3.74477900	2.18799300	1.70973800
C	3.37791200	2.78849000	-0.99373500
C	3.76337400	3.68335700	1.30415700
H	2.97678200	2.02631800	2.47330800
C	4.21200000	3.79163200	-0.16335700
H	3.93694500	2.43604300	-1.86679100
H	2.75590400	4.10260400	1.40717300
H	4.41418000	4.25840800	1.97334500
H	4.09234900	4.81299400	-0.54452600
H	5.27981300	3.55129400	-0.23846400
P	3.08438000	1.32140700	0.15485700
C	2.24330300	-2.63949800	-2.82474800
H	2.04963200	-1.60544800	-3.12633200
H	3.32382300	-2.80419200	-2.86146300
H	1.77839300	-3.29390300	-3.57089100

C	1.91590100	-2.82235200	2.62723200	H	-4.79370600	1.84428800	-2.75992100
H	1.97412100	-3.68349300	3.30328300	H	-1.80640600	3.38340900	0.92459200
H	2.54280600	-2.02865400	3.04642900	H	-4.94757400	4.22026500	-1.93950900
H	0.88204300	-2.46153400	2.62510300	H	-4.20282100	3.90599700	0.38401100
C	5.08126800	1.69338700	2.27533300	C	-3.30282200	1.02882000	1.06098500
H	5.06766900	0.61662700	2.46815700	C	-3.70127000	1.78121300	2.09859600
H	5.92039600	1.89577200	1.60401000	H	-4.24304600	1.35880200	2.94073800
H	5.28677700	2.20101900	3.22498000	H	-3.48923500	2.84390700	2.18219500
C	2.03738700	3.37796200	-1.46342200	C	-2.48310500	1.58408900	-0.11598100
H	2.21153900	4.18245800	-2.18750400	C	-1.06863500	0.94967400	-0.06594800
H	1.39718900	2.62057400	-1.92333700	O	-0.42069300	0.76001200	-1.13250100
H	1.47265100	3.80102900	-0.62531600	O	-0.56489800	0.69011400	1.07760500
Cu	1.22089100	0.12834700	0.24596300	**8A**			
Si	-3.75572700	-0.82218700	1.12613800	Sum of electronic and thermal Free Energies= -4981.811008			
C	-2.41344300	-1.93432800	0.38588300	C	3.02064500	1.32369600	2.75109600
H	-1.47993500	-1.77200400	0.93272000	C	4.69104300	2.41725000	0.84011300
H	-2.69333100	-2.99025000	0.47551900	C	4.29505400	3.32638000	2.02605900
H	-2.21454700	-1.72020800	-0.66848900	C	3.96950700	2.43861600	3.23590200
C	-3.99961700	-1.34537200	2.93250700	H	2.03425500	1.77288900	2.58440300
H	-3.10422400	-1.13672800	3.52730200	H	5.71560800	2.06076000	1.00025700
H	-4.84638200	-0.83776300	3.40529900	H	5.09328400	4.04584500	2.24313000
H	-4.19941400	-2.42168500	2.98272900	H	3.40636700	3.90990400	1.75524700
C	-5.39802500	-1.12585100	0.21427700	H	4.89009300	2.00194100	3.64556300
C	-5.57129700	-2.18965200	-0.68918800	H	3.50910100	3.01403400	4.04815800
C	-6.51391000	-0.30341500	0.46334900	P	3.56357900	0.90794800	0.99125300
C	-6.79908100	-2.42636700	-1.31279000	C	4.75061000	-0.51582900	1.14142600
H	-4.73575300	-2.84685300	-0.91726800	C	4.55931800	-1.67576700	0.35105600
C	-7.74468000	-0.53440100	-0.15241000	C	5.81912800	-0.48918300	2.05487200
H	-6.41559400	0.54052000	1.14280200	C	5.41767800	-2.77314100	0.53968000
C	-7.89033800	-1.59950600	-1.04404700	C	6.66670100	-1.58185600	2.22079000
H	-6.90245700	-3.25513900	-2.00861800	H	5.98929900	0.39771800	2.65622300
H	-8.58825700	0.11771600	0.05902200	C	6.45746900	-2.73563200	1.46531600
H	-8.84649200	-1.78101300	-1.52762000	H	5.27916300	-3.67491200	-0.04802400
C	-3.15173700	1.26321100	-1.48152900	H	7.47943800	-1.53471800	2.93984300
C	-4.38899200	2.12145100	-1.77867700	H	7.10418100	-3.59939800	1.58994000
C	-2.21989800	3.12186300	-0.05527900	C	4.03987800	-1.70775700	-2.60317700
C	-4.05166400	3.61743300	-1.74507800	C	2.67256900	-3.52695900	-0.99089300
C	-3.43593600	4.00078200	-0.39286300	C	3.46051800	-2.96623400	-3.29166900
H	-2.39418700	1.42140100	-2.25584600	H	3.68080600	-0.80847200	-3.11364500
H	-5.17853700	1.90826100	-1.04706600	C	3.37223500	-4.09287200	-2.24863900
H	-3.33767300	3.84607500	-2.54978900	H	3.02147500	-4.03058200	-0.08388800
H	-1.43153400	3.33352100	-0.78937600	H	2.45723800	-2.74703100	-3.67602200
H	-3.12577800	5.05387000	-0.39853700	H	4.07252200	-3.25496400	-4.15437900
H	-3.41820400	0.20182000	-1.53190300	H	2.83304200	-4.96308500	-2.64144600

H	4.38354000	-4.43504700	-1.99766400	H	-2.62202800	1.38403400	1.89573500
P	3.18785600	-1.71150600	-0.90111600	H	-4.80643000	-0.74946300	2.15782100
C	2.83407000	0.14029800	3.70118000	H	-3.16940600	0.60358700	4.36464700
H	2.10231500	-0.56867300	3.30276900	H	-0.98417700	-0.05969100	3.11302500
H	3.76984000	-0.39651700	3.88194200	H	-2.09502200	-1.59433200	4.72101100
H	2.45907300	0.49454900	4.66827600	H	-3.56742200	0.75339800	0.57306100
C	4.61546100	3.10296800	-0.52655900	H	-4.92199500	0.93156600	2.65098700
H	5.27059500	3.98155800	-0.55376700	H	-0.69512000	-1.71626700	2.67604400
H	4.92919700	2.43010400	-1.33138600	H	-4.42160200	-0.61393600	4.59032800
H	3.59670600	3.43649200	-0.74931800	H	-3.04339000	-2.30964700	3.42310600
C	5.57224200	-1.66686700	-2.60478900	C	-2.58245000	-1.86648300	0.56307000
H	5.95496500	-0.80869100	-2.04492500	C	-2.04856700	-3.07681700	0.80940300
H	6.01472800	-2.56602200	-2.16733100	H	-2.34295300	-3.96163400	0.25297500
H	5.93490100	-1.58414900	-3.63593000	H	-1.29712500	-3.25249400	1.57535100
C	1.14286500	-3.65025600	-1.05769500	C	-2.05436900	-0.62634900	1.34157300
H	0.84656400	-4.70543900	-1.07673700	C	-0.91628900	-0.05018000	0.46512700
H	0.66046700	-3.17527700	-0.19969900	O	0.26938300	-0.10004500	0.84279600
H	0.73626800	-3.17602000	-1.95750800	O	-1.31534200	0.46510800	-0.65454200
Cu	1.99287600	0.11008100	-0.36293500	B	-0.53313900	1.40446000	-1.60172300
Si	-3.94753900	-1.86807900	-0.79677900	O	0.83590300	0.86012600	-1.90585200
C	-4.20643500	-0.30221800	-1.81640300	O	-1.24908500	1.33119200	-2.87047700
H	-3.26667000	0.05349200	-2.24622100	C	0.76236000	0.19984700	-3.17362300
H	-4.89184300	-0.53908700	-2.63986500	C	-0.36297200	0.94202200	-3.89655400
H	-4.64346100	0.52842000	-1.25561400	H	0.03734200	1.82027400	-4.42895500
C	-3.50490700	-3.23472000	-2.04272900	H	-0.87733600	0.30748800	-4.62934200
H	-2.51918200	-3.06075900	-2.48800500	H	1.72766400	0.27462000	-3.68696400
H	-3.50987700	-4.23887100	-1.60814100	H	0.51726200	-0.86406300	-3.03450100
H	-4.24308200	-3.23010500	-2.85248400	Si	-0.49818500	3.33775800	-0.87918700
C	-5.60198200	-2.35445600	0.01413100	C	0.45382000	4.44344700	-2.11246500
C	-6.80930400	-1.75018200	-0.38330600	H	0.50017900	5.48546500	-1.77601800
C	-5.68105900	-3.37107000	0.98557100	H	1.48126400	4.08406600	-2.24686300
C	-8.03654200	-2.14344700	0.15609100	H	-0.02814400	4.43530500	-3.09635200
H	-6.79712500	-0.95617900	-1.12501400	C	0.34882100	3.57526400	0.81630200
C	-6.90291300	-3.77071100	1.52859900	H	-0.14140500	2.99419700	1.60509400
H	-4.77056000	-3.85280300	1.33414400	H	1.38599900	3.23032200	0.75000300
C	-8.08670500	-3.15672200	1.11372800	H	0.36917300	4.62525600	1.13133200
H	-8.95176700	-1.65592800	-0.16968100	C	-2.26782700	4.03781500	-0.72678000
H	-6.93168900	-4.55806200	2.27753500	C	-3.23143300	3.76680300	-1.72003400
H	-9.03956100	-3.46374200	1.53653000	C	-2.67175000	4.83891700	0.35719800
C	-3.13090700	0.48031200	1.53357300	C	-4.52710300	4.28054200	-1.63768900
C	-4.22228700	0.09396500	2.54398400	H	-2.96272200	3.13215800	-2.56051100
C	-1.48405400	-0.96346400	2.74435300	C	-3.96772800	5.35405200	0.44789100
C	-3.62914500	-0.28463300	3.90736000	H	-1.96499800	5.06963100	1.15088500
C	-2.56475100	-1.37945700	3.75298400	C	-4.90001400	5.07742800	-0.55259700

H	-5.24888800	4.05534300	-2.41925200
H	-4.24866100	5.96980400	1.29910000
H	-5.90925300	5.47586700	-0.48617200

TS7A

Sum of electronic and thermal Free Energies= -4981.775658

C	-0.86807300	3.23746100	0.19942800
C	-0.05258600	3.64773000	-2.40183900
C	-1.43628300	4.21331000	-1.99889500
C	-1.44330400	4.48538000	-0.49150300
H	-1.60023200	2.42545500	0.12149600
H	0.64604800	4.47817100	-2.54459400
H	-1.67979300	5.10666100	-2.58690200
H	-2.20637100	3.46535200	-2.23188700
H	-0.82246200	5.35984800	-0.25715500
H	-2.45236600	4.70929400	-0.12178500
P	0.54988500	2.62058300	-0.90921300
C	2.00466200	3.60214100	-0.26265900
C	3.03343800	2.96015700	0.47634500
C	2.09182300	4.99546200	-0.44612500
C	4.07574200	3.74565300	1.00567800
C	3.14024200	5.75111600	0.07126000
H	1.31749900	5.51453300	-0.99851400
C	4.14038100	5.12137100	0.80845900
H	4.85803100	3.27644000	1.58919600
H	3.16691500	6.82486400	-0.09212800
H	4.96230700	5.69282600	1.22996600
C	4.67452100	0.37434800	0.27168700
C	3.45835000	0.98275800	2.62933600
C	4.74760400	-0.77825300	1.30021400
H	4.52943200	-0.04587300	-0.72592100
C	4.43388600	-0.23024100	2.71388800
H	4.00678900	1.89240700	2.89393200
H	4.00537800	-1.53578400	1.03287200
H	5.72896000	-1.26422100	1.25978400
H	3.99695400	-1.02010500	3.33183200
H	5.35527200	0.08543500	3.21587000
P	3.03143700	1.12942200	0.79934300
C	-0.54284900	3.41994000	1.68167700
H	-0.21424100	2.47886900	2.13040800
H	0.23622700	4.17263000	1.83906300
H	-1.43799700	3.74881200	2.22337200
C	-0.09974600	2.84548600	-3.70756600
H	-0.47135000	3.47272600	-4.52724600
H	0.88696700	2.47053400	-3.99381400
H	-0.76899500	1.98342100	-3.61967800
C	5.94153700	1.23539400	0.25442700
H	5.84392100	2.10767900	-0.39735600
H	6.22349200	1.58678700	1.25241600
H	6.77562900	0.63058500	-0.12029600
C	2.23905500	0.88388100	3.55114900
H	2.56068000	0.77815300	4.59419600
H	1.62232200	1.78644600	3.48872500
H	1.62014400	0.02293100	3.28676700
Cu	1.29649800	-0.12529700	0.08407300
Si	-4.15717800	-1.15991200	-1.27490400
C	-2.81819900	-0.06346400	-2.04070200
H	-1.94964000	-0.66941200	-2.31572400
H	-3.19420700	0.40583600	-2.95701200
H	-2.46581900	0.72334500	-1.36957800
C	-4.53859900	-2.54123700	-2.51291000
H	-3.68019500	-3.20748700	-2.64736600
H	-5.39924700	-3.14964000	-2.21787700
H	-4.77633800	-2.09758900	-3.48616500
C	-5.74827500	-0.14778500	-1.04461300
C	-5.83055500	1.21595600	-1.37700800
C	-6.91853800	-0.76682400	-0.56345300
C	-7.02232800	1.93162500	-1.23600900
H	-4.95292400	1.73497000	-1.75439700
C	-8.11311300	-0.06019600	-0.42072500
H	-6.89798100	-1.81957000	-0.28865000
C	-8.16731900	1.29439100	-0.75746900
H	-7.05614300	2.98517700	-1.50101700
H	-9.00049500	-0.56417200	-0.04694100
H	-9.09579600	1.84798500	-0.64747600
C	-3.35234900	0.27927400	1.66079000
C	-4.65932600	0.27522900	2.46833600
C	-2.64757500	-1.84405800	2.81280900
C	-4.48410400	-0.41815700	3.82511900
C	-3.94425100	-1.84111000	3.63583200
H	-2.59704200	0.86276500	2.19813000
H	-5.44819900	-0.22964000	1.89907100
H	-3.78127300	0.15931300	4.44307300
H	-1.87787000	-1.30146100	3.37914500
H	-3.75051500	-2.31148200	4.60784900
H	-3.50852400	0.79457400	0.70798800
H	-4.99536000	1.30964600	2.60846500
H	-2.26224300	-2.85792400	2.68083600
H	-5.43581200	-0.43987800	4.36959900

H	-4.70615300	-2.45172200	3.13779100
C	-3.59387100	-1.93666900	0.37853000
C	-3.90294700	-3.22995500	0.56120700
H	-4.43776800	-3.80285100	-0.19055000
H	-3.62912700	-3.79053600	1.45059100
C	-2.77450100	-1.13950900	1.42174000
C	-1.31566400	-1.04259300	0.91809500
O	-0.71291800	0.03910400	0.81084000
O	-0.76146200	-2.19759000	0.68390900
B	0.74545800	-2.34637600	0.61276000
O	1.38022200	-1.87212100	1.83038400
O	1.02755200	-3.74973000	0.49569900
C	1.64825200	-3.03020900	2.62645500
C	1.84778400	-4.13914100	1.59016100
H	2.89864100	-4.20532600	1.27350100
H	1.53372600	-5.12437300	1.95493800
H	2.52919900	-2.85536300	3.25318000
H	0.79146000	-3.24592800	3.28190600
Si	1.45646500	-1.90858700	-1.57584700
C	1.48435300	-0.46203400	-2.84937000
H	1.72525600	-0.88510700	-3.83335700
H	0.49754500	0.00127100	-2.92022300
H	2.20149400	0.33727900	-2.64369800
C	0.12887600	-3.05168500	-2.32752200
H	0.11449700	-4.02643100	-1.83614000
H	-0.86736400	-2.61442500	-2.20828100
H	0.31078800	-3.19894700	-3.39831000
C	3.15104100	-2.76288300	-1.81852300
C	4.23374600	-2.07642100	-2.40207000
C	3.35784800	-4.12307300	-1.51201500
C	5.46556600	-2.69426600	-2.63413400
H	4.11297200	-1.03942700	-2.70426000
C	4.58394300	-4.75027000	-1.74298700
H	2.53900200	-4.69602600	-1.09106300
C	5.64735900	-4.03623200	-2.29892900
H	6.27728000	-2.13045400	-3.08765500
H	4.70667000	-5.80205800	-1.49579900
H	6.60170700	-4.52350000	-2.48074400

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Sum of electronic and thermal Free Energies= -1355.349899

Si	-0.88577200	-1.35693600	0.54874200
C	0.07115700	-2.21459700	-0.83622100
H	1.12399300	-2.33955400	-0.56361600
H	-0.34819100	-3.21261800	-1.00783400
H	0.05174700	-1.66924600	-1.78304500
C	-0.78664800	-2.45571300	2.08979200
H	0.23893000	-2.53491000	2.46498800
H	-1.42131000	-2.09989300	2.90743700
H	-1.12867300	-3.46416800	1.83254600
C	-2.71842500	-1.21275100	0.07317200
C	-3.21522400	-1.69925500	-1.14869600
C	-3.64490800	-0.64617600	0.96948100
C	-4.57403000	-1.62492600	-1.46408000
H	-2.53438900	-2.14370800	-1.86989700
C	-5.00347300	-0.56945500	0.66277400
H	-3.30027100	-0.25147600	1.92308200
C	-5.47152900	-1.06003000	-0.55808300
H	-4.93050100	-2.00817500	-2.41636500
H	-5.69644100	-0.12688100	1.37325300
H	-6.52890300	-1.00139000	-0.80065500
C	-0.73444600	1.51174000	-1.25150200
C	-1.94208900	2.36086300	-0.83121500
C	0.70942900	2.76562500	0.39257400
C	-1.51223100	3.75025800	-0.34520500
C	-0.49431300	3.63215700	0.79576800
H	-0.23551100	1.98437800	-2.10493100
H	-2.49930400	1.84982600	-0.03718600
H	-1.06222000	4.30633800	-1.18016500
H	1.23756000	3.27274900	-0.42650600
H	-0.13295400	4.62415500	1.09312900
H	-1.06827700	0.53321900	-1.60786000
H	-2.62855100	2.44874000	-1.68130300
H	1.43055500	2.68558300	1.20968100
H	-2.38414400	4.32876000	-0.01748400
H	-0.98945200	3.20233000	1.67375800
C	-0.15869300	0.36425500	0.97955500
C	-0.03130400	0.65589500	2.28335000
H	-0.32867600	-0.04476100	3.05784400
H	0.38001200	1.59255600	2.64930300
C	0.31668800	1.34429700	-0.12254200
C	1.59309900	0.74609900	-0.73486900
O	1.75673400	0.45135700	-1.89463600
O	2.59643600	0.63187000	0.18872800
B	3.70737100	-0.16444600	-0.01458300
O	4.96429700	0.28862100	0.27963500
O	3.65102200	-1.47271000	-0.41581800
C	5.85631200	-0.82966100	0.14586600
C	5.00626500	-1.93373800	-0.53470700

H	5.24786000	-2.04876600	-1.59697900
H	5.10297600	-2.90720300	-0.04602300
H	6.72290400	-0.53236800	-0.45109200
H	6.20345100	-1.12662400	1.14191000

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Sum of electronic and thermal Free Energies= -952.693767

C	1.08054000	-1.14578500	1.25204600
C	1.07884000	-2.60363200	0.74453300
C	3.13939600	-0.66279200	-0.09412200
C	2.48842900	-3.07674700	0.36882000
C	3.14782500	-2.11248900	-0.62475500
H	1.64642400	-1.10900500	2.19637900
H	0.42101300	-2.67014700	-0.13150900
H	3.10626400	-3.13622700	1.27659100
H	3.75174100	-0.62938100	0.82065800
H	4.17836000	-2.42288700	-0.83553900
H	0.05701200	-0.84759800	1.48686500
H	0.64682100	-3.25796400	1.51102900
H	3.62576600	0.00037700	-0.81168100
H	2.45175800	-4.08996400	-0.04930500
H	2.60631000	-2.14492000	-1.57979000
C	1.73632500	-0.19843700	0.26214700
C	1.14067300	0.91219200	-0.23838000
C	1.87028900	1.82602000	-1.22449100
H	2.51517300	1.24219400	-1.89069400
H	1.14554000	2.31682800	-1.88224200
Si	-0.59533000	1.47915400	0.30724000
C	-1.09429900	3.03728200	-0.65537100
H	-0.39488100	3.86537600	-0.49896100
H	-1.16445300	2.85266100	-1.73211600
H	-2.08244000	3.37048200	-0.31895100
C	-0.64484600	1.93153300	2.15005300
H	0.10104600	2.70563700	2.36147900
H	-1.62227300	2.33620200	2.43575100
H	-0.43028400	1.08061700	2.80286000
C	-1.90119600	0.15087900	-0.06889300
C	-3.07833800	0.03843300	0.69352100
C	-1.75705900	-0.71888300	-1.16612500
C	-4.06661400	-0.89565200	0.37673100
H	-3.23061300	0.68578900	1.55387800
C	-2.74168500	-1.65314500	-1.49141100
H	-0.85380100	-0.67188000	-1.76964700
C	-3.90066500	-1.74390300	-0.71865100
H	-4.96410400	-0.96275300	0.98584400
H	-2.60365800	-2.31171400	-2.34482100
H	-4.66775500	-2.47205500	-0.96717200
C	2.71751500	2.91290200	-0.53876600
H	3.20210600	3.56122600	-1.27735900
H	2.10483800	3.54817300	0.11022900
H	3.49793100	2.46612900	0.08555400

TS8A

Sum of electronic and thermal Free Energies= -3938.357823

C	0.30601600	-2.02408500	2.59797400
C	0.26703600	0.61504600	3.35053500
C	-0.83135400	-0.24824200	4.00095300
C	-0.32844300	-1.69800300	3.98064900
H	-0.42614400	-2.53012300	1.96191600
H	1.16191900	0.53242000	3.98175900
H	-1.04444100	0.09478900	5.02025600
H	-1.76541100	-0.15397700	3.43093400
H	0.44030400	-1.81184100	4.75583200
H	-1.12503100	-2.41100700	4.21797600
P	0.55960300	-0.33482600	1.75904200
C	2.35540900	-0.18493500	1.33891800
C	2.86215200	-0.84047900	0.18602900
C	3.22233200	0.60611100	2.11055300
C	4.22577600	-0.70262800	-0.11853500
C	4.56988000	0.74181500	1.77794500
H	2.85137400	1.12629900	2.98692600
C	5.07745500	0.07786900	0.66274800
H	4.63511200	-1.21141700	-0.98562500
H	5.21922000	1.35666900	2.39481500
H	6.12706900	0.16910400	0.39805800
C	1.54615100	-1.05734400	-2.52014800
C	2.83591400	-3.28926100	-1.46714300
C	1.97317100	-2.16229100	-3.51419200
H	0.47810100	-0.85085100	-2.63991700
C	3.18180400	-2.90307300	-2.92253100
H	3.73743200	-3.32991800	-0.84724700
H	1.14677900	-2.86851800	-3.66014800
H	2.19691600	-1.73455600	-4.49901500
H	3.44591500	-3.78745200	-3.51595400
H	4.05633800	-2.24091600	-2.93821600
P	1.69931400	-1.90407400	-0.81061600
C	1.53945900	-2.92041100	2.73689200
H	1.94352900	-3.21451600	1.76540300
H	2.33724600	-2.42505900	3.30062800
H	1.26859500	-3.83667500	3.27531100

C	-0.10557100	2.08650500	3.17853200
H	-0.35720700	2.53422300	4.14703800
H	0.71538200	2.66508800	2.74542400
H	-0.96938400	2.20136200	2.51690600
C	2.30774100	0.25644300	-2.72371300
H	2.01671300	1.00888300	-1.98636700
H	3.39219300	0.13186100	-2.65398800
H	2.08202500	0.66058800	-3.71805400
C	2.12146600	-4.64742700	-1.37174800
H	2.76718400	-5.44877700	-1.75064100
H	1.85586000	-4.88816300	-0.33781100
H	1.19464100	-4.66247000	-1.95526500
Cu	-0.98442700	-0.06177700	0.12958300
C	1.61892500	3.35947400	-0.04985000
C	2.53695600	3.97953800	-1.12244200
C	-0.17179200	5.09506800	-0.60510200
C	2.23488000	5.47050300	-1.33221000
C	0.75594400	5.69766200	-1.67731600
H	1.86126400	3.82215200	0.91985300
H	2.39382800	3.44444200	-2.07042000
H	2.48162200	6.02348600	-0.41412100
H	-0.02952000	5.64767200	0.33664100
H	0.54799000	6.76893700	-1.78641100
H	1.80622000	2.28865700	0.05481400
H	3.58510700	3.83601900	-0.83420900
H	-1.22194700	5.20697200	-0.88810100
H	2.87572800	5.87851700	-2.12290400
H	0.53233500	5.23074400	-2.64577300
C	0.15649300	3.62510000	-0.35519600
C	-0.78749800	2.71733300	-0.42957600
C	-1.86745300	1.96091200	-0.57326600
H	-2.22279700	1.66512800	-1.55737200
H	-2.59311000	1.84976900	0.23283300
Si	-2.59384300	-1.39000100	-0.85293900
C	-2.71714500	-3.18528100	-0.18421000
H	-1.76251100	-3.70418700	-0.33224600
H	-2.93810100	-3.21200100	0.88912100
H	-3.49673600	-3.76279100	-0.69617500
C	-2.41422900	-1.61585000	-2.75338000
H	-3.27549400	-2.13843400	-3.18827600
H	-2.29951000	-0.66564400	-3.28841500
H	-1.52304400	-2.21687600	-2.97261900
C	-4.33270300	-0.62585700	-0.59578100
C	-4.97776700	-0.70835200	0.65507000
C	-4.99833400	0.10269500	-1.60047800
C	-6.21564500	-0.10893200	0.89055500
H	-4.50263200	-1.26101000	1.46429200
C	-6.23637300	0.71153900	-1.37494400
H	-4.54903700	0.18909400	-2.58743800
C	-6.85185400	0.60727000	-0.12706100
H	-6.68750300	-0.20102100	1.86628600
H	-6.72290400	1.26326800	-2.17618400
H	-7.81581700	1.07651800	0.05154700

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Sum of electronic and thermal Free Energies= -3938.357823

C	-0.78156600	-2.11678700	2.29847700
C	-0.40309100	0.45496500	3.18591900
C	-1.10107000	-0.52796500	4.16726300
C	-0.71560000	-1.97361700	3.82790000
H	-1.82968300	-2.02988600	1.98599500
H	0.55526200	0.78173200	3.60286400
H	-0.86711200	-0.27068200	5.20665900
H	-2.18655800	-0.41619200	4.05342000
H	0.29946300	-2.20011200	4.17717400
H	-1.38358400	-2.69312900	4.31737500
P	-0.01357900	-0.53466400	1.62047000
C	1.80472800	-0.92633900	1.69136600
C	2.48663200	-1.27556500	0.49736500
C	2.49976800	-0.99127900	2.91175900
C	3.80911400	-1.74308200	0.58937700
C	3.82541000	-1.41759700	2.97466200
H	2.00468700	-0.71242300	3.83532100
C	4.47860700	-1.81490700	1.80918500
H	4.32894700	-2.05621400	-0.30990800
H	4.33704700	-1.45375300	3.93222300
H	5.50346100	-2.17299200	1.84670700
C	2.68008100	-0.02405600	-2.26706400
C	2.05262300	-2.72959000	-2.04951800
C	2.75143000	-0.86642100	-3.56106600
H	2.08212100	0.87815300	-2.42802400
C	3.05053000	-2.31982800	-3.15924200
H	2.52418400	-3.41358700	-1.33651600
H	1.79078600	-0.82306700	-4.08914400
H	3.50748500	-0.46608200	-4.24727500
H	2.98301000	-2.99818600	-4.01835200
H	4.07897100	-2.38997600	-2.78486600
P	1.60802500	-1.11520600	-1.13473700
C	-0.21283000	-3.42587900	1.75316900

H	-0.27827600	-3.46839500	0.66263200
H	0.83519200	-3.55708800	2.03984900
H	-0.77865300	-4.27637800	2.14969800
C	-1.26169600	1.69744300	2.91658400
H	-1.45092900	2.23207900	3.85507300
H	-0.77991200	2.38840500	2.22164500
H	-2.23213600	1.41848400	2.49376400
C	4.06574600	0.42019400	-1.78398300
H	4.03205100	0.86406200	-0.78666500
H	4.78485900	-0.40319900	-1.75418400
H	4.46414500	1.17446400	-2.47326600
C	0.79385800	-3.40233900	-2.61654100
H	1.05421100	-4.34517400	-3.11213700
H	0.06356700	-3.62224600	-1.83292200
H	0.29280600	-2.76473500	-3.35250900
Cu	-0.65404600	0.16007300	-0.43219400
C	1.67248600	2.97024200	0.96739400
C	3.10018100	3.51251400	0.74838600
C	0.86092700	4.36731100	-0.99870100
C	3.08785200	4.90162400	0.09465700
C	2.29461700	4.88447600	-1.21904200
H	1.19070500	3.59905300	1.73405000
H	3.65378100	2.82042100	0.10127900
H	2.62986200	5.62526900	0.78476400
H	0.32629900	5.09778900	-0.36957100
H	2.26615500	5.88739200	-1.66269200
H	1.70351600	1.95187700	1.36434100
H	3.63480600	3.54341800	1.70576000
H	0.31801500	4.30741300	-1.94611000
H	4.11400700	5.24655400	-0.08183400
H	2.80532500	4.23367600	-1.94222800
C	0.83364300	3.01442400	-0.29406700
C	0.10439700	2.01143600	-0.77718900
C	-0.81623400	1.65104700	-1.74931000
H	-0.48567300	1.28571000	-2.72187500
H	-1.82666800	2.05827600	-1.74875500
Si	-2.59468100	-0.92471300	-1.21623500
C	-2.70259200	-0.97578200	-3.13361300
H	-2.61704700	0.02393500	-3.57377200
H	-1.89584300	-1.59002900	-3.55186100
H	-3.65300500	-1.40484400	-3.47481600
C	-2.97972100	-2.74747100	-0.73502100
H	-2.17768000	-3.41934100	-1.06221100
H	-3.10805000	-2.88663600	0.34370300
H	-3.90299000	-3.09357800	-1.21720200
C	-4.17000800	0.04579000	-0.67702800
C	-5.46483700	-0.40344600	-1.00199400
C	-4.08491400	1.24361500	0.05524200
C	-6.60813000	0.29889500	-0.61627100
H	-5.58689400	-1.32321300	-1.57061700
C	-5.22068900	1.95855200	0.44692000
H	-3.10327900	1.62886500	0.32229000
C	-6.48958300	1.48545200	0.11196800
H	-7.59285200	-0.07738200	-0.88378300
H	-5.11423800	2.88250000	1.01061000
H	-7.37787800	2.03473800	0.41316100

TS9A

Sum of electronic and thermal Free Energies= -3938.346537

C	2.23559200	-2.46272100	-0.64267000
C	1.04013500	-1.20271300	-2.78859500
C	2.56489700	-1.40738900	-2.87522700
C	2.91440100	-2.63018100	-2.01877500
H	2.84798000	-1.77840600	-0.04467800
H	0.55598600	-2.03817800	-3.31043400
H	2.87876500	-1.53097100	-3.91863500
H	3.08141800	-0.52055000	-2.48588800
H	2.53914100	-3.54047700	-2.50699100
H	3.99746400	-2.75607700	-1.90455700
P	0.66613000	-1.43178900	-0.95020400
C	-0.75686400	-2.62030200	-0.89962200
C	-1.85945100	-2.37735800	-0.04425300
C	-0.73577500	-3.79716900	-1.66728300
C	-2.86729700	-3.35294200	0.04424300
C	-1.75299300	-4.74491500	-1.57763900
H	0.09477200	-3.98472500	-2.34076700
C	-2.81810900	-4.52697900	-0.70486200
H	-3.71191700	-3.19508100	0.70592700
H	-1.70823300	-5.64901400	-2.17805000
H	-3.61298600	-5.26175800	-0.61324000
C	-3.43948700	0.16929200	0.23011900
C	-2.81522300	-1.25977100	2.53164300
C	-4.39487100	0.32661100	1.43691200
H	-3.01910100	1.14034400	-0.04644500
C	-4.30982000	-0.93789700	2.30636300
H	-2.66154100	-2.32926800	2.70968700
H	-4.09496200	1.19773500	2.03136900
H	-5.42080600	0.51709700	1.10014400
H	-4.83399700	-0.80858300	3.26167600

H	-4.80417600	-1.76846200	1.78869500
P	-1.94098500	-0.78422000	0.91350400
C	2.07986500	-3.77213200	0.13541300
H	1.53703600	-3.63478000	1.07492400
H	1.54402900	-4.52923400	-0.44339400
H	3.06833900	-4.17807000	0.38030300
C	0.54201400	0.10795200	-3.39366900
H	0.86702800	0.18789800	-4.43810400
H	-0.54945200	0.16612600	-3.37689000
H	0.91681600	0.97512400	-2.84309200
C	-4.11303300	-0.42749900	-1.01005700
H	-3.39528700	-0.58474500	-1.82080600
H	-4.59596900	-1.38799600	-0.80677200
H	-4.88255700	0.26226500	-1.37581300
C	-2.22975300	-0.47334000	3.71466300
H	-2.75639200	-0.72974700	4.64143600
H	-1.16908600	-0.69325700	3.85659300
H	-2.32125600	0.60862900	3.56948500
Cu	0.04574100	0.30116200	0.32076000
C	-1.59821900	2.96380400	-2.23076000
C	-2.91784100	3.76201300	-2.17960000
C	-0.53532900	4.61717100	-0.63961900
C	-2.66786500	5.24546600	-1.87104600
C	-1.85369900	5.41583300	-0.58015800
H	-1.02497100	3.31492100	-3.10605000
H	-3.56205100	3.33717800	-1.39645900
H	-2.11509200	5.69860000	-2.70730000
H	0.09743900	5.06875300	-1.42243000
H	-1.64756000	6.47857100	-0.39748000
H	-1.79973600	1.89977500	-2.38653800
H	-3.46289000	3.65712300	-3.12683700
H	0.01108100	4.72086100	0.30358100
H	-3.61957200	5.78718100	-1.79798300
H	-2.44940800	5.05844400	0.27143500
C	-0.77323700	3.14822000	-0.96921800
C	-0.34018700	2.12560800	-0.21907300
C	0.43521800	2.20745400	1.03084000
H	-0.13244600	2.49434300	1.91952500
H	1.36641100	2.78290900	0.98423800
Si	1.77065500	0.68755800	2.03567200
C	1.88512900	1.81912400	3.56891300
H	1.97772800	2.88111800	3.32426800
H	0.99841300	1.69660300	4.20324800
H	2.75672200	1.53911900	4.17140200
C	1.80213200	-1.03631100	2.88418300
H	0.86928800	-1.22037000	3.42549700
H	1.94531900	-1.85556500	2.17887400
H	2.61418800	-1.07599700	3.62245400
C	3.41355800	0.84144200	1.07061200
C	4.59886300	0.30086500	1.60720900
C	3.51687200	1.49324000	-0.17425900
C	5.82297600	0.40527400	0.94274000
H	4.57129900	-0.21297100	2.56534600
C	4.73791400	1.60487900	-0.84459500
H	2.63043200	1.91985500	-0.63652900
C	5.89649200	1.06031100	-0.28759200
H	6.71850500	-0.02231000	1.38659300
H	4.78358400	2.12009000	-1.80073200
H	6.84737800	1.14692000	-0.80643100

10A

Sum of electronic and thermal Free Energies= -3938.408638

C	0.65320000	-3.04298800	-0.01621000
C	-0.07382600	-2.11890000	-2.51804300
C	1.16625500	-3.03481700	-2.44293500
C	1.01566400	-3.94169100	-1.21631300
H	1.56619100	-2.51767400	0.28902300
H	-0.93041800	-2.71819900	-2.85114900
H	1.27908900	-3.60709300	-3.37165000
H	2.06823700	-2.42018000	-2.33053200
H	0.22067600	-4.68059200	-1.38795300
H	1.93386800	-4.50484400	-1.01139100
P	-0.40829000	-1.63908200	-0.71944800
C	-2.17956300	-2.14238800	-0.44111700
C	-3.04858300	-1.24080700	0.21941600
C	-2.67148900	-3.40263100	-0.82320900
C	-4.36198500	-1.65065800	0.50809800
C	-3.97994300	-3.78818900	-0.54053900
H	-2.01911900	-4.09947900	-1.34044900
C	-4.82697000	-2.91038500	0.13831000
H	-5.03526400	-0.97603400	1.02819100
H	-4.33396000	-4.77058000	-0.84011000
H	-5.84633600	-3.20360800	0.37314900
C	-3.35558800	1.69792500	-0.36535000
C	-3.28399400	0.86756100	2.29918000
C	-3.92040100	2.67163100	0.69557400
H	-2.60177500	2.21364500	-0.96846800
C	-4.41031700	1.84814300	1.89743100
H	-3.69797900	-0.05259700	2.72408000

H	-3.12924300	3.35776000	1.01980600
H	-4.72015400	3.28844500	0.26895900
H	-4.69105800	2.49222700	2.73972400
H	-5.31113100	1.28971200	1.61408200
P	-2.39431100	0.43638200	0.68396600
C	0.09849700	-3.78330400	1.20173300
H	-0.11484600	-3.09824100	2.02754600
H	-0.82227800	-4.32576300	0.96861000
H	0.83459000	-4.51226300	1.56040500
C	0.09413400	-0.92554100	-3.46034600
H	0.32515100	-1.27030000	-4.47536900
H	-0.81605800	-0.31995800	-3.51534500
H	0.90648400	-0.27220000	-3.12867900
C	-4.42759700	1.14737800	-1.31276900
H	-4.01802900	0.40772800	-2.00665300
H	-5.25525300	0.67140700	-0.77934900
H	-4.84421600	1.96882300	-1.90744400
C	-2.29825200	1.47343400	3.31007300
H	-2.81781400	1.73140000	4.24046600
H	-1.49521600	0.77112100	3.55155200
H	-1.82766500	2.38277600	2.92236400
Cu	-0.16198300	0.46918500	0.13968100
C	0.41883900	2.65046700	-2.06510100
C	-0.34067900	3.96551400	-2.33066800
C	2.29574700	3.91155700	-0.98562500
C	0.63063100	5.14668700	-2.46586000
C	1.55831600	5.24351200	-1.24636900
H	1.00805700	2.41499200	-2.96922600
H	-1.02292000	4.15705900	-1.48957200
H	1.23994800	5.00685200	-3.37114100
H	2.97083000	3.72782700	-1.83926000
H	2.28181900	6.05795000	-1.38524800
H	-0.29037300	1.82412600	-1.92936300
H	-0.96156600	3.87858300	-3.23282200
H	2.93865100	4.02150300	-0.10834000
H	0.07893600	6.08548900	-2.60494500
H	0.96254100	5.49674500	-0.35857500
C	1.32593600	2.74460300	-0.84815400
C	1.18102100	1.89559900	0.20078500
C	2.06595900	2.04545600	1.43577800
H	1.44830800	2.42246600	2.27001600
H	2.87548600	2.78379800	1.32798500
Si	2.81914000	0.45950400	2.14835800
C	1.44576000	-0.57448300	2.95997900
H	1.07887700	-0.07896900	3.86648700
H	0.59966400	-0.66610400	2.26839000
H	1.77392300	-1.58180500	3.23679700
C	4.07684400	0.91582800	3.49735900
H	3.60438900	1.51859600	4.28185300
H	4.50322700	0.02700300	3.97600200
H	4.90743700	1.49865600	3.08496200
C	3.71873000	-0.59569500	0.85071800
C	4.35387400	-1.79840300	1.21872000
C	3.82459900	-0.19395700	-0.49454400
C	5.05978100	-2.56872600	0.29220200
H	4.30402100	-2.14359800	2.25008700
C	4.53630400	-0.95627100	-1.42586500
H	3.32730500	0.71678000	-0.81576100
C	5.15453700	-2.14618800	-1.03593900
H	5.54104900	-3.49158600	0.60618700
H	4.61031100	-0.61832000	-2.45661000
H	5.70951800	-2.73801700	-1.75923200

TS10A

Sum of electronic and thermal Free Energies= -4126.969204

C	2.54177600	-2.84234500	-1.25913000
C	2.59048200	-2.89809400	1.51491500
C	2.35433400	-4.23827800	0.78368400
C	3.02137900	-4.14920000	-0.59494800
H	1.50793400	-2.98294800	-1.59742800
H	3.64251500	-2.84598200	1.82159200
H	2.73893800	-5.07398100	1.37974900
H	1.27470900	-4.39253900	0.66319800
H	4.11492400	-4.13450700	-0.48354400
H	2.77807600	-5.01367300	-1.22389500
P	2.33793200	-1.61270700	0.16183300
C	3.84608000	-0.53557100	0.16736300
C	3.70606500	0.85166500	-0.08966300
C	5.13235300	-1.06243100	0.37468500
C	4.86324600	1.64795400	-0.15174900
C	6.26574100	-0.25432200	0.32427600
H	5.25451800	-2.12390500	0.56684100
C	6.13050300	1.10797400	0.05429200
H	4.77732800	2.70750700	-0.36965300
H	7.24883300	-0.68737400	0.48480900
H	7.00721200	1.74705700	0.00227800
C	1.66892900	2.92260500	0.84497500
C	2.27601300	2.72514700	-1.87877400
C	1.32594600	4.13960200	-0.04976700

H	0.76591800	2.59284200	1.36894900
C	2.27477400	4.14266100	-1.25847800
H	3.24799300	2.49631000	-2.32713000
H	0.29003100	4.05536200	-0.39862500
H	1.39159900	5.07152300	0.52362100
H	1.97931300	4.89420900	-2.00037900
H	3.28664400	4.40824000	-0.92837400
P	2.01649900	1.55155800	-0.41564000
C	3.37616600	-2.36774600	-2.44868200
H	2.96533800	-1.45367400	-2.88946800
H	4.41577100	-2.16974900	-2.16968600
H	3.37817500	-3.13539900	-3.23061400
C	1.69591500	-2.69222400	2.74038200
H	1.87429600	-3.48562500	3.47570400
H	1.89834400	-1.73524900	3.23277700
H	0.64034200	-2.71744100	2.45626400
C	2.75031800	3.21078500	1.89210700
H	3.03536200	2.30791800	2.43981800
H	3.65973900	3.63092500	1.45383900
H	2.36826100	3.93633400	2.61929800
C	1.18715800	2.53452400	-2.94532500
H	1.35167800	3.22484900	-3.78066100
H	1.19238800	1.51536500	-3.34368100
H	0.18567200	2.72010500	-2.54525000
Cu	0.52497800	-0.24385100	-0.10690400
C	-1.41032900	-0.05799200	2.48739000
C	-1.07400400	0.98835800	3.56861900
C	-3.06853000	1.52839100	1.44464800
C	-2.25076100	1.94080200	3.81868800
C	-2.72206700	2.58951900	2.51083400
H	-2.19666700	-0.71978000	2.88411700
H	-0.19879300	1.57402400	3.24966200
H	-3.08381700	1.37406300	4.25856400
H	-3.93828100	0.95510100	1.79787400
H	-3.59384900	3.22986200	2.69503700
H	-0.54842200	-0.69773900	2.29050100
H	-0.78690700	0.48419500	4.50034100
H	-3.38459800	2.02136200	0.52224100
H	-1.97455800	2.70955500	4.55158700
H	-1.92774600	3.24524300	2.12501900
C	-1.91813500	0.56510200	1.20088300
C	-1.39389000	0.27352600	-0.01555700
C	-1.96952000	0.82948500	-1.30929000
H	-1.25534000	0.66225200	-2.12539400
H	-2.08884500	1.92170100	-1.23357200
Si	-3.63615500	0.17818700	-2.03258400
C	-3.34739800	-1.21247800	-3.28125400
H	-2.69552200	-0.87342400	-4.09486000
H	-2.86147900	-2.07351300	-2.81728800
H	-4.29741100	-1.53521100	-3.72189900
C	-4.40126300	1.64711300	-2.96595300
H	-3.69645900	2.01998500	-3.71850400
H	-5.31927200	1.36280700	-3.49187500
H	-4.64123100	2.48381000	-2.30021900
C	-4.86750600	-0.42319700	-0.72078400
C	-6.11802900	0.19990700	-0.55176500
C	-4.57903400	-1.52926500	0.10422700
C	-7.03969900	-0.25087300	0.39638000
H	-6.38331600	1.05520100	-1.16808800
C	-5.49468900	-1.98221500	1.05583500
H	-3.62423500	-2.04027800	0.02390200
C	-6.72809300	-1.34399400	1.20558700
H	-7.99790900	0.25155000	0.50309300
H	-5.24268200	-2.83458800	1.68138700
H	-7.44096500	-1.69731500	1.94622500
C	-0.89245000	-1.84757900	-0.37266000
O	-1.14529300	-2.51104800	0.61202500
O	-0.74456800	-1.94957200	-1.58335400

TS11A

Sum of electronic and thermal Free Energies= -4126.971639

C	-0.15985300	3.14472700	-0.59587200
C	-1.77963200	2.86444400	1.62424600
C	-0.73950500	4.00218200	1.65970500
C	-0.45848500	4.42520100	0.21155400
H	0.84729900	2.80763100	-0.31587400
H	-2.74197600	3.29589800	1.32054300
H	-1.10243600	4.83619500	2.27161400
H	0.18581300	3.64048100	2.12735300
H	-1.33806600	4.93474900	-0.20481800
H	0.37717300	5.13212700	0.14381600
P	-1.22953500	1.78321000	0.17183600
C	-2.78687600	1.60802000	-0.82207500
C	-3.32563700	0.31412500	-1.03752800
C	-3.45960100	2.72192700	-1.35391500
C	-4.49223000	0.18639900	-1.81026600
C	-4.61560300	2.57565700	-2.11707900
H	-3.07815200	3.72082200	-1.16712500
C	-5.12893200	1.29964400	-2.35383600

H	-4.91716800	-0.79702000	-1.98520000
H	-5.11257400	3.45177300	-2.52355900
H	-6.02874500	1.17265000	-2.94894600
C	-3.50597600	-1.65027000	1.23513500
C	-2.94944000	-2.64789800	-1.31609000
C	-3.75357700	-3.15669600	0.98784000
H	-2.84545500	-1.52268400	2.09790900
C	-4.05973300	-3.35611300	-0.50516500
H	-3.32325400	-2.30670000	-2.28690200
H	-2.85209200	-3.71561600	1.26141300
H	-4.56783700	-3.52323100	1.62402800
H	-4.11752300	-4.41887100	-0.76888200
H	-5.03682500	-2.91625700	-0.74172600
P	-2.47216600	-1.14325900	-0.27585500
C	-0.19331700	3.29847500	-2.11785800
H	0.04783200	2.35847600	-2.62291800
H	-1.17153900	3.62573600	-2.47912800
H	0.54548600	4.04377600	-2.43397300
C	-1.96865900	2.12765800	2.95140500
H	-2.26621200	2.83515700	3.73429800
H	-2.74917300	1.36440000	2.88131300
H	-1.05336200	1.62599400	3.27463800
C	-4.79327700	-0.85330400	1.47063200
H	-4.59601600	0.21681800	1.58499200
H	-5.51448500	-0.96556600	0.65517700
H	-5.27351300	-1.20325200	2.39173600
C	-1.72447000	-3.54835600	-1.54530500
H	-2.02208300	-4.46043200	-2.07573400
H	-0.97008800	-3.03864700	-2.15087900
H	-1.24760100	-3.83375500	-0.60301200
Cu	-0.41877900	-0.34404200	0.40970800
C	1.83809100	0.59952700	2.61951400
C	2.36716400	0.26510500	4.02797700
C	3.81260000	-0.53550900	1.56725200
C	3.89364700	0.11418400	4.03216600
C	4.34803000	-0.89715800	2.97198400
H	2.22233900	1.59361400	2.33177600
H	1.89704100	-0.66927900	4.35833400
H	4.35599300	1.08986700	3.82079000
H	4.25947900	0.42193100	1.26027000
H	5.44328800	-0.95660500	2.94204400
H	0.75161600	0.65451300	2.63122600
H	2.05651300	1.04275400	4.73738700
H	4.15233000	-1.27486800	0.84134900
H	4.24698700	-0.18962700	5.02548900
H	3.98428400	-1.89676700	3.24502900
C	2.30029600	-0.39541000	1.57434100
C	1.43651000	-1.08622200	0.77429000
C	1.95155300	-2.08335700	-0.25386900
H	1.16690700	-2.82779600	-0.43237600
H	2.79765800	-2.67304200	0.12923200
Si	2.45199100	-1.44062900	-1.97462500
C	0.96915900	-0.62861900	-2.83838300
H	0.25322700	-1.38516900	-3.17677200
H	0.43502900	0.03751600	-2.15207800
H	1.27644800	-0.04615800	-3.71333600
C	3.01482700	-2.93005500	-3.00604500
H	2.20448300	-3.66294000	-3.09040200
H	3.30500700	-2.63346200	-4.01977100
H	3.86821800	-3.44609400	-2.55274700
C	3.86395500	-0.17242800	-1.92782400
C	5.21272700	-0.57083100	-1.98456100
C	3.60666200	1.20795000	-1.83127500
C	6.25401000	0.35806100	-1.93589000
H	5.46094500	-1.62617100	-2.06997000
C	4.64080000	2.14492300	-1.78170800
H	2.57923200	1.56269200	-1.79966800
C	5.97000800	1.72084200	-1.83180700
H	7.28568900	0.01913200	-1.98162900
H	4.41090900	3.20488600	-1.70776600
H	6.77775400	2.44678800	-1.79480800
C	0.01994700	-1.99632500	1.90500500
O	0.03666400	-3.15956900	1.56291100
O	-0.48137200	-1.26825700	2.75603100

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Sum of electronic and thermal Free Energies= -4127.029324

C	-2.86952500	2.91439500	-1.36905100
C	-3.12567600	2.60754800	1.36709100
C	-2.87709900	4.03775800	0.84109500
C	-3.43030600	4.12033200	-0.58872000
H	-1.81315900	3.12255300	-1.58463000
H	-4.19750600	2.50026500	1.57753600
H	-3.33361300	4.77953200	1.50678200
H	-1.79773000	4.24042700	0.83005000
H	-4.52792500	4.07630400	-0.56704800
H	-3.16220500	5.06421200	-1.07886400
P	-2.73741100	1.50669400	-0.11348800
C	-4.23832800	0.43060400	-0.29962100

C	-4.07243300	-0.97718600	-0.35114800
C	-5.53318300	0.96688100	-0.40260700
C	-5.20769400	-1.78418100	-0.53891500
C	-6.64742100	0.15016300	-0.58255400
H	-5.67497700	2.04186300	-0.34417800
C	-6.48168700	-1.23314000	-0.65918900
H	-5.10022900	-2.86345800	-0.58848000
H	-7.63697900	0.59049600	-0.66525200
H	-7.34121000	-1.88145200	-0.80402400
C	-2.31946700	-2.61871300	1.48637400
C	-2.39585800	-3.26903800	-1.23125400
C	-1.85817100	-4.03959100	1.08434500
H	-1.53192100	-2.12174200	2.06186400
C	-2.56370000	-4.43207300	-0.22525800
H	-3.25052700	-3.21320000	-1.91299800
H	-0.77332900	-4.04014600	0.92883200
H	-2.06416500	-4.75613400	1.88830300
H	-2.16216400	-5.36728500	-0.63380400
H	-3.62878800	-4.60618700	-0.02745400
P	-2.36613000	-1.70210700	-0.17368000
C	-3.56024600	2.59758400	-2.69593300
H	-3.09642000	1.73892900	-3.19197700
H	-4.62190300	2.37153500	-2.56391500
H	-3.48182900	3.45392600	-3.37545500
C	-2.32680800	2.24278500	2.62156200
H	-2.50396200	2.97748700	3.41601900
H	-2.62080600	1.26124700	3.00725600
H	-1.25263800	2.19786500	2.41843600
C	-3.60709500	-2.60642400	2.31681200
H	-3.94475300	-1.58718900	2.52622300
H	-4.43030700	-3.12858300	1.82081600
H	-3.42789800	-3.10312200	3.27745400
C	-1.11130300	-3.37968000	-2.06643100
H	-1.13782600	-4.28272600	-2.68747300
H	-0.98999100	-2.51608700	-2.72722200
H	-0.21885700	-3.43257700	-1.43478100
Cu	-1.06112500	0.07453200	-0.14959000
C	2.70978400	2.88546500	-0.65565200
C	2.84235300	4.33849300	-0.15212800
C	4.78526800	2.25367700	0.61513800
C	4.30164600	4.70731200	0.14549900
C	4.93331600	3.70492800	1.12001300
H	3.23418300	2.80700400	-1.62144500
H	2.24519000	4.45481200	0.76317300
H	4.87253600	4.70472700	-0.79441900
H	5.36335700	2.14865900	-0.31610500
H	5.99442500	3.93711200	1.27477100
H	1.66869800	2.63279400	-0.85200700
H	2.41891400	5.02696500	-0.89456100
H	5.23903500	1.56525600	1.33048200
H	4.36750300	5.72595000	0.54815400
H	4.44431800	3.79295700	2.09987000
C	3.34202600	1.90092000	0.31056400
C	2.69051000	0.85173200	0.86301600
C	3.28724800	-0.12631800	1.85178800
H	2.54583100	-0.30973700	2.63827500
H	4.18413000	0.26939400	2.33688200
Si	3.72952500	-1.82791200	1.09576800
C	2.14595600	-2.74815000	0.60964600
H	1.48915200	-2.86740900	1.47819100
H	1.58919600	-2.19476600	-0.15298400
H	2.38060600	-3.74183300	0.21172500
C	4.65755200	-2.83658700	2.40517600
H	4.02777000	-2.97671400	3.29102500
H	4.93041300	-3.83061900	2.03422300
H	5.57624300	-2.33809800	2.73341400
C	4.80943700	-1.61458000	-0.44537700
C	6.14590800	-2.05179400	-0.48635700
C	4.28736200	-1.00586000	-1.60609800
C	6.93292900	-1.89118900	-1.62941100
H	6.58579000	-2.52839000	0.38650500
C	5.07035100	-0.84243300	-2.75009400
H	3.26198100	-0.64437200	-1.61669100
C	6.39533200	-1.28481500	-2.76507500
H	7.96274200	-2.23932500	-1.63262500
H	4.64531500	-0.36910600	-3.63149700
H	7.00386300	-1.15806000	-3.65673400
C	1.25375200	0.53119100	0.53246500
O	0.85832900	0.54425400	-0.68648500
O	0.46872600	0.20280700	1.46860600

TS12A

Sum of electronic and thermal Free Energies= -4981.817363

C	0.87175900	-3.53367100	0.70135800
C	1.84545200	-2.87920800	3.20009000
C	0.73394900	-3.95188400	3.13161300
C	0.80810000	-4.64228300	1.76507800
H	-0.11027000	-3.04939500	0.63153000
H	2.79412000	-3.36834100	3.44222900

H	0.82316800	-4.66047100	3.96402100	O	-0.56326100	-0.90794600	-0.69833100
H	-0.24461000	-3.46402200	3.23605500	O	-1.51574500	1.06343100	-0.14504200
H	1.70793100	-5.27003000	1.70602000	B	-0.06902400	2.53885800	-0.59010500
H	-0.05018200	-5.30464800	1.59403000	O	0.73696200	1.80440300	-1.49338900
P	1.95994100	-2.16011200	1.43720900	O	-0.89746200	3.41558100	-1.28087000
C	3.67684400	-2.62736500	0.86051700	C	0.09211800	1.88218500	-2.77763300
C	4.30906500	-1.85762700	-0.15108200	C	-0.83759800	3.10975300	-2.67594000
C	4.38954600	-3.70959000	1.40612000	H	-0.43908600	3.97782800	-3.21606800
C	5.61998700	-2.18315100	-0.54069400	H	-1.84219000	2.89896700	-3.05804700
C	5.68559000	-4.02476600	1.00194000	H	0.85107800	1.99123400	-3.55858000
H	3.92714700	-4.33207200	2.16365600	H	-0.46533100	0.95499800	-2.95501500
C	6.31052100	-3.25100600	0.02707300	C	-2.55003800	-2.58627100	-2.04701400
H	6.12006800	-1.59262400	-1.30139000	C	-2.51825300	-4.10814000	-1.78722700
H	6.20101200	-4.87057500	1.44826000	C	-4.76418400	-2.42326900	-0.88713600
H	7.32366400	-3.47546000	-0.29347400	C	-3.93027800	-4.69591900	-1.66642500
C	4.24937800	1.15759000	-0.47819600	C	-4.75119200	-3.94287900	-0.61213300
C	4.13058200	-0.45069500	-2.76110900	H	-3.04290500	-2.42112200	-3.01922500
C	4.43363200	1.86383700	-1.84059700	H	-1.96570200	-4.29643600	-0.85691600
H	3.51405700	1.70404600	0.11728200	H	-4.43700200	-4.61885900	-2.63937400
C	4.98927500	0.83806700	-2.84339500	H	-5.27164600	-2.25708300	-1.85082500
H	4.75168000	-1.34042100	-2.89307500	H	-5.78025800	-4.32109200	-0.58292600
H	3.46058300	2.23527000	-2.18192500	H	-1.53902900	-2.19212800	-2.11369800
H	5.08906200	2.73539000	-1.73551600	H	-1.96377300	-4.60806500	-2.59130800
H	4.99506700	1.23535400	-3.86508600	H	-5.36865300	-1.91413900	-0.13534600
H	6.03146200	0.60795200	-2.59077500	H	-3.88255400	-5.76472000	-1.42311700
P	3.43353400	-0.46062700	-1.00011300	H	-4.32072700	-4.12104600	0.38284400
C	1.26011200	-3.99263900	-0.70369900	C	-3.35698600	-1.86101300	-0.98727800
H	1.25835800	-3.14006400	-1.38969000	C	-2.92936100	-0.81895700	-0.23122700
H	2.25400800	-4.45054400	-0.72506500	C	-3.82214700	-0.09126500	0.76087400
H	0.53815200	-4.72478700	-1.08176400	H	-3.19535400	0.37356500	1.52733700
C	1.58493700	-1.79735000	4.25451500	H	-4.48014600	-0.79678400	1.27622700
H	1.46785100	-2.24733300	5.24795400	Si	-4.90746400	1.31068700	0.00792900
H	2.41023800	-1.08053400	4.30886400	C	-4.69298200	1.42633900	-1.86699700
H	0.67415500	-1.23268400	4.03067400	H	-3.63454600	1.59676600	-2.08588000
C	5.53985800	1.05250400	0.34144400	H	-5.00370500	0.51461700	-2.38665800
H	5.38890100	0.47561000	1.25812000	H	-5.26163200	2.26624800	-2.28116700
H	6.35742500	0.58119100	-0.21207100	C	-4.44690400	2.97229900	0.78047600
H	5.86023500	2.05974400	0.62800300	H	-3.42630500	3.23651100	0.48739700
C	3.01817300	-0.49770600	-3.81707500	H	-5.12025300	3.76895100	0.44595000
H	3.45435600	-0.50696400	-4.82273300	H	-4.49301300	2.93689200	1.87475100
H	2.39979600	-1.39491900	-3.71318400	C	-6.72554600	0.91712700	0.40861400
H	2.35820500	0.37129200	-3.74752800	C	-7.11435000	0.57464300	1.71872200
Cu	1.28206100	-0.42438400	-0.75348900	C	-7.73727200	0.96689300	-0.56750100
C	-1.56603200	-0.17586900	-0.37492200	C	-8.44364600	0.29751000	2.04065400

H	-6.36621800	0.52092700	2.50787300
C	-9.07086100	0.69069100	-0.25535500
H	-7.48375500	1.22290000	-1.59332400
C	-9.42756900	0.35469500	1.05106000
H	-8.71247000	0.03645900	3.06105700
H	-9.82998100	0.73584300	-1.03213900
H	-10.46365600	0.13798400	1.29711400
Si	0.47008300	3.05100300	1.30275600
C	-0.78129200	4.29048700	2.01351600
H	-0.46600600	4.64703300	3.00057400
H	-0.88877700	5.16011600	1.35753000
H	-1.76955400	3.83118600	2.11640100
C	0.60678300	1.59530400	2.50968200
H	-0.36248000	1.08945000	2.56739900
H	1.34139500	0.84831100	2.19383400
H	0.87194000	1.92824300	3.51995200
C	2.15973800	3.93969000	1.21755100
C	3.15433500	3.77966500	2.20027600
C	2.44309700	4.82396400	0.15742600
C	4.37003600	4.46682600	2.13314600
H	2.98111300	3.10783500	3.03770000
C	3.65313300	5.51616700	0.08217700
H	1.70073000	4.97753200	-0.62330900
C	4.62313200	5.33792100	1.07186100
H	5.11636700	4.32594200	2.91118400
H	3.83967300	6.19526300	-0.74610400
H	5.56554700	5.87662700	1.01831100

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Sum of electronic and thermal Free Energies= -4981.823008

C	-1.40559100	3.43782100	0.61062900
C	-2.67719700	2.87223000	2.99073100
C	-1.69734600	4.06978500	2.97855200
C	-1.62778100	4.63121000	1.55361600
H	-0.38324900	3.06424600	0.74997200
H	-3.70027800	3.25339600	3.06366600
H	-1.99751100	4.82766100	3.71222500
H	-0.69925000	3.72102500	3.27632100
H	-2.56815200	5.13763900	1.29751800
H	-0.82892900	5.37638900	1.44599000
P	-2.46830600	2.01991600	1.29643000
C	-4.11450600	2.29698600	0.45054600
C	-4.52573300	1.41764100	-0.58496300
C	-4.98876000	3.33512400	0.81796100
C	-5.79311600	1.59120300	-1.16767600
C	-6.23662300	3.50228500	0.21993600
H	-4.69521200	4.04045000	1.58704000
C	-6.64814100	2.61748300	-0.77343900
H	-6.12834400	0.91220800	-1.94461100
H	-6.88111000	4.31925300	0.53210800
H	-7.62210600	2.72389000	-1.24209800
C	-4.11807600	-1.58779000	-0.66799500
C	-3.85498600	-0.13652700	-3.03915900
C	-3.93899200	-2.41376100	-1.96119400
H	-3.45258100	-1.97507100	0.10758000
C	-4.43972900	-1.57158300	-3.14856100
H	-4.61384300	0.60421800	-3.30328700
H	-2.87526700	-2.64543000	-2.08162100
H	-4.46883700	-3.36975300	-1.88386600
H	-4.16574800	-2.02760400	-4.10679300
H	-5.53486400	-1.52377500	-3.12645400
P	-3.41476100	0.07198200	-1.21013900
C	-1.59907500	3.72422100	-0.87802300
H	-1.42525800	2.81107200	-1.45616200
H	-2.61049700	4.08021800	-1.09688100
H	-0.88808300	4.48256400	-1.22287100
C	-2.44691500	1.91187800	4.16370300
H	-2.52665700	2.44593800	5.11848400
H	-3.18408300	1.10269400	4.17331700
H	-1.45464500	1.45255700	4.11675700
C	-5.54910200	-1.59401600	-0.12211700
H	-5.65372600	-0.93189200	0.74179300
H	-6.28995600	-1.28526300	-0.86624200
H	-5.79944500	-2.60928200	0.20318800
C	-2.64245200	0.10357400	-3.94947100
H	-2.93036600	-0.01437400	-5.00058600
H	-2.24274300	1.11556900	-3.82635400
H	-1.83321300	-0.60177300	-3.74307800
Cu	-1.30024600	0.18039000	-0.71855100
C	1.59186700	0.21341000	-0.24855200
O	0.49952300	0.83810600	-0.34176400
O	1.70810700	-1.07181500	-0.28054900
B	0.58635800	-2.20105900	-0.28665900
O	-0.43589800	-1.82974900	-1.28299200
O	1.24526900	-3.37530700	-0.81735500
C	0.07180800	-2.28708700	-2.54116900
C	0.89208600	-3.53879800	-2.18080000
H	0.29263900	-4.45327900	-2.30612600
H	1.78604100	-3.63473600	-2.81118400

H	-0.76059000	-2.50552100	-3.21913200
H	0.70302700	-1.51449200	-3.00581500
C	2.27647700	2.92257900	-1.51253800
C	2.14854500	4.37369100	-0.99912000
C	4.56575100	2.75756500	-0.50748300
C	3.51787900	5.04901500	-0.84643500
C	4.45511000	4.20331700	0.02407700
H	2.71920700	2.96143700	-2.52086900
H	1.63691000	4.36346400	-0.02742700
H	3.96918100	5.17969000	-1.84056400
H	5.02058300	2.79586700	-1.50978300
H	5.45310300	4.65530100	0.06780800
H	1.29438000	2.46384400	-1.59985500
H	1.51539500	4.94960900	-1.68495900
H	5.25143700	2.18172000	0.11482900
H	3.40345900	6.05375000	-0.42144100
H	4.07477800	4.17633900	1.05410300
C	3.20202000	2.10439900	-0.63478800
C	2.90643100	0.91398500	-0.05382300
C	3.90740700	0.09990300	0.74981200
H	3.36961800	-0.51574700	1.47703700
H	4.55726300	0.76185300	1.32816100
Si	5.02489600	-1.10265700	-0.26996400
C	4.67292900	-0.97059200	-2.12242600
H	3.62540900	-1.22784800	-2.30505900
H	4.84705600	0.03576700	-2.51640700
H	5.29417900	-1.67026100	-2.69230500
C	4.74183200	-2.88000300	0.29968700
H	3.72226800	-3.19471200	0.05237800
H	5.44436400	-3.56373600	-0.18994000
H	4.88079500	-2.98638100	1.38154700
C	6.83350900	-0.61421600	0.06000100
C	7.31881500	-0.51021800	1.37872700
C	7.74511300	-0.35880600	-0.98043300
C	8.64535100	-0.17061900	1.64718600
H	6.65078600	-0.69955900	2.21733800
C	9.07523800	-0.01794800	-0.72179100
H	7.41555900	-0.42500000	-2.01434600
C	9.52897900	0.07697000	0.59414200
H	8.99052000	-0.09991000	2.67546900
H	9.75594400	0.17380500	-1.54732700
H	10.56283600	0.34173400	0.79893900
Si	-0.00727000	-2.56510400	1.65672200
C	1.30633600	-3.65749300	2.50113600
H	0.99601700	-3.95626900	3.50879700
H	1.49154800	-4.56265400	1.91508100
H	2.25940300	-3.12287700	2.58558200
C	-0.24830800	-1.04487600	2.77940900
H	0.65642200	-0.42541200	2.77466600
H	-1.07801400	-0.41033900	2.45401800
H	-0.43336400	-1.34034900	3.81927000
C	-1.63860600	-3.55844400	1.65547500
C	-2.70761000	-3.28450000	2.52867400
C	-1.80218900	-4.63407700	0.75889000
C	-3.88102800	-4.04532100	2.51490700
H	-2.62612200	-2.46375000	3.23741200
C	-2.96944800	-5.39920100	0.73765300
H	-0.99652100	-4.87508700	0.06927400
C	-4.01531000	-5.10633200	1.61757800
H	-4.68690000	-3.81267500	3.20696700
H	-3.06390900	-6.22664000	0.03844400
H	-4.92335400	-5.70384600	1.60753500

TS13A

Sum of electronic and thermal Free Energies= -4981.801107

C	-1.59758100	-3.61143900	-0.29554700
C	-2.13565500	-2.94114900	-2.90593900
C	-1.59927600	-4.37340300	-2.63955300
C	-1.94782200	-4.79391300	-1.21099100
H	-0.50971100	-3.47221700	-0.29115000
H	-3.15492400	-2.99762800	-3.29997400
H	-1.98222700	-5.07601700	-3.38898300
H	-0.50670000	-4.36300200	-2.74844500
H	-3.01828000	-5.02171900	-1.12404000
H	-1.40536100	-5.69919200	-0.90973500
P	-2.21018600	-2.06883400	-1.20918500
C	-4.01541500	-2.04529900	-0.73575800
C	-4.44324900	-1.20226700	0.32767900
C	-4.96425200	-2.88526200	-1.34447500
C	-5.77830000	-1.28578700	0.76022500
C	-6.29210900	-2.92419900	-0.92349100
H	-4.66837700	-3.53675900	-2.15890700
C	-6.70021700	-2.12958400	0.14558800
H	-6.10665200	-0.68384900	1.59911000
H	-6.99720900	-3.58525700	-1.41950900
H	-7.72600400	-2.16522600	0.50093400
C	-4.00522700	1.63178800	1.44484600
C	-3.31958200	-0.59705400	2.98172800
C	-3.98889400	1.80336900	2.98450100

H	-3.28336000	2.32272000	1.00178100	H	4.03672500	-5.29364000	1.82353700
C	-4.26229100	0.43928800	3.63441500	H	5.03841500	-2.86661200	1.55192200
H	-3.75882400	-1.59889400	3.01880300	H	5.55282800	-4.69884700	-0.03639600
H	-3.00260200	2.16196200	3.29810700	H	1.31378700	-2.63653900	1.59032600
H	-4.71798700	2.55965800	3.29799300	H	1.58067200	-5.11849200	1.61728700
H	-4.11351400	0.47209500	4.72070600	H	5.28760700	-2.22680500	-0.06108100
H	-5.30887400	0.15517400	3.46958900	H	3.52625800	-6.15348000	0.37523300
P	-3.22106400	-0.07559500	1.16064000	H	4.18834400	-4.23863600	-1.05045000
C	-2.06764400	-3.78295700	1.14754000	C	3.21936800	-2.22274600	0.63988600
H	-1.77484400	-2.93452500	1.77008200	C	2.88015100	-1.05638400	0.03448600
H	-3.15473700	-3.89543000	1.20712300	C	3.84483100	-0.20012300	-0.76766600
H	-1.61539200	-4.68173700	1.58303000	H	3.28919000	0.33171000	-1.54637000
C	-1.27052100	-2.20133600	-3.93550400	H	4.57217900	-0.83119200	-1.28466100
H	-1.12197900	-2.83267200	-4.81980100	Si	4.81706900	1.14003300	0.22723600
H	-1.73106800	-1.26989300	-4.27203600	C	4.40026600	1.06986800	2.06884000
H	-0.28200100	-1.96038600	-3.52931500	H	3.33281500	1.26447000	2.20720400
C	-5.37184900	1.92694500	0.81343900	H	4.62080900	0.09127500	2.50733500
H	-5.42021300	1.62083100	-0.23572100	H	4.95793300	1.82680200	2.63119200
H	-6.19463000	1.43471800	1.33871500	C	4.41704700	2.85065900	-0.46618800
H	-5.55844200	3.00589900	0.85459200	H	3.35229700	3.06866100	-0.33001300
C	-1.93647000	-0.62887500	3.64909700	H	5.00028000	3.62805000	0.03983300
H	-2.03653500	-0.91783700	4.70213900	H	4.64566500	2.91317500	-1.53625700
H	-1.26825200	-1.34461200	3.16279500	C	6.67147000	0.78598800	-0.00441200
H	-1.43801300	0.34098700	3.59595600	C	7.23228200	0.72609000	-1.29571500
Cu	-1.33782300	-0.03304700	-0.08179500	C	7.54017100	0.57848700	1.08217600
C	1.51638700	-0.45520700	0.17740000	C	8.58979100	0.47203400	-1.49426400
O	0.46228000	-1.11181100	0.27804800	H	6.59975600	0.88292600	-2.16794100
O	1.52714900	0.85233200	0.14319000	C	8.90115200	0.32384600	0.89357700
B	0.32830300	1.73612700	0.39917700	H	7.15199300	0.61494500	2.09694200
O	-0.26023900	1.56984100	1.70808400	C	9.42948500	0.26943400	-0.39648100
O	0.84977600	3.07679900	0.31682400	H	8.99345200	0.43327300	-2.50275500
C	0.19211900	2.66588900	2.50755200	H	9.54753400	0.16758800	1.75345100
C	0.44398100	3.77783100	1.48581100	H	10.48735600	0.07142100	-0.54681600
H	-0.47005300	4.35464000	1.28941500	Si	-0.92546700	1.98795400	-1.53893800
H	1.23559400	4.47167100	1.79028500	C	0.52892200	2.00597700	-2.76858400
H	-0.57026700	2.92392800	3.25193300	H	0.25022600	2.48864500	-3.71231600
H	1.11715400	2.39552000	3.03943000	H	1.39871200	2.52592800	-2.35924500
C	2.30596900	-3.07250600	1.50053100	H	0.83419100	0.97767000	-2.99720300
C	2.21651100	-4.51558100	0.95742400	C	-2.35550200	1.21758700	-2.58652800
C	4.60548900	-2.82907600	0.54032700	H	-2.05195600	0.26781500	-3.02530600
C	3.60541400	-5.15466700	0.82177900	H	-3.29407500	1.04910400	-2.04966800
C	4.54332600	-4.27154000	-0.01159200	H	-2.57149000	1.91417700	-3.40663900
H	2.74483700	-3.12005100	2.50986900	C	-1.57410900	3.78286500	-1.36007000
H	1.72615800	-4.49593000	-0.02532500	C	-0.72290300	4.90045900	-1.46548200

C	-2.94816000	4.04847200	-1.21094700
C	-1.21389200	6.20619200	-1.40601000
H	0.34460600	4.74463500	-1.57998000
C	-3.44939100	5.35117200	-1.13974800
H	-3.65245500	3.22274400	-1.16524700
C	-2.58064000	6.43821500	-1.23610400
H	-0.52776400	7.04517800	-1.49390200
H	-4.51789500	5.51535300	-1.02134000
H	-2.96383800	7.45417800	-1.18788500

$P_{0\text{-}2}$

Sum of electronic and thermal Free Energies= -1355.368192

C	0.63725100	2.82681200	-0.88866400
C	0.89464200	4.23616600	-0.31211400
C	2.17708900	1.84793000	0.84074600
C	2.26712100	4.34295000	0.36157200
C	2.43535900	3.25265900	1.42550600
H	1.36489800	2.64269200	-1.69406700
H	0.11045800	4.46900800	0.42101900
H	3.05466000	4.23252600	-0.39756900
H	2.94373300	1.63927400	0.07968500
H	3.44179600	3.28714600	1.85909100
H	-0.34688600	2.77894800	-1.34968500
H	0.80142100	4.97594100	-1.11589700
H	2.30973100	1.09158500	1.61498400
H	2.39935000	5.33606100	0.80749700
H	1.73051900	3.43311600	2.24831000
C	0.82628200	1.74788600	0.16050700
C	0.07693800	-0.24891900	1.56213000
H	0.82095400	0.05371300	2.30345900
H	-0.86432100	-0.37597500	2.10674700
Si	0.59036900	-1.97597600	0.89532400
C	2.14859400	-1.81574500	-0.16779200
C	2.08814000	-1.22505900	-1.44604700
C	3.40376000	-2.26727400	0.27830900
C	3.22966200	-1.08765400	-2.23670000
H	1.13928300	-0.86016100	-1.83094600
C	4.54959500	-2.13475200	-0.50888500
H	3.49398600	-2.73458500	1.25574100
C	4.46450900	-1.54235600	-1.76893700
H	3.15516100	-0.62933200	-3.21914700
H	5.50603100	-2.49474700	-0.13937700
H	5.35354600	-1.43815800	-2.38481400
C	-0.80428400	-2.71615800	-0.14447800
H	-0.51965700	-3.70853800	-0.51090600
H	-1.72244000	-2.82519800	0.44226500
H	-1.05215200	-2.10104000	-1.01468100
C	0.93128200	-3.08772400	2.38960600
H	0.02713300	-3.19703900	2.99873000
H	1.24317800	-4.09100200	2.08034600
H	1.71405800	-2.67901000	3.03754800
C	-0.10028600	0.81287100	0.49475500
C	-1.39340600	0.74348600	-0.25043900
O	-1.56195500	0.92739400	-1.43828000
O	-2.45025400	0.43846200	0.57294500
B	-3.67975300	0.05387200	0.06562500
O	-3.86269800	-0.96838000	-0.82552800
O	-4.83645300	0.62533200	0.52401300
C	-5.26767100	-1.02462000	-1.11576700
C	-5.92609900	-0.11947700	-0.04285200
H	-6.65972900	0.57384900	-0.46340500
H	-6.40923100	-0.69983700	0.75144100
H	-5.43348400	-0.65096400	-2.13225100
H	-5.60838900	-2.06255600	-1.06471300

P2

Sum of electronic and thermal Free Energies= -952.697643

C	3.02973900	-0.11923200	1.08496300
C	4.31644900	0.24798200	0.31506400
C	1.62760600	0.83674800	-0.75816000
C	4.09254200	1.44864200	-0.61316400
C	2.90014600	1.20991700	-1.54858100
H	2.77663100	0.72509200	1.74589000
H	4.63409100	-0.61905700	-0.27977400
H	3.89828500	2.34322800	-0.00385800
H	1.34286700	1.69646600	-0.13332600
H	2.70995100	2.10082600	-2.15960000
H	3.22772900	-0.97183900	1.73691500
H	5.12622500	0.45910400	1.02441500
H	0.79477700	0.68202900	-1.44588300
H	4.99962900	1.65780200	-1.19334800
H	3.14116500	0.39401700	-2.24357800
C	1.86398500	-0.36271400	0.14254300
C	1.15321800	-1.51097900	0.07844400
C	0.00392700	-1.74166400	-0.88754800
H	0.12883900	-1.17203300	-1.81446100
H	-0.00049900	-2.79848500	-1.19212900
Si	-1.76886200	-1.36414500	-0.26313400
C	-1.98050500	0.48058600	0.11042600
C	-1.44754200	1.05099000	1.28275400

C	-2.67002400	1.33680600	-0.76740700
C	-1.59034100	2.41040700	1.56220800
H	-0.90587300	0.42721000	1.98912300
C	-2.81828600	2.69820500	-0.49435600
H	-3.10415000	0.93885900	-1.68114700
C	-2.27722100	3.23858900	0.67218900
H	-1.16905000	2.82330300	2.47484900
H	-3.35732700	3.33495200	-1.19064500
H	-2.39165300	4.29712100	0.88853000
C	-2.19055000	-2.35278100	1.29682200
H	-3.23573000	-2.18412200	1.57850400
H	-2.05947100	-3.42842300	1.13521800
H	-1.57047300	-2.06668600	2.15210500
C	-2.95916100	-1.87531600	-1.64597300
H	-2.88134700	-2.95185500	-1.83498500
H	-4.00024900	-1.66079800	-1.38231800
H	-2.74104600	-1.36351000	-2.58949400
C	1.43251800	-2.72487900	0.94192600
H	1.82931100	-3.54434300	0.32666600
H	2.14305700	-2.54514300	1.74885100
H	0.50938400	-3.10350100	1.39446100

1B

Sum of electronic and thermal Free Energies= -3147.513475

C	1.32298700	-2.34065600	0.33866000
C	2.40765800	-3.02926100	1.18687100
C	0.85184100	-0.74215000	2.25842300
C	2.11751700	-2.90376700	2.68910300
C	1.93389600	-1.43571900	3.10023800
H	0.37440400	-2.87323700	0.48173700
H	3.38294300	-2.57263900	0.96569400
H	1.20206200	-3.46361300	2.92797100
H	-0.12242900	-1.19692400	2.47935700
H	1.67623700	-1.36478300	4.16316200
H	1.57156700	-2.42884200	-0.72434300
H	2.48588300	-4.08426800	0.89841800
H	0.76387400	0.31379900	2.53661600
H	2.92453500	-3.36430400	3.27064800
H	2.88603300	-0.90088100	2.97440600
C	1.15499000	-0.86260700	0.74607500
H	2.11575100	-0.35862700	0.58017100
C	-4.28933800	-1.73786300	-1.12316200
C	-3.38986700	-2.40213700	-0.07374000
C	-2.30815700	-0.34590200	-1.91619800
C	-2.23648200	-1.47818300	0.34683600
C	-1.39349700	-1.00590700	-0.86019500
H	-4.79484800	-0.87285800	-0.67216000
H	-2.97686600	-3.33461800	-0.48441400
H	-2.64154900	-0.59202300	0.85526300
H	-2.71625300	0.58811700	-1.50433300
H	-5.07706000	-2.42891400	-1.44493400
H	-3.97349500	-2.68291100	0.81067400
H	-1.73740800	-0.07386000	-2.80997800
H	-1.60669300	-1.99239300	1.07905500
H	-0.91115800	-1.87997700	-1.31793500
C	-3.46540600	-1.27166600	-2.32976400
H	-4.10428700	-0.75254800	-3.05371400
H	-3.05448500	-2.14883600	-2.84981000
C	3.76341800	1.01403100	-2.10738600
C	3.05301500	-0.33630300	-2.28574700
C	1.55331000	2.12652800	-1.57135400
C	1.58322900	-0.16330900	-2.70809700
C	0.77114100	0.81183100	-1.82179900
H	3.83125900	1.52031100	-3.08086900
H	3.11729600	-0.90111600	-1.34870000
H	1.57362200	0.24779600	-3.72763700
H	1.56259000	2.68793400	-2.51604000
H	-0.12106800	1.10032200	-2.38960900
H	4.79343900	0.85519900	-1.76744700
H	3.57192500	-0.94010100	-3.03977800
H	1.00857000	2.74456600	-0.84861300
H	1.08587700	-1.13834200	-2.77512800
C	3.00654500	1.91872500	-1.12471200
H	3.50309100	2.89229700	-1.04338300
H	3.03552100	1.47945500	-0.11861800
P	-0.05652400	0.16492200	-0.26332300
Cu	-0.82718600	1.80401300	0.89916200
Cl	-1.55373200	3.42544000	2.05318300

OAc$^-$

Sum of electronic and thermal Free Energies= -228.480089

C	0.21991200	0.00054300	-0.01300400
O	0.73573700	1.14711400	0.00297300
O	0.76936500	-1.12991700	0.00306400
C	-1.35471800	-0.01654500	-0.00426400
H	-1.71651400	0.09450300	1.02870200
H	-1.76299200	0.82501700	-0.57818900
H	-1.75246500	-0.96108600	-0.39520400

Cl$^-$

Sum of electronic and thermal Free Energies= -460.267256

Cl	0.00000000	0.00000000	0.00000000

2B

Sum of electronic and thermal Free Energies= -2915.737156

C	1.69885800	1.79849500	1.49521500
C	1.52059200	2.90605800	2.54894300
C	-0.51851500	0.77140400	2.21531800
C	0.67724700	2.42458500	3.73820100
C	-0.67848600	1.87588100	3.27131900
H	2.28677700	0.98521500	1.93918700
H	1.02966300	3.77217600	2.08273500
H	1.22467800	1.63413000	4.27167500
H	-0.04261300	-0.10511900	2.67683800
H	-1.25026500	1.49118800	4.12376600
H	2.28315100	2.18048600	0.65033700
H	2.50375400	3.25198100	2.89032600
H	-1.49978000	0.44592500	1.85423800
H	0.53252800	3.24120900	4.45528900
H	-1.27354700	2.69501800	2.84357200
C	0.33555300	1.25760700	1.02099300
H	-0.21271800	2.09048100	0.56504200
C	3.60468400	-3.45290700	-0.10835000
C	3.33331600	-2.61919700	1.15023600
C	2.30026500	-1.75979800	-1.49303200
C	2.03016500	-1.81473500	1.02413000
C	2.01622600	-0.91407500	-0.23279700
H	2.82785400	-4.22399200	-0.20721500
H	4.17220600	-1.92863100	1.31785200
H	1.17535000	-2.50291900	0.96220100
H	1.45980100	-2.44876400	-1.66131400
H	4.56069200	-3.98180300	-0.01783700
H	3.28096800	-3.26530300	2.03444200
H	2.36723300	-1.12111600	-2.37959300
H	1.87678600	-1.21745200	1.92904200
H	2.80863900	-0.15993000	-0.13638300
C	3.60269600	-2.56766600	-1.36080300
H	3.74772900	-3.17594600	-2.26143300
H	4.45287800	-1.87225300	-1.31447300
C	-0.40182800	3.69590900	-2.41092200
C	0.99164700	3.30566800	-1.89627600
C	-1.09676400	1.25355100	-2.42095500
C	1.38559800	1.88561300	-2.33707300
C	0.33191700	0.79690000	-2.01938000
H	-0.37918300	3.74681200	-3.50912300
H	1.00790200	3.38435300	-0.80294600
H	1.51526400	1.89854600	-3.42898100
H	-1.15221400	1.21526600	-3.51805000
H	0.55743000	-0.06663500	-2.65712500
H	-0.66677500	4.69979100	-2.05871800
H	1.74384400	4.01459000	-2.26295900
H	-1.83772000	0.54074700	-2.04310800
H	2.36474300	1.61581900	-1.92335100
C	-1.46406200	2.67669000	-1.97576000
H	-2.44042200	2.94031500	-2.39779900
H	-1.59178800	2.71239800	-0.88669000
P	0.36293100	-0.04319200	-0.34053100
Cu	-1.35010800	-1.30725400	-0.13888300
O	-3.59790400	-0.38812000	0.22078200
C	-3.78475800	-1.62208800	0.20057900
O	-2.83248700	-2.48115800	0.03058000
C	-5.17515900	-2.20874200	0.37886700
H	-5.18533400	-2.87907400	1.24417400
H	-5.91301000	-1.41751000	0.51609400
H	-5.43735000	-2.81243500	-0.49573500

TS1B

Sum of electronic and thermal Free Energies= -3770.515272

C	4.00395700	0.82683400	0.42856500
C	4.98941700	1.85470300	-0.15512100
C	2.06310700	2.13975600	-0.54376900
C	4.34478200	3.24160400	-0.28636700
C	3.05147600	3.17208400	-1.10958600
H	3.75411200	1.12674000	1.45337500
H	5.32429400	1.51381500	-1.14531400
H	4.11653300	3.63002200	0.71637900
H	1.70195800	2.48042400	0.43459300
H	2.56670800	4.15420500	-1.14878900
H	4.48833700	-0.15213400	0.50102100
H	5.88510600	1.90520400	0.47578900
H	1.17957600	2.08493100	-1.18399500
H	5.05029500	3.94731800	-0.74084700
H	3.29896700	2.90262900	-2.14671200
C	2.71332500	0.74695700	-0.41648600
H	2.99982100	0.43656500	-1.42934100
C	0.61854400	-0.95361200	4.73966500
C	1.35488700	0.29432100	4.23664900
C	0.96777200	-2.05614100	2.46959400
C	1.21924600	0.45337700	2.71392600
C	1.70743800	-0.80175000	1.95376900
H	-0.46099300	-0.82556000	4.57930900

H	2.41959200	0.22123200	4.50146100
H	0.16532000	0.63288200	2.46249500
H	-0.09135700	-1.98808200	2.19042900
H	0.76342300	-1.07329000	5.81997500
H	0.97187500	1.19376100	4.73323400
H	1.35268400	-2.95895800	1.98711600
H	1.76494600	1.34408600	2.38749800
H	2.78094400	-0.92953500	2.14685500
C	1.09673800	-2.20618400	3.99444000
H	0.53127200	-3.08659400	4.32166800
H	2.14866400	-2.39924300	4.25028900
C	3.90714900	-2.56832000	-2.92696900
C	4.40310700	-2.32700400	-1.49403900
C	1.50950800	-2.34314800	-2.14509700
C	3.36899500	-2.77488700	-0.44574200
C	1.94061400	-2.21869800	-0.66023100
H	3.79378300	-3.64883700	-3.09510100
H	4.63588100	-1.26241700	-1.37308800
H	3.29302400	-3.87046200	-0.49801000
H	1.30022500	-3.40574300	-2.32620000
H	1.24025500	-2.86158300	-0.11807600
H	4.65252600	-2.21634300	-3.65003800
H	5.34333000	-2.86507000	-1.32225200
H	0.55762600	-1.82349200	-2.30170700
H	3.73084000	-2.55189200	0.56498500
C	2.55713200	-1.87891200	-3.16655900
H	2.19500200	-2.09368200	-4.17898800
H	2.68899000	-0.78957600	-3.11692600
P	1.47205000	-0.56954700	0.10641500
Cu	-0.69218400	-0.36454800	-0.25834200
O	-0.97782400	-3.64165800	-0.14176700
C	-2.05737500	-3.07722800	-0.11410900
O	-2.12015900	-1.75351500	0.12258900
C	-3.36502900	-3.81239700	-0.28429600
H	-3.91607000	-3.39422000	-1.12878200
H	-3.15945200	-4.87292900	-0.42978400
H	-3.98959900	-3.67465700	0.60398500
B	-3.11588800	-0.60519200	-0.22586100
O	-3.63233200	-0.01764600	0.97900200
O	-4.21647600	-1.10669900	-1.00237100
C	-4.94427400	-0.54276500	1.15956300
C	-5.41667700	-0.87673200	-0.26784400
H	-6.05199000	-1.77059400	-0.30192000
H	-5.97532700	-0.04273600	-0.71370900
H	-4.91410700	-1.44626000	1.78928300
H	-5.57700100	0.19813100	1.66027600
Si	-2.37862300	1.13803900	-1.40138400
C	-4.06447400	1.72960700	-2.06050300
H	-4.75022000	1.97269400	-1.24408400
H	-3.92524600	2.63645800	-2.66022900
H	-4.52760600	0.96053500	-2.68446200
C	-1.33403100	0.89265500	-2.99156900
H	-0.26031700	0.77196000	-2.81516800
H	-1.68219600	-0.00449900	-3.51726200
H	-1.46258800	1.73606200	-3.68092700
C	-1.68343100	2.63056200	-0.43162700
C	-1.09183500	3.71802800	-1.10273200
C	-1.80971800	2.72700600	0.96848600
C	-0.63473500	4.84387000	-0.41386800
H	-0.98392000	3.69116800	-2.18501300
C	-1.35190700	3.84945600	1.66389800
H	-2.29330700	1.92070600	1.51455200
C	-0.75898000	4.91002400	0.97586300
H	-0.18637600	5.67002000	-0.96048700
H	-1.46455400	3.89872700	2.74422400
H	-0.40497900	5.78434500	1.51575600

3B

Sum of electronic and thermal Free Energies= -3288.112070

C	2.68423200	0.56142900	-2.32224600
C	3.89581900	0.09404300	-3.14819100
C	2.56274900	-1.70765600	-1.22291100
C	3.86588200	-1.42251300	-3.38625400
C	3.75503800	-2.19278500	-2.06238000
H	1.77320900	0.36000100	-2.89902300
H	4.82092000	0.36352500	-2.61898000
H	3.00300500	-1.66973800	-4.02047800
H	1.62288600	-1.94269900	-1.74087200
H	3.66199100	-3.26848700	-2.25232000
H	2.73272500	1.64506400	-2.17025900
H	3.91763900	0.62936400	-4.10493400
H	2.52597600	-2.25206400	-0.27249100
H	4.75896100	-1.73880900	-3.93785900
H	4.68122700	-2.05721400	-1.48549200
C	2.62309300	-0.18257100	-0.97392700
H	3.55793700	0.03700000	-0.44737900
C	-1.77513600	3.83205300	-0.69553200
C	-1.04944300	3.17474700	-1.87517900
C	-0.18057400	2.65466700	0.90654100

C	-0.40721200	1.84004400	-1.46768500
C	0.56889400	1.99398400	-0.27452000
H	-2.63203400	3.20863800	-0.40688500
H	-0.27062200	3.85345700	-2.25262200
H	-1.19063900	1.12901900	-1.17203800
H	-0.96297300	1.96788800	1.26048800
H	-2.17978000	4.80760700	-0.99020300
H	-1.74451100	3.00453100	-2.70559300
H	0.49377800	2.83060300	1.74977700
H	0.09863400	1.39947100	-2.33067500
H	1.40328100	2.64604300	-0.56818400
C	-0.82937600	3.98973300	0.50122500
H	-1.36564000	4.40678500	1.36188400
H	-0.03779700	4.71004800	0.24828800
C	4.82421900	-0.06330300	2.69247500
C	4.48556800	1.21990500	1.92213100
C	2.40025000	-0.80084000	2.58237900
C	3.02241100	1.64640200	2.13461100
C	1.96471600	0.53190700	1.91883400
H	4.75394400	0.13312900	3.77196500
H	4.69140500	1.06825200	0.85531100
H	2.92309400	1.98202300	3.17720600
H	2.27639100	-0.67957300	3.66770500
H	1.06018500	0.84594400	2.45319300
H	5.86091500	-0.36117200	2.49659800
H	5.14236100	2.03833500	2.24070400
H	1.71530900	-1.60492400	2.28792700
H	2.79627700	2.52238300	1.51663000
C	3.86086800	-1.19974200	2.32272500
H	4.09508200	-2.10026100	2.90255900
H	4.00563200	-1.46878800	1.26945700
P	1.22431400	0.29649200	0.20445800
Cu	-0.52264900	-1.09336000	0.22181000
Si	-2.52145200	-2.20026000	0.23952000
C	-2.83075800	-3.39495800	-1.22818300
H	-2.10463000	-4.21627700	-1.20545300
H	-3.83475900	-3.83499400	-1.19158300
H	-2.72134000	-2.89592400	-2.19747200
C	-2.89095300	-3.24160600	1.80510200
H	-2.77233800	-2.66501700	2.72930600
H	-3.90737300	-3.65439100	1.79541900
H	-2.19135600	-4.08398200	1.86144700
C	-3.90144200	-0.87201000	0.13237900
C	-4.61371100	-0.43097400	1.26360300
C	-4.19698000	-0.23474000	-1.08946200
C	-5.56409300	0.59038700	1.18489800
H	-4.42714600	-0.89587100	2.22911800
C	-5.14599800	0.78542700	-1.18069500
H	-3.67618400	-0.54553400	-1.99375800
C	-5.83379500	1.20542000	-0.03899900
H	-6.09805000	0.90385900	2.07912900
H	-5.35456800	1.24933400	-2.14216800
H	-6.57419800	1.99842200	-0.10448100

4B

Sum of electronic and thermal Free Energies= -3599.985972

C	3.38610100	1.94326400	1.47640300
C	4.49940700	2.99759900	1.33891300
C	2.81878100	2.23584200	-0.96233100
C	4.20167800	4.00461200	0.21934300
C	3.92797400	3.28944600	-1.11095900
H	2.45945600	2.43942100	1.79168300
H	5.44984700	2.48799500	1.12529000
H	3.32082500	4.60153500	0.49502100
H	1.87892500	2.73441000	-0.70200000
H	3.64924500	4.01470200	-1.88455000
H	3.65768100	1.23848600	2.26856100
H	4.63366700	3.51781900	2.29490700
H	2.64089700	1.74054400	-1.92082200
H	5.03418200	4.70980600	0.11102000
H	4.84959500	2.80077700	-1.45853600
C	3.15634400	1.20648500	0.14063600
H	4.10614800	0.72497200	-0.12223900
C	1.07935500	-2.41175900	4.32102500
C	1.47884300	-0.93123200	4.32674600
C	1.62794400	-2.51570700	1.83180600
C	1.27656000	-0.28951200	2.94470300
C	2.06712500	-1.03250700	1.84215100
H	-0.00408300	-2.49225600	4.15517600
H	2.53440400	-0.83720200	4.61995200
H	0.20938600	-0.32091900	2.68862900
H	0.57091300	-2.57730400	1.54091000
H	1.28153000	-2.86912900	5.29672100
H	0.89810600	-0.37962400	5.07564800
H	2.18926500	-3.09180900	1.09274700
H	1.55279000	0.76638400	2.98514800
H	3.13596900	-0.99679600	2.09962700
C	1.81782300	-3.17051100	3.21177800
H	1.47837200	-4.21218200	3.16880800

H	2.89151000	-3.20263400	3.44684900
C	4.85727200	-1.40539000	-2.99402900
C	5.13101400	-1.50785700	-1.49012600
C	2.37147200	-1.15000400	-2.54180100
C	3.93529300	-2.11236000	-0.73356500
C	2.54211000	-1.48717400	-1.03406900
H	4.71251600	-2.41262300	-3.41049500
H	5.37150800	-0.50895900	-1.10405600
H	3.87426300	-3.17276300	-1.01754600
H	2.13229200	-2.09232200	-3.05334200
H	1.80310400	-2.26852700	-0.83782000
H	5.72189000	-0.97310700	-3.51124000
H	6.01602000	-2.12734000	-1.30044500
H	1.49531500	-0.50849300	-2.68881000
H	4.14192900	-2.10701300	0.34180900
C	3.60443800	-0.55936700	-3.24527000
H	3.39646500	-0.48918700	-4.31956000
H	3.80038500	0.46380300	-2.90460400
P	1.87304000	-0.18343300	0.15987600
Cu	-0.36097300	0.41561500	-0.20433800
C	-3.76883500	1.77771100	-1.16082100
C	-5.17878000	1.63263200	-0.55212000
C	-3.28825800	3.69200100	0.43562700
C	-5.68665700	2.95774700	0.03316200
C	-4.69173200	3.53190000	1.05167600
H	-3.83244400	2.44260700	-2.03739300
H	-5.14463100	0.86985700	0.23505700
H	-5.83027400	3.68558000	-0.77911700
H	-3.34193100	4.45258500	-0.35979800
H	-5.04293400	4.50001500	1.43046900
H	-3.40993700	0.81210700	-1.51183000
H	-5.87043600	1.26091500	-1.31701200
H	-2.57310900	4.05305600	1.18001900
H	-6.66870200	2.81555200	0.50067000
H	-4.62626600	2.85755900	1.91608900
C	-2.79681800	2.38556300	-0.17914600
C	-1.61699000	1.90051200	0.19032000
C	-0.45032900	2.14270100	0.88565300
H	0.23600300	2.91813400	0.54838100
H	-0.36590400	1.88583700	1.94126500
Si	-1.53463200	-1.25451500	-1.38723100
C	-1.83775200	-0.85749000	-3.24138000
H	-2.35992000	-1.67265400	-3.75824900
H	-2.40928200	0.06196400	-3.40195100
H	-0.87323600	-0.72864900	-3.74764100
C	-0.73062200	-3.00424300	-1.48818400
H	0.16869100	-3.00769100	-2.11397100
H	-0.46268300	-3.40631200	-0.50468500
H	-1.44037900	-3.70831100	-1.93967500
C	-3.23719600	-1.68825900	-0.60531500
C	-4.34723500	-2.08309200	-1.37594100
C	-3.40416500	-1.69535900	0.79209200
C	-5.55559700	-2.46563600	-0.78745500
H	-4.27284000	-2.09166200	-2.46092500
C	-4.60334200	-2.08448500	1.39331700
H	-2.57949700	-1.37970400	1.42968700
C	-5.68742200	-2.47078300	0.60219400
H	-6.39412500	-2.76083400	-1.41391500
H	-4.69474400	-2.08112600	2.47701300
H	-6.62510500	-2.76914400	1.06374900

TS2B

Sum of electronic and thermal Free Energies= -3599.960133

C	3.50345100	-1.33699200	-1.87366300
C	4.14134000	-2.68473800	-2.25558700
C	1.80478800	-2.54324400	-0.46315300
C	3.11974800	-3.82948500	-2.21302200
C	2.41991400	-3.89739200	-0.84891700
H	2.73557600	-1.08441300	-2.61560700
H	4.96478800	-2.90379700	-1.56071900
H	2.36601600	-3.66880700	-2.99629400
H	1.01283000	-2.27891700	-1.17528800
H	1.63978500	-4.66762500	-0.85781400
H	4.26445800	-0.55043900	-1.91436000
H	4.58862600	-2.60913700	-3.25393200
H	1.32358400	-2.62095700	0.51726400
H	3.60819400	-4.78444600	-2.44017700
H	3.14688600	-4.19889700	-0.08075000
C	2.85712500	-1.40966000	-0.47632100
H	3.64929000	-1.65506500	0.24030700
C	3.23246700	4.36338100	-1.81166400
C	3.34945100	3.09031700	-2.65823500
C	2.88429400	2.91764700	0.25896500
C	2.56773600	1.92208700	-2.03630700
C	3.02152100	1.62931800	-0.58610900
H	2.19046600	4.71215400	-1.82484600
H	4.40874900	2.81081400	-2.75303200
H	1.49683900	2.16016900	-2.02799700
H	1.82180400	3.18549700	0.33872400

H	3.83808200	5.16950000	-2.24235200
H	2.98427200	3.27156100	-3.67596800
H	3.24480600	2.76226800	1.27899400
H	2.66968400	1.03576200	-2.66444500
H	4.08362500	1.34433800	-0.60038700
C	3.65757400	4.09355500	-0.36328000
H	3.51358300	4.98917000	0.25282100
H	4.73326500	3.86759800	-0.33652300
C	3.74761300	-1.77997900	3.76542500
C	4.59226800	-0.93308500	2.80651500
C	1.62374400	-0.72653400	2.85511100
C	3.89947400	0.39612600	2.45799900
C	2.41985300	0.28988600	1.99329900
H	3.64357700	-1.25256900	4.72452200
H	4.79454300	-1.51376000	1.89759800
H	3.90188200	1.01512000	3.36681000
H	1.40430000	-0.23449600	3.81258500
H	1.95790000	1.26338400	2.19531700
H	4.25395400	-2.72763900	3.98324700
H	5.57146600	-0.71395500	3.24912500
H	0.64942500	-0.92688200	2.39391100
H	4.50204500	0.94348700	1.72529600
C	2.35839900	-2.03941800	3.17018700
H	1.74822000	-2.62935400	3.86433200
H	2.46978100	-2.65006600	2.26645900
P	2.05636900	0.18483200	0.14340600
Cu	-0.06240800	0.14155200	-0.44566200
C	-2.90799100	-1.84810100	0.61184700
C	-4.37398800	-2.25978000	0.85137300
C	-3.23437700	-2.25286300	-1.89661200
C	-4.87668700	-3.22907800	-0.22628400
C	-4.70549900	-2.61527500	-1.62147000
H	-2.26485700	-2.71310600	0.85150500
H	-5.00275500	-1.36216900	0.84804500
H	-4.31078900	-4.17144000	-0.17124000
H	-2.66315500	-3.19438800	-1.98780100
H	-5.06695500	-3.30558800	-2.39435800
H	-2.61195100	-1.06015600	1.31721200
H	-4.46987800	-2.71037000	1.84751000
H	-3.13169700	-1.74074800	-2.85845600
H	-5.92800900	-3.48555900	-0.04559200
H	-5.31905500	-1.70756000	-1.69044500
C	-2.61642300	-1.40106100	-0.80104600
C	-1.78122100	-0.38598900	-1.13997900
C	-0.95236900	-0.17129400	-2.27920400
H	-0.71557800	-1.02768600	-2.90873100
H	-0.98639300	0.77925800	-2.81357700
Si	-1.89613000	1.39816100	0.50910100
C	-1.37618000	1.74710300	2.32592200
H	-1.94650800	2.58269600	2.75138400
H	-1.52117500	0.87620500	2.97382800
H	-0.31480700	2.01263300	2.36880800
C	-1.44907400	2.97157700	-0.48954000
H	-0.37811200	3.20277000	-0.48038200
H	-1.75515900	2.87095800	-1.53610800
H	-1.97637100	3.83765900	-0.07235900
C	-3.80096400	1.40215700	0.54004200
C	-4.53345300	1.41582400	1.73998700
C	-4.53697100	1.46097300	-0.65961900
C	-5.93022700	1.48156900	1.74778300
H	-4.01267400	1.37047600	2.69276400
C	-5.93018400	1.53798800	-0.66228200
H	-4.01070800	1.43936300	-1.61029300
C	-6.63377100	1.54486900	0.54497000
H	-6.46652600	1.48522500	2.69351300
H	-6.46813600	1.58867300	-1.60570300
H	-7.71923000	1.59904500	0.54658200

5B

Sum of electronic and thermal Free Energies= -3600.027131

C	3.90191300	0.09877400	-2.17245000
C	3.84233300	0.00877800	-3.70814700
C	1.43060400	0.68251700	-2.11611100
C	2.73859000	0.90597400	-4.28622900
C	1.37647600	0.59540200	-3.64959600
H	4.19672700	1.11812700	-1.89251500
H	3.65480900	-1.03383100	-4.00208000
H	2.99460600	1.95849300	-4.09842100
H	1.62345200	1.72199000	-1.82005600
H	0.61032200	1.28004100	-4.03138800
H	4.68438900	-0.56631400	-1.79163300
H	4.81691900	0.28017600	-4.13151900
H	0.45932800	0.42051200	-1.68268700
H	2.68628200	0.78847200	-5.37497700
H	1.06151100	-0.41691500	-3.94028800
C	2.53525200	-0.23654200	-1.54167000
H	2.27324400	-1.26140200	-1.83467300
C	4.51553800	3.22701300	2.71214000
C	4.29105800	3.40288700	1.20536000

C	3.99789100	0.74422900	2.48100300
C	3.31243000	2.35455100	0.65399000
C	3.76312100	0.90740400	0.96268300
H	3.57735200	3.43509100	3.24508600
H	5.25319300	3.31332100	0.68073900
H	2.31836500	2.50365300	1.09837100
H	3.03320200	0.83254500	3.00135900
H	5.25123800	3.95330200	3.07701300
H	3.91059400	4.40789100	0.98817900
H	4.38957100	-0.25256700	2.70799800
H	3.19131400	2.49864700	-0.42432400
H	4.70931100	0.71017800	0.44110600
C	4.97405900	1.79850400	3.03009100
H	5.08611200	1.66264800	4.11227800
H	5.96777600	1.63059600	2.59061300
C	3.18735800	-4.43069100	-0.77601800
C	4.28382400	-3.35684800	-0.82272400
C	1.87806900	-3.03545400	0.88448800
C	4.35870200	-2.55570800	0.48883200
C	3.00511300	-1.97336100	0.96408100
H	3.44337800	-5.17869400	-0.01202900
H	4.09088200	-2.68732500	-1.66881000
H	4.71298000	-3.23563200	1.27712800
H	2.05307900	-3.75799800	1.69404200
H	3.11138400	-1.73720800	2.02966500
H	3.14042900	-4.96511700	-1.73204500
H	5.25959500	-3.81854700	-1.01583600
H	0.91254500	-2.56347300	1.09748800
H	5.11667200	-1.76750200	0.41198300
C	1.82303700	-3.81406000	-0.43751100
H	1.05854100	-4.59588700	-0.36310000
H	1.50269200	-3.15613500	-1.25584000
P	2.45593000	-0.28658300	0.34050600
Cu	0.46974100	0.30140500	1.11135200
C	-3.52107400	1.33285700	-1.50217500
C	-4.65279500	2.37802800	-1.59593800
C	-2.03787200	3.01705800	-0.37803700
C	-4.09842100	3.80816700	-1.64120000
C	-3.15826800	4.07470600	-0.45804700
H	-2.94711900	1.37230400	-2.44501800
H	-5.30816700	2.26621700	-0.72235500
H	-3.54287300	3.94986800	-2.58040600
H	-1.40374600	3.12633200	-1.27589900
H	-2.72288500	5.07964100	-0.53548300
H	-3.96303700	0.33477000	-1.45213800
H	-5.27110700	2.18074900	-2.48101600
H	-1.39384900	3.22685500	0.47819200
H	-4.91868900	4.53714600	-1.65234100
H	-3.73478100	4.05097200	0.47670500
C	-2.58586200	1.60141200	-0.33613800
C	-2.24415000	0.68877300	0.61691100
C	-1.25454800	0.94068500	1.72257200
H	-1.18705700	2.00170200	1.99115500
H	-1.54358700	0.41238000	2.63825200
Si	-2.87876700	-1.10096900	0.54485300
C	-2.33433700	-2.07855700	2.07974400
H	-1.24701000	-2.07226800	2.20599200
H	-2.77472000	-1.66953700	2.99487000
H	-2.66283400	-3.12069100	1.99366100
C	-2.16312100	-2.02106700	-0.95898400
H	-1.06771100	-1.98115300	-0.92152000
H	-2.44851800	-3.07925100	-0.97115800
H	-2.47612600	-1.57603000	-1.90823100
C	-4.77826100	-1.20405200	0.51390000
C	-5.45285000	-2.28697300	-0.07942000
C	-5.56375100	-0.23036500	1.15991000
C	-6.84444300	-2.39705000	-0.03081700
H	-4.88693200	-3.06073700	-0.59357000
C	-6.95495000	-0.33444800	1.21600900
H	-5.07755600	0.62952700	1.61424100
C	-7.59979100	-1.42005000	0.61964400
H	-7.33859100	-3.24341300	-0.50136900
H	-7.53608700	0.43263500	1.72162600
H	-8.68274300	-1.50253400	0.65937000

TS3B

Sum of electronic and thermal Free Energies= -3788.583361

C	5.11716800	-0.69108000	-0.60637600
C	5.91821800	-1.97190500	-0.89963200
C	3.01629900	-1.80407900	-1.50335400
C	5.30582000	-2.76908500	-2.06021300
C	3.82422600	-3.07727900	-1.80144900
H	5.19326700	-0.02486900	-1.47503600
H	5.93817100	-2.60026300	0.00224000
H	5.39850900	-2.18489100	-2.98714100
H	2.99139700	-1.17397400	-2.40273400
H	3.38679800	-3.60007900	-2.66011000
H	5.56890900	-0.15603100	0.23589400
H	6.96069800	-1.71279400	-1.12091400

H	1.97940200	-2.06177600	-1.26848300
H	5.86651600	-3.69752700	-2.22044000
H	3.74014900	-3.76191000	-0.94559900
C	3.63418900	-1.01223500	-0.32704700
H	3.59398600	-1.67319300	0.54708100
C	2.97883400	4.44342100	-2.27026000
C	3.58634400	3.16261200	-2.85489600
C	2.68809400	3.26102000	-0.03218900
C	3.06025200	1.91016600	-2.13690200
C	3.29132800	1.96136200	-0.60855800
H	1.89873200	4.45784300	-2.47262900
H	4.68097900	3.20288700	-2.76056100
H	1.97959500	1.80858500	-2.31129900
H	1.59319600	3.21791600	-0.12534800
H	3.40157000	5.32738500	-2.76207900
H	3.36904200	3.08849200	-3.92704100
H	2.91155700	3.35154000	1.03558800
H	3.52576600	1.01820400	-2.56849600
H	4.37127300	1.96206500	-0.40976200
C	3.21309900	4.51287600	-0.75622600
H	2.73532400	5.40492600	-0.33401300
H	4.29023000	4.61509900	-0.56118200
C	3.71918000	-1.35204100	3.94387500
C	4.68591200	-0.51408100	3.09379400
C	1.74222900	-0.21379600	2.84409800
C	4.06773200	0.83250100	2.67672200
C	2.66717600	0.72353000	2.02658900
H	3.54070300	-0.83893800	4.89979500
H	4.97711900	-1.09083100	2.20858300
H	3.95545700	1.44486300	3.58326900
H	1.47829000	0.31557000	3.77072500
H	2.20630100	1.71687900	2.08425200
H	4.17506700	-2.31819900	4.19024600
H	5.61187500	-0.32402800	3.65001800
H	0.80912600	-0.37820600	2.29633700
H	4.75775000	1.38416500	2.02737900
C	2.37701500	-1.55742700	3.22730000
H	1.68390200	-2.11222400	3.86994800
H	2.51750100	-2.17738300	2.33289700
P	2.53144500	0.43276800	0.17271500
Cu	0.42323600	0.20248800	-0.43635000
C	-3.91869000	-2.12771500	-0.21108600
C	-5.01067100	-2.08714000	-1.30510600
C	-2.14126600	-2.19398300	-1.97970700
C	-4.53021400	-2.71853900	-2.62061300
C	-3.20435400	-2.10290600	-3.09415300
H	-3.72987500	-3.17165700	0.06761600
H	-5.29798800	-1.04383800	-1.48480700
H	-4.38607600	-3.79883700	-2.47228500
H	-1.97476100	-3.25996100	-1.76436100
H	-2.85070500	-2.61116500	-4.00084800
H	-4.29251800	-1.63533500	0.69045800
H	-5.90994300	-2.60418600	-0.94649100
H	-1.18189400	-1.79358900	-2.31716600
H	-5.29996700	-2.61125100	-3.39522300
H	-3.36016500	-1.04845100	-3.35889700
C	-2.62939000	-1.49569400	-0.71157100
C	-2.31189100	-0.15301600	-0.46130200
C	-1.33583100	0.59115400	-1.23215700
H	-1.26015200	0.29688000	-2.28425100
H	-1.44170000	1.67585300	-1.16036300
Si	-3.08203700	0.79867500	1.01588900
C	-2.25381800	2.49784300	1.19634200
H	-1.16502400	2.41667600	1.27974400
H	-2.47641700	3.16220100	0.35539800
H	-2.62623800	2.98494500	2.10466500
C	-1.07981400	-2.39213000	0.70282900
O	-1.71675800	-3.11887100	1.39910000
O	-0.01582300	-1.95489500	0.34185300
C	-2.83362100	-0.09811000	2.66610200
H	-3.33671400	0.43865400	3.47854900
H	-3.18609900	-1.13207700	2.66304600
H	-1.76517300	-0.12160900	2.90999100
C	-4.92540200	1.12994200	0.70789200
C	-5.92241500	0.78068300	1.63574900
C	-5.33714500	1.78591300	-0.46867500
C	-7.26912100	1.07154300	1.40330300
H	-5.64998200	0.26923600	2.55574300
C	-6.67997100	2.08015800	-0.70831400
H	-4.59738500	2.06828200	-1.21525000
C	-7.65110000	1.72271400	0.22995100
H	-8.01878200	0.78836400	2.13761700
H	-6.96953100	2.58588800	-1.62579500
H	-8.69783300	1.94949100	0.04632000

6B

Sum of electronic and thermal Free Energies= -3788.617977

C	-4.39723000	2.21869700	-0.94015600
C	-4.27036200	3.74285100	-1.11533600

C	-1.86478700	2.00299300	-1.10872300	H	-1.80757000	-0.50750000	2.56508300
C	-3.01906600	4.11817700	-1.92205700	H	-5.92126700	-0.04519700	1.26649900
C	-1.75166800	3.52403500	-1.29144800	C	-2.83712700	1.19068500	3.44369900
H	-4.55946900	1.76554100	-1.92633400	H	-2.15906500	1.25879400	4.30193400
H	-4.22033500	4.21766500	-0.12512000	H	-2.43821600	1.88494000	2.69346000
H	-3.12536300	3.73981600	-2.94885200	P	-3.13713800	-0.21934000	0.06912300
H	-1.90180300	1.52112200	-2.09539000	Cu	-1.13947600	-0.98794400	-0.01902400
H	-0.87225900	3.75787900	-1.90238300	C	3.37685400	-1.86254000	-0.55790700
H	-5.28505900	1.98658400	-0.34097900	C	4.72735100	-2.57513400	-0.39955200
H	-5.17189500	4.13367900	-1.60230800	C	2.72838100	-2.58559000	1.76476000
H	-0.97591200	1.61096300	-0.60322500	C	4.61867200	-3.77258000	0.55304100
H	-2.93173000	5.20822700	-1.99964500	C	4.06537900	-3.33081500	1.91399100
H	-1.58136700	3.99041000	-0.31076500	H	2.65101300	-2.54769000	-1.00752700
C	-3.12691600	1.62624500	-0.29739600	H	5.48096800	-1.87297000	-0.02241900
H	-3.00862700	2.08453600	0.69183000	H	3.94839900	-4.52591500	0.11427000
C	-4.94098800	-3.11312800	-3.18153100	H	1.98433700	-3.28256600	1.36230100
C	-4.61122800	-1.67253700	-3.59200400	H	3.91808200	-4.20103500	2.56669100
C	-4.66961400	-2.46216200	-0.73359400	H	3.48227200	-1.02443900	-1.25558900
C	-3.71480400	-0.98186100	-2.55259100	H	5.07815100	-2.90375300	-1.38579600
C	-4.33202300	-1.00997900	-1.13492800	H	2.35159700	-2.26458600	2.74257400
H	-4.01949600	-3.71188700	-3.18877000	H	5.59574400	-4.25573300	0.67789100
H	-5.54424000	-1.10195600	-3.70382800	H	4.80567300	-2.69145100	2.40814000
H	-2.73991500	-1.48801200	-2.51201200	C	2.76739000	-1.36767700	0.78761700
H	-3.73461600	-3.02949900	-0.61915800	C	3.50948600	-0.13482700	1.33116800
H	-5.61857400	-3.57286900	-3.91040100	C	3.95777700	-0.05697600	2.59391000
H	-4.11705300	-1.65573400	-4.57047700	H	3.84733600	-0.85979200	3.31814300
H	-5.17505400	-2.48762700	0.23714300	H	4.44125600	0.83676100	2.97931400
H	-3.51258600	0.04775600	-2.86554800	Si	3.81281900	1.39970800	0.23760400
H	-5.26241200	-0.42645000	-1.14143600	C	3.92270300	2.93712500	1.34230500
C	-5.56153800	-3.15314400	-1.77932200	H	3.01754900	3.04792400	1.94833700
H	-5.74898400	-4.18868000	-1.47179600	H	4.78338200	2.91126000	2.01791800
H	-6.54031700	-2.65319100	-1.80216200	H	4.02799200	3.83277200	0.71964600
C	-4.25398200	1.62095900	3.84680000	C	1.28224000	-0.97914200	0.56742500
C	-5.23588600	1.46732200	2.67652400	O	0.79347900	0.04334300	1.09413900
C	-2.81591000	-0.24702000	2.90518600	O	0.57664100	-1.79876600	-0.14028200
C	-5.24450900	0.03087700	2.12623100	C	2.46105900	1.73081000	-1.04514600
C	-3.84562200	-0.53334200	1.77824600	H	2.71017800	2.61719100	-1.64006900
H	-4.59463000	1.00013100	4.68795500	H	2.30130600	0.89668300	-1.73488700
H	-4.96781500	2.17792400	1.88566200	H	1.51794700	1.91497800	-0.52513600
H	-5.67177000	-0.62175200	2.90119200	C	5.48212100	1.21800800	-0.66193000
H	-3.05097500	-0.92468700	3.73790400	C	5.62461900	1.48589000	-2.03516900
H	-3.94020900	-1.62542000	1.73426700	C	6.64259300	0.84753300	0.04513700
H	-4.25224800	2.65690800	4.20550700	C	6.86388900	1.39354300	-2.67420700
H	-6.25111400	1.73406900	2.99397800	H	4.75538000	1.77006700	-2.62281700

C	7.88483600	0.75538800	-0.58391300
H	6.57225800	0.61562000	1.10571600
C	7.99854200	1.02917200	-1.94890900
H	6.94220900	1.60460000	-3.73773500
H	8.76279400	0.46653900	-0.01172200
H	8.96378400	0.95589300	-2.44285300

7B

Sum of electronic and thermal Free Energies= -4643.426945

C	5.40059400	-2.41950000	-0.29617000
C	5.66466800	-3.78557700	-0.95371700
C	3.29430100	-2.16461900	-1.69224100
C	5.06828500	-3.85803600	-2.36632900
C	3.56965200	-3.52432600	-2.35319200
H	5.93568100	-1.64793700	-0.86404900
H	5.22391500	-4.57799300	-0.33220000
H	5.59345200	-3.14425500	-3.01698000
H	3.71979100	-1.36534300	-2.31407800
H	3.16683500	-3.52978200	-3.37281100
H	5.81985100	-2.40745700	0.71551400
H	6.74377600	-3.97814100	-0.98377900
H	2.21532000	-1.97913100	-1.64199500
H	5.23291400	-4.85217000	-2.79792700
H	3.02977600	-4.30621500	-1.80067200
C	3.89337500	-2.09355200	-0.26896100
H	3.39407300	-2.87326000	0.31854600
C	6.05801800	3.31523500	-0.16404100
C	6.17846600	2.13096400	-1.13184700
C	4.75533400	1.84338300	1.45687400
C	5.00863200	1.14907300	-0.96553400
C	4.86744000	0.64499400	0.48905500
H	5.17260000	3.91032200	-0.42771200
H	7.12517300	1.60355100	-0.94682100
H	4.06878100	1.64153800	-1.25089300
H	3.80839700	2.37158800	1.27676100
H	6.92367300	3.98047200	-0.26370900
H	6.21686300	2.48475300	-2.16899800
H	4.73171700	1.50002200	2.49609100
H	5.13544800	0.30551600	-1.65274500
H	5.76805100	0.07573900	0.75438900
C	5.92612800	2.82625200	1.28377500
H	5.79219600	3.67548900	1.96393000
H	6.85935600	2.32925400	1.58528800
C	2.87194500	-3.60025200	3.60082200
C	4.25332700	-3.06251000	3.19948900
C	1.78301700	-1.47208400	2.75733500
C	4.29904600	-1.52421000	3.21976600
C	3.15849400	-0.83355600	2.43260400
H	2.67243500	-3.33892100	4.64998800
H	4.50881000	-3.44020500	2.20256400
H	4.20797500	-1.20161200	4.26700700
H	1.51460200	-1.15848200	3.77592400
H	3.09474300	0.19949800	2.79565900
H	2.86263300	-4.69522500	3.54573400
H	5.02303500	-3.45085300	3.87735200
H	1.01620300	-1.05986500	2.09420200
H	5.27986200	-1.16787500	2.88278700
C	1.76592500	-3.00654900	2.71731800
H	0.78320900	-3.36340600	3.04651700
H	1.88485200	-3.36299300	1.68576500
P	3.38454100	-0.49755400	0.59747500
Cu	1.59710000	0.28629300	-0.28800900
C	-2.20727400	-2.41828200	-0.66516900
C	-2.99963600	-3.57045100	-1.30050700
C	-1.93654800	-1.36630200	-2.93519700
C	-2.57514200	-3.81447000	-2.75391700
C	-2.70983200	-2.52775800	-3.57789200
H	-1.14635600	-2.68639800	-0.62300700
H	-4.07284600	-3.35119400	-1.26506900
H	-1.52926600	-4.15474900	-2.77743500
H	-0.86718200	-1.62256100	-2.94369400
H	-2.33847500	-2.68323000	-4.59870600
H	-2.52071400	-2.28054400	0.37380800
H	-2.85188700	-4.47810900	-0.70289800
H	-2.03303900	-0.44986800	-3.52320900
H	-3.17539300	-4.61688000	-3.19967700
H	-3.77024500	-2.26621200	-3.66559100
C	-2.32984600	-1.08375600	-1.44621800
C	-3.72174100	-0.43553900	-1.27361000
C	-4.39052700	0.09504900	-2.30893300
H	-4.01871400	0.08697300	-3.33002500
H	-5.34772300	0.59104600	-2.17788200
Si	-4.55292000	-0.28308700	0.44159400
C	-5.88334700	1.06040900	0.37662900
H	-5.46126400	2.02434500	0.07488500
H	-6.70487100	0.81373000	-0.30360900
H	-6.31762200	1.18385200	1.37507200
C	-1.24632700	-0.08304600	-0.96670000
O	-1.35562800	1.09902900	-1.47197200

O	-0.31171400	-0.45748100	-0.22248600
C	-3.30956200	0.19468300	1.78246900
H	-3.78026600	0.16044400	2.77150900
H	-2.42004300	-0.44140400	1.80574300
H	-2.98192700	1.22563500	1.61587500
C	-5.41494000	-1.91168200	0.91515200
C	-5.08812200	-2.62886800	2.07968000
C	-6.45095700	-2.42572600	0.11115400
C	-5.75961000	-3.80414200	2.42702400
H	-4.29644900	-2.26822200	2.73184500
C	-7.12796100	-3.59760500	0.45077400
H	-6.73277500	-1.90551300	-0.80215500
C	-6.78210100	-4.29161600	1.61266000
H	-5.48480800	-4.33724700	3.33358900
H	-7.92359200	-3.97005000	-0.18928400
H	-7.30667100	-5.20481100	1.88054700
B	-0.32521600	2.26095100	-1.32766000
O	1.04346000	1.70677500	-1.60350500
O	-0.59242300	3.15149300	-2.43629900
C	1.26262000	1.83544400	-3.01503700
C	0.46493300	3.09777900	-3.37272200
H	1.10144000	3.99298300	-3.28888100
H	0.07517900	3.05646200	-4.39838600
H	2.33607600	1.92335600	-3.21485000
H	0.87550800	0.95267200	-3.54402800
Si	-0.37627500	3.25464400	0.47579500
C	0.89826600	4.67282600	0.38031700
H	0.90966500	5.27802300	1.29389000
H	1.90897900	4.27504300	0.22574900
H	0.67467000	5.33846800	-0.45998800
C	0.10896400	2.22687300	2.01597400
H	1.03882900	1.67694400	1.82324400
H	0.28295200	2.86028600	2.89373000
H	-0.65186900	1.48579800	2.27682700
C	-2.08994500	4.02075000	0.80555000
C	-2.93196700	4.36823200	-0.27032100
C	-2.56488100	4.27787900	2.10560600
C	-4.18346900	4.95077900	-0.05512400
H	-2.59959400	4.18056100	-1.28842200
C	-3.81637800	4.85757000	2.32793700
H	-1.94995100	4.02057500	2.96543400
C	-4.63002300	5.19669400	1.24557600
H	-4.81122900	5.21268100	-0.90344700
H	-4.15647300	5.04334700	3.34390200
H	-5.60455200	5.64773800	1.41406200

TS4B

Sum of electronic and thermal Free Energies= -4643.406863

C	-4.49504800	-3.00943800	0.74203600
C	-4.39909800	-4.29749300	1.57887700
C	-2.48189800	-2.06463300	1.95840400
C	-3.75343100	-4.03616300	2.94722600
C	-2.38825500	-3.34894500	2.79767100
H	-5.17341800	-2.31200000	1.24914000
H	-3.80164600	-5.03996500	1.03065300
H	-4.41867300	-3.39360300	3.54155600
H	-3.08945100	-1.32476000	2.49514000
H	-1.96812700	-3.11757600	3.78363600
H	-4.94727700	-3.23214400	-0.22973600
H	-5.39788100	-4.73309200	1.70379200
H	-1.49489300	-1.61174300	1.83375300
H	-3.64980200	-4.97532600	3.50353500
H	-1.68466700	-4.04247700	2.31515800
C	-3.10930100	-2.35337200	0.57526400
H	-2.45303000	-3.08110400	0.08154500
C	-6.51310400	2.29967600	-0.11790900
C	-6.29294200	1.27854700	1.00531400
C	-4.94051100	0.97179500	-1.61408800
C	-4.91979100	0.59668000	0.89065400
C	-4.71353300	-0.06369600	-0.49227700
H	-5.79810700	3.12619500	-0.00229100
H	-7.08248500	0.51465000	0.96070800
H	-4.12301900	1.33470700	1.05208300
H	-4.15774900	1.73960500	-1.56486400
H	-7.51463000	2.73970300	-0.04404600
H	-6.38273700	1.76117800	1.98588600
H	-4.86167700	0.50069300	-2.59931600
H	-4.81210000	-0.14390600	1.68931400
H	-5.46232100	-0.85871200	-0.61095800
C	-6.31647100	1.64924900	-1.49312200
H	-6.42806600	2.39461400	-2.28943800
H	-7.10333000	0.89881700	-1.65565000
C	-2.04865400	-4.25833700	-3.13836400
C	-3.48158800	-3.95227100	-2.67949200
C	-1.38461100	-1.85078300	-2.70395600
C	-3.85490700	-2.47743000	-2.90923300
C	-2.83997400	-1.45302200	-2.34430700
H	-1.97957300	-4.12739100	-4.22782800
H	-3.57905700	-4.21246100	-1.61931900

H	-3.90505600	-2.31323400	-3.99543000
H	-1.24740900	-1.64779300	-3.77536400
H	-3.02132000	-0.50605100	-2.86549100
H	-1.80230900	-5.30705800	-2.93443500
H	-4.19609900	-4.58843800	-3.21577200
H	-0.68130800	-1.20050800	-2.17393600
H	-4.86414100	-2.27595000	-2.53191600
C	-1.03959200	-3.32592800	-2.45458300
H	-0.02658100	-3.52420800	-2.82385400
H	-1.01451000	-3.53442300	-1.37741400
P	-3.01119100	-0.85278600	-0.56752300
Cu	-1.31192800	0.43546500	-0.00337500
C	2.72339300	-1.80381900	1.43714100
C	3.91152200	-2.48005400	2.13746300
C	2.73401700	0.00440000	3.18483000
C	3.93458400	-2.18004200	3.64090100
C	3.92284300	-0.66602600	3.88712400
H	1.78879600	-2.22430800	1.82715200
H	4.85068400	-2.14277500	1.68545100
H	3.05409400	-2.63297600	4.11988300
H	1.80526700	-0.39426600	3.61688600
H	3.87258500	-0.45130200	4.96184300
H	2.73124200	-2.04247900	0.37027900
H	3.85977000	-3.56159100	1.96345100
H	2.70913000	1.07830200	3.37920700
H	4.81509100	-2.63738900	4.10830000
H	4.86194500	-0.23188700	3.52378500
C	2.67979200	-0.26757700	1.64898200
C	3.77512000	0.47156600	0.83310600
C	4.40373100	1.54553600	1.33753600
H	4.21359600	1.93232800	2.33486700
H	5.13268600	2.10683100	0.76166800
Si	4.22242400	-0.00161900	-0.96790400
C	5.27087300	1.37968800	-1.72575800
H	4.74492700	2.33913900	-1.70798400
H	6.23513900	1.50561000	-1.22280000
H	5.48367200	1.13073000	-2.77162800
C	1.31705100	0.27343300	1.16554400
O	1.04978000	1.48893100	1.54175100
O	0.53423000	-0.42477700	0.49193000
C	2.67552500	-0.21060700	-2.03618900
H	2.95397000	-0.49241600	-3.05805300
H	1.97504400	-0.95306600	-1.64574200
H	2.14752200	0.74703000	-2.08610200
C	5.26997600	-1.58612700	-1.05879700
C	4.80904200	-2.75721200	-1.68583000
C	6.57601000	-1.60807500	-0.53193100
C	5.60887400	-3.89897800	-1.78051800
H	3.80877600	-2.78325700	-2.11114900
C	7.38191000	-2.74372400	-0.62161100
H	6.97388200	-0.72341100	-0.03882200
C	6.89829200	-3.89497800	-1.24745500
H	5.22575300	-4.78994100	-2.27133900
H	8.38576500	-2.73124000	-0.20516000
H	7.52303700	-4.78110200	-1.31991900
B	-0.33606700	2.08183700	1.38620900
O	-1.33479000	1.27364300	2.08991200
O	-0.32599600	3.37550600	2.01898200
C	-1.70582400	1.97552700	3.27763100
C	-1.40101100	3.44030200	2.94213700
H	-2.27495700	3.93107700	2.48673800
H	-1.09955000	4.02360000	3.81994800
H	-2.76215500	1.79170800	3.50429000
H	-1.10014900	1.62579000	4.12629300
Si	-0.67976900	2.80461500	-0.72428100
C	-2.06518300	4.09927700	-0.53648900
H	-2.21385900	4.65563100	-1.46886600
H	-3.01941600	3.62819800	-0.27274300
H	-1.82032400	4.81910900	0.24891200
C	-1.05604100	1.99207200	-2.43618300
H	-2.08226900	1.62314700	-2.50101300
H	-0.95173200	2.76439900	-3.20910200
H	-0.38487300	1.17092600	-2.70644100
C	0.96313000	3.73976700	-1.05298900
C	1.51513700	4.62741300	-0.10556400
C	1.64245300	3.62213000	-2.28090800
C	2.67355500	5.35730000	-0.37436300
H	1.03307000	4.73533900	0.85991600
C	2.80556300	4.34835600	-2.55625300
H	1.26205700	2.95954300	-3.05237300
C	3.32543300	5.22293900	-1.60223000
H	3.06905500	6.03469100	0.37865200
H	3.29846000	4.23373600	-3.51861300
H	4.22552300	5.79452000	-1.81351200

8B

Sum of electronic and thermal Free Energies= -3599.994184

C	3.94873300	-0.55714900	-0.99702900
C	5.23069700	-0.75673800	-0.16103900

C	3.97152700	-3.01146200	-1.61333600	C	2.49483800	1.88876000	1.82948600
C	6.07726800	-1.91927600	-0.69854700	H	0.44553900	2.20939600	2.36360400
C	5.25445100	-3.21248900	-0.78128300	C	1.52103100	0.46334400	4.24041100
H	4.24483100	-0.22719100	-2.00600500	H	1.52185300	-0.65442800	2.38730600
H	4.94728000	-0.96746300	0.87964700	H	-0.08189500	-0.18360900	2.92960900
H	6.44891200	-1.66156500	-1.70102000	C	3.05949200	2.19623800	3.22851200
H	4.26442200	-2.81388300	-2.65732000	H	3.11766700	1.11771900	1.35941200
H	5.85676400	-4.02190500	-1.21194800	H	2.57402700	2.78518400	1.20662600
H	3.33463100	0.23487600	-0.56767600	C	2.96217000	0.98388500	4.16346400
H	5.81736200	0.17032100	-0.14863200	H	1.47176900	-0.44123300	4.85794600
H	3.36589300	-3.92184800	-1.61716300	H	0.88915800	1.21359600	4.73704700
H	6.96175100	-2.06884700	-0.06753600	H	4.10101900	2.52731600	3.13775900
H	4.97580800	-3.53034200	0.23259200	H	2.50206900	3.03758800	3.66450600
C	3.14753500	-1.83392900	-1.10380700	H	3.32995600	1.24344000	5.16324100
C	1.86484400	-1.98639200	-0.78237900	H	3.61614900	0.18459400	3.78708800
C	0.87939100	-2.96020000	-0.69675300	C	-1.41683700	1.97785400	0.44987500
H	0.33077600	-3.29096300	-1.57987600	C	-2.29356200	1.96626200	-0.81953700
H	0.88169500	-3.68953300	0.11308900	C	-2.25020700	1.51055000	1.65981000
Cu	0.09584300	-1.25180200	-0.09556700	H	-1.10266000	3.01459200	0.64046100
Si	-1.94019700	-2.33066200	0.52840400	C	-3.54015500	2.85244400	-0.63956600
C	-1.97889100	-4.20551000	0.10821000	H	-2.60503500	0.93808200	-1.03689800
H	-1.86581100	-4.39066100	-0.96611200	H	-1.73037900	2.31687500	-1.68931100
H	-1.18244800	-4.75639200	0.62240900	C	-3.49580700	2.39474100	1.85072600
H	-2.93469000	-4.64538800	0.41605200	H	-2.55755000	0.47217700	1.49754000
P	0.18791200	1.01656200	0.25993700	H	-1.65453200	1.52785200	2.57885400
C	1.13584500	1.98395700	-1.05298200	C	-4.36408900	2.43952600	0.58658200
C	0.93541600	1.39015600	-2.46613600	H	-4.15681700	2.80292500	-1.54465200
C	0.93572400	3.51472200	-1.06022400	H	-3.22341700	3.90065300	-0.53300000
H	2.18326900	1.79769600	-0.79052200	H	-4.08046600	2.02457100	2.70157000
C	1.84860300	2.08038000	-3.49346700	H	-3.17529900	3.41384800	2.11286800
H	-0.10938300	1.50549400	-2.78027700	H	-5.20345100	3.13132500	0.72873600
H	1.14178000	0.31459100	-2.44331800	H	-4.79675900	1.44789500	0.40961300
C	1.86139900	4.18880400	-2.08875400	C	-2.24669700	-2.33595500	2.42489000
H	-0.10313900	3.75708300	-1.31326200	H	-1.38934900	-2.79980800	2.92787900
H	1.11787100	3.93545200	-0.06414600	H	-2.37490000	-1.33897200	2.85837400
C	1.66085700	3.60421700	-3.49416600	H	-3.13023000	-2.93135500	2.68728900
H	1.65682000	1.67113900	-4.49247100	C	-3.55855800	-1.72797300	-0.30726500
H	2.89589800	1.84569700	-3.25642200	C	-4.74589200	-1.47488200	0.40459800
H	1.68108500	5.27060000	-2.09473100	C	-3.62118300	-1.60202800	-1.70952000
H	2.90785000	4.04864400	-1.78267900	C	-5.93114000	-1.11385900	-0.24437000
H	2.35356200	4.07331400	-4.20293200	H	-4.75355600	-1.56831800	1.48794800
H	0.64653100	3.84496700	-3.84321300	C	-4.79826400	-1.24252100	-2.36834300
C	1.03527300	1.39903000	1.91270200	H	-2.72801000	-1.79483800	-2.30284000
C	0.95130500	0.16686100	2.84361800	C	-5.96110100	-0.99394400	-1.63473700

H	-6.83224600	-0.93009500	0.33610000
H	-4.81081400	-1.15799300	-3.45238600
H	-6.88064000	-0.71432300	-2.14194400

TS5B

Sum of electronic and thermal Free Energies= -3599.970760

C	4.08440300	0.31040500	1.30161000
C	5.43049600	0.13784200	0.56863000
C	4.19687700	2.81051300	0.94742300
C	6.29995200	1.39755000	0.69826700
C	5.54794600	2.64801200	0.21831000
H	4.29406700	0.38345400	2.38272500
H	5.23292700	-0.05608600	-0.49522400
H	6.58426100	1.53092400	1.75261200
H	4.40708300	3.02324900	2.00912500
H	6.16750300	3.54277700	0.36202000
H	3.44804300	-0.56898500	1.15727100
H	5.96886400	-0.73709400	0.95599600
H	3.65886600	3.67967800	0.55443400
H	7.23560400	1.27710600	0.13751300
H	5.36130700	2.56294700	-0.86122800
C	3.34546600	1.55320800	0.84131300
C	2.09237500	1.51334300	0.37340200
C	1.28695100	2.67281000	-0.09314600
H	1.05680800	3.42153800	0.67277800
H	1.65920000	3.17569000	-0.99392100
Cu	0.39656100	0.82142000	-0.15541800
Si	-0.80784100	2.81717900	-0.92140000
C	-0.59706000	4.71032500	-1.02168300
H	-0.43975300	5.16308700	-0.03719200
H	0.24278600	5.00143300	-1.66255500
H	-1.50690100	5.15337100	-1.44236100
P	-0.35092900	-1.23708900	-0.20542600
C	0.23806700	-2.04240500	1.38861100
C	0.03992700	-1.13656200	2.62428900
C	-0.26572200	-3.47445900	1.65579600
H	1.32248200	-2.08879700	1.23008600
C	0.70735800	-1.74941600	3.86650500
H	-1.02782000	-0.98515100	2.82467200
H	0.47361400	-0.15246000	2.41481200
C	0.41065900	-4.07471700	2.90108900
H	-1.35114300	-3.46334400	1.81543500
H	-0.08594200	-4.11873400	0.78654700
C	0.21726400	-3.18014800	4.13401100
H	0.52020900	-1.11242600	4.73923000
H	1.79599600	-1.76015300	3.71705300
H	0.01371100	-5.07945400	3.09077600
H	1.48544200	-4.19538400	2.70514500
H	0.74051400	-3.60744700	4.99774500
H	-0.85013900	-3.15525200	4.39697000
C	0.55291200	-2.14843400	-1.59616300
C	0.72966700	-1.20919800	-2.81273500
C	1.92340100	-2.73566700	-1.19642100
H	-0.09888900	-2.98313500	-1.89353100
C	1.40161600	-1.91844800	-3.99838900
H	1.35023600	-0.35750400	-2.50192100
H	-0.23332700	-0.79417100	-3.12523200
C	2.60109000	-3.44528200	-2.38212900
H	2.57279400	-1.92642100	-0.83779100
H	1.81727500	-3.44845700	-0.37293300
C	2.75377200	-2.52118700	-3.59683800
H	1.52697100	-1.21143200	-4.82717900
H	0.74077300	-2.71647600	-4.36686500
H	3.57945800	-3.82700000	-2.06663700
H	2.00204100	-4.32245600	-2.66695300
H	3.19504400	-3.06800400	-4.43863500
H	3.45154600	-1.70930100	-3.34870100
C	-2.12576900	-1.82811700	-0.42267000
C	-3.05373900	-1.30019300	0.69074800
C	-2.70441600	-1.47027900	-1.80689700
H	-2.09032800	-2.92568700	-0.35190600
C	-4.49090500	-1.82320300	0.52662200
H	-3.06055700	-0.20434700	0.66848100
H	-2.67840900	-1.59244300	1.67546100
C	-4.13989600	-1.99903900	-1.97217800
H	-2.70537300	-0.37907200	-1.92317600
H	-2.07828900	-1.87669800	-2.60775900
C	-5.06495300	-1.49351400	-0.85755600
H	-5.12559500	-1.39750400	1.31276000
H	-4.49918100	-2.91320100	0.67294800
H	-4.52835600	-1.70596500	-2.95517100
H	-4.12153000	-3.09838800	-1.96049900
H	-6.06668000	-1.92593600	-0.96893200
H	-5.17829800	-0.40511800	-0.94722400
C	-1.14466400	2.31667400	-2.72960900
H	-0.21445100	2.37158200	-3.30707300
H	-1.53463400	1.30152500	-2.83123100
H	-1.85334300	3.00938500	-3.19978000
C	-2.36552300	2.61403700	0.15480400

C	-3.63933400	2.43741500	-0.41837800	H	0.20656100	-1.38453200	2.48609800
C	-2.29746800	2.70415400	1.55899900	H	-0.08838100	0.30771400	2.15248500
C	-4.78950900	2.35239500	0.37062900	C	3.28160300	-0.91532700	3.84542500
H	-3.74180700	2.37382800	-1.49916300	H	2.73003200	-2.26859300	2.25521800
C	-3.44132800	2.61313700	2.35389700	H	3.98546400	-1.12424000	1.80104400
H	-1.33483400	2.84781700	2.04634900	C	1.97827700	-0.98960300	4.65442700
C	-4.69366600	2.43580700	1.76130500	H	-0.03942700	-0.17675100	4.61907200
H	-5.76102600	2.22644700	-0.10084100	H	1.21054500	0.97315400	4.16152600
H	-3.35634500	2.68468500	3.43515300	H	4.02526900	-1.61103300	4.25264200
H	-5.58651600	2.36948600	2.37683700	H	3.71149100	0.09183900	3.94177200
9B				H	2.16782600	-0.72506500	5.70145100
Sum of electronic and thermal Free Energies= -3600.035639				H	1.61355000	-2.02676400	4.65586500
C	-0.66836600	3.30092500	1.04277000	C	3.17584000	0.33315200	-0.91319000
C	-0.17942800	4.72844900	0.73068100	C	2.77939700	0.88659400	-2.30322500
C	-2.98774800	3.88921300	0.28678100	C	3.84833100	1.45249500	-0.08985400
C	-1.32800200	5.74070900	0.84381600	H	3.91135200	-0.47308500	-1.05042300
C	-2.51928800	5.32652000	-0.03134900	C	3.98278900	1.47930100	-3.05184300
H	-0.95077200	3.26297700	2.10944600	H	2.02024400	1.66734000	-2.15951200
H	0.22148600	4.74903000	-0.29245500	H	2.30420800	0.11132100	-2.91180500
H	-1.65455700	5.79710200	1.89282300	C	5.04832200	2.06312000	-0.83573200
H	-3.37926800	3.88187000	1.31824800	H	3.11300600	2.24229700	0.11964400
H	-3.34979400	6.03227600	0.10093100	H	4.18932000	1.07324000	0.87847600
H	0.14891400	2.58101000	0.90513400	C	4.66336400	2.57989700	-2.22790100
H	0.64319000	5.00883200	1.40221900	H	3.65576600	1.87311000	-4.02137600
H	-3.82722400	3.62964000	-0.36324200	H	4.70866200	0.68193100	-3.26736200
H	-0.98302700	6.74635700	0.57117800	H	5.47923700	2.87120900	-0.23263000
H	-2.22584200	5.37705500	-1.08877700	H	5.83214400	1.29869000	-0.93646500
C	-1.84595700	2.88851700	0.17250600	H	5.54919100	2.95966700	-2.75048600
C	-1.78897000	1.78703600	-0.61732500	H	3.97353100	3.42868300	-2.12150400
C	-2.97346300	1.39889500	-1.49954100	C	1.81244800	-2.25851300	-0.50286600
H	-3.91124100	1.90995900	-1.23474500	C	0.66138600	-3.07254600	0.12683800
H	-2.76554000	1.70839700	-2.53872100	C	1.88522100	-2.50789100	-2.02495200
Cu	-0.21795000	0.67050400	-0.51354200	H	2.76118900	-2.59889200	-0.06322500
Si	-3.32442900	-0.45769900	-1.65399600	C	0.75775000	-4.56803800	-0.21623900
C	-4.99648700	-0.71972400	-2.51399200	H	-0.30110200	-2.67989000	-0.22466600
H	-5.81675900	-0.30276200	-1.91980900	H	0.66123800	-2.95421700	1.21397700
H	-5.01397500	-0.23095300	-3.49512400	C	1.98049000	-4.00787200	-2.35275100
H	-5.20933400	-1.78331300	-2.66916100	H	0.99139500	-2.09145700	-2.50695000
P	1.65867100	-0.43374300	-0.08679700	H	2.74887900	-1.99246600	-2.45670600
C	1.96131600	-0.29817100	1.76367100	C	0.82497000	-4.80190400	-1.73056100
C	0.64753200	-0.38474800	2.57433000	H	-0.10048500	-5.09488800	0.21687900
C	3.04389700	-1.22145000	2.35558100	H	1.65604000	-4.99209900	0.25538300
H	2.31064300	0.73755000	1.87056600	H	1.99785900	-4.14266900	-3.44085100
C	0.89728500	-0.07547000	4.05865100	H	2.93536400	-4.40084600	-1.97500800

H	0.93567300	-5.87074100	-1.94867500
H	-0.12169300	-4.48386500	-2.18931400
C	-1.96275200	-1.23713900	-2.72320500
H	-2.03211300	-0.89228200	-3.76126200
H	-0.99083900	-0.91542200	-2.33116600
H	-1.98902100	-2.33190100	-2.72716500
C	-3.37195200	-1.34943600	0.02186300
C	-3.48456300	-2.75238000	0.08128500
C	-3.33799600	-0.65172200	1.24395500
C	-3.55896200	-3.43128000	1.29917800
H	-3.51857800	-3.33196600	-0.83966500
C	-3.41622900	-1.32404800	2.46674000
H	-3.22713800	0.42880900	1.23698100
C	-3.52573700	-2.71545400	2.49799700
H	-3.64781600	-4.51473300	1.31352100
H	-3.39158900	-0.76005000	3.39587000
H	-3.58713600	-3.23890400	3.44859500

TS6B

Sum of electronic and thermal Free Energies= -3788.582699

C	1.79813600	-1.78478400	2.28137400
C	2.35214700	-3.01111700	3.03558400
C	4.01978700	-1.42632700	1.17306200
C	3.86835000	-2.90823400	3.24227100
C	4.59122300	-2.65878700	1.91237300
H	1.95187900	-0.89135900	2.90877800
H	2.11181600	-3.90860400	2.45246400
H	4.08610600	-2.07920100	3.93153000
H	4.20936200	-0.53174400	1.78464200
H	5.66640100	-2.51819600	2.07855200
H	0.72801200	-1.90434000	2.12005200
H	1.83897400	-3.11388100	3.99950000
H	4.55128800	-1.27331500	0.23286200
H	4.25323800	-3.81858800	3.71813500
H	4.48398200	-3.54129400	1.26782200
C	2.52190500	-1.55622200	0.96819500
C	1.88907400	-1.49050600	-0.24313100
C	2.65897900	-1.28314400	-1.53561600
H	3.64597100	-1.76487100	-1.50784400
H	2.10992200	-1.80368300	-2.32954400
C	-2.76600500	2.32859000	-1.53683000
C	-3.11690800	3.82718800	-1.56250100
C	-1.20159600	2.73264600	0.39456100
C	-1.96794300	4.69193200	-1.02503000
C	-1.53335900	4.23347500	0.37399800
H	-1.92255300	2.14942900	-2.21550300
H	-4.01652800	3.99580800	-0.95346500
H	-1.11137200	4.61915300	-1.70941100
H	-0.33310700	2.54698300	-0.24977800
H	-0.66230100	4.80763500	0.71044800
H	-3.61244400	1.74899700	-1.91874000
H	-3.37342500	4.12636200	-2.58563900
H	-0.90264700	2.42797300	1.40284900
H	-2.26334000	5.74750300	-1.00594400
H	-2.33997800	4.43742400	1.09278400
C	-2.38713300	1.88071500	-0.11049000
H	-3.25402400	2.08104100	0.53052200
C	-3.34534800	-3.14131800	-3.13040600
C	-3.09127400	-1.69922400	-3.58444000
C	-3.30492300	-2.36981800	-0.70243200
C	-2.30589000	-0.91921300	-2.51898100
C	-3.03155500	-0.91200100	-1.14960400
H	-2.38244900	-3.65929300	-3.03031500
H	-4.05005800	-1.19694400	-3.78089000
H	-1.32665000	-1.39656000	-2.39267100
H	-2.35522300	-2.87458600	-0.48787100
H	-3.92780900	-3.68539300	-3.88353800
H	-2.53178600	-1.68537400	-4.52721000
H	-3.88767200	-2.38961300	0.22267500
H	-2.11846600	0.09950300	-2.86791200
H	-3.99588500	-0.39534700	-1.26084700
C	-4.07094300	-3.15768200	-1.78007300
H	-4.21369300	-4.18803900	-1.43378700
H	-5.07591900	-2.72652400	-1.90142100
C	-3.90732600	1.21542400	3.95668700
C	-4.70385300	0.90120300	2.68589000
C	-1.88464800	0.01526700	3.00780700
C	-4.21540800	-0.39116800	2.00823100
C	-2.68161200	-0.49819800	1.77797300
H	-4.07276000	0.42031200	4.69761500
H	-4.62955700	1.75191300	1.99624000
H	-4.49603500	-1.23194400	2.65834700
H	-1.94212400	-0.77036400	3.77366000
H	-2.44164700	-1.56511000	1.70182100
H	-4.26521700	2.14676900	4.41076000
H	-5.77023500	0.79430700	2.91825600
H	-0.82081900	0.10822700	2.76130200
H	-4.76195800	-0.54475900	1.07236000
C	-2.41055200	1.31340000	3.63967600

H	-1.83836100	1.52228700	4.55143600	C	2.10219600	-1.24521600	-0.83868700
H	-2.24464300	2.16728300	2.97162000	C	2.21989400	1.28238500	-0.96141700
P	-2.00589800	0.04767600	0.10737900	H	2.41062300	1.26596300	-2.04454100
Cu	0.08773800	-0.65248200	-0.08517800	H	1.50589300	2.09843000	-0.79136700
Si	2.89860900	0.49814300	-2.16192200	C	-2.83161800	1.25891400	2.38247500
C	1.24886400	1.14429400	-2.84287000	C	-3.37132200	1.13094200	3.81771800
H	0.46786900	1.06689800	-2.07790100	C	-2.69998800	-1.25781600	2.22329300
H	1.31769500	2.19275200	-3.15146000	C	-2.87951300	-0.15140100	4.50003500
H	0.91969500	0.55178700	-3.70384400	C	-3.23689600	-1.38253300	3.65878000
C	0.49982400	-2.84752400	-0.51446100	H	-1.74010800	1.36331600	2.41642900
O	0.54985500	-3.17888100	-1.68412800	H	-4.47091000	1.13311800	3.79397300
O	-0.10502400	-3.16605400	0.50781900	H	-1.78917700	-0.10215500	4.62074200
C	4.17837900	0.47666400	-3.55685600	H	-1.60349000	-1.24164600	2.24887800
H	3.86043400	-0.21140700	-4.34800200	H	-2.83287700	-2.29207700	4.11823200
H	4.30614100	1.46539500	-4.01078400	H	-3.22629300	2.17777700	1.93856300
H	5.15950100	0.13831100	-3.20616400	H	-3.06992000	2.01280300	4.39508500
C	3.46111500	1.69046700	-0.79855900	H	-2.98866700	-2.14389500	1.65335300
C	2.63225800	1.94177000	0.31286600	H	-3.30732300	-0.23674000	5.50598900
C	4.68679400	2.37743700	-0.85599100	H	-4.32996400	-1.50348700	3.63242300
C	3.00731900	2.83245500	1.31895300	C	-3.20984100	0.02409900	1.52838600
H	1.68758600	1.40996400	0.39661900	H	-4.30659800	-0.01752400	1.45627600
C	5.07024400	3.27224900	0.14660200	C	-2.67956100	4.46999400	-2.27657100
H	5.35739400	2.21611200	-1.69627500	C	-2.13340800	4.30625100	-0.85259000
C	4.23075800	3.50213500	1.23702500	C	-3.54938900	2.07307000	-2.19944900
H	2.34881000	3.00358400	2.16678400	C	-1.80546100	2.83884400	-0.54291200
H	6.02360700	3.78937100	0.07593100	C	-3.03035000	1.91508900	-0.75557000
H	4.52662200	4.19728100	2.01810600	H	-1.88589400	4.22809400	-2.99755800
TS7B				H	-2.87673000	4.67321000	-0.13039100
Sum of electronic and thermal Free Energies= -3788.580100				H	-1.00225500	2.49764200	-1.21144900
C	1.49130600	-2.54174000	-0.34213600	H	-2.78798100	1.71755800	-2.90882400
C	1.20494400	-3.53537600	-1.48561500	H	-2.96343300	5.51236900	-2.46299100
C	3.31603600	-1.47414500	-1.72196100	H	-1.23623400	4.91990700	-0.71217700
C	2.44935800	-3.78210600	-2.34800300	H	-4.44565500	1.46626700	-2.36373900
C	3.01952900	-2.45844700	-2.87335800	H	-1.40529000	2.74432500	0.46963800
H	2.19916700	-3.01243100	0.35778100	H	-3.83613100	2.23525500	-0.08191700
H	0.40516600	-3.13183900	-2.12382900	C	-3.87904600	3.54367200	-2.51575000
H	3.21363000	-4.29025200	-1.74285400	H	-4.22590500	3.62379200	-3.55289900
H	4.11979100	-1.89674400	-1.10128100	H	-4.71772900	3.86404700	-1.88146500
H	3.93509700	-2.63711900	-3.45028900	C	-4.73443300	-3.63277000	-0.72012200
H	0.58402100	-2.34251000	0.23237000	C	-5.38297400	-2.32365500	-0.24554100
H	0.83070800	-4.47989200	-1.07139800	C	-2.81085100	-2.31770000	-1.72581800
H	3.70155800	-0.53466000	-2.12424900	C	-5.02315700	-1.14558100	-1.16598100
H	2.21126500	-4.45463300	-3.18151100	C	-3.50430700	-0.96680400	-1.40776200
H	2.29662500	-2.00096200	-3.56341900	H	-5.14358700	-3.90123400	-1.70477400

H	-5.06598200	-2.11285100	0.78240900	H	-3.90601800	2.46499400	1.99378700
H	-5.48939000	-1.32786300	-2.14490800	H	-3.00892600	4.67496500	0.07291100
H	-3.08432600	-2.57684200	-2.75851000	H	-5.73532600	4.28432100	1.41821900
H	-3.39307400	-0.37726100	-2.32313100	H	-5.85382000	1.84008800	0.41068100
H	-4.99610600	-4.45212500	-0.04067300	H	-6.61835800	3.82906700	-0.85024000
H	-6.47368000	-2.43165300	-0.21382400	H	-2.28994900	2.64219700	1.33843600
H	-1.72326300	-2.18272300	-1.72207400	H	-3.35676700	4.86772900	1.78916500
H	-5.47025400	-0.21795000	-0.78885800	H	-5.55376600	1.62449200	-1.30243200
C	-3.20902800	-3.49543600	-0.82706000	H	-5.29166500	5.61034900	0.34831600
H	-2.77276100	-4.41587800	-1.23225900	H	-5.01472900	4.03857400	-1.55026400
H	-2.77787700	-3.37314000	0.17297000	C	-3.78263700	1.96877800	-0.07988300
P	-2.55466100	0.15987600	-0.23268200	C	-3.35319600	0.29510000	-1.95657800
Cu	-0.35343600	-0.03623300	-0.32886100	H	-4.30875300	0.60748500	-2.38732100
Si	3.84590900	1.92663800	-0.14535800	H	-2.59214800	0.41614000	-2.73674100
C	4.97414800	0.54665300	0.50446400	C	4.26822600	-1.08566500	-1.99166600
C	4.55986800	-0.32087500	1.53529200	C	4.89775900	-2.32490000	-2.65173200
C	6.27384700	0.36815100	-0.00520000	C	2.73246300	-2.57705200	-0.66733200
C	5.40197200	-1.32049200	2.02579000	C	3.91339400	-3.49861500	-2.72091400
H	3.56327000	-0.23403300	1.95747000	C	3.34923100	-3.81879000	-1.33145500
C	7.12266000	-0.62806000	0.48311000	H	3.44006600	-0.72708900	-2.61844100
H	6.63628800	1.01601300	-0.79921600	H	5.78467900	-2.62613500	-2.07620700
C	6.68668100	-1.47766800	1.50053800	H	3.08687700	-3.23957700	-3.39730400
H	5.05332400	-1.97648000	2.81911200	H	1.85718500	-2.24507900	-1.24266500
H	8.12173500	-0.74008600	0.06948400	H	2.59427600	-4.61090400	-1.39629100
H	7.34292000	-2.25504300	1.88314800	H	5.01204300	-0.28449900	-1.95956800
C	3.47658300	3.12906200	1.26666700	H	5.25312800	-2.06168000	-3.65506100
H	4.40827400	3.53735200	1.67417700	H	2.36225400	-2.84232000	0.32500000
H	2.86688300	3.96833400	0.91229100	H	4.40220600	-4.38169600	-3.14874100
H	2.92191200	2.64566600	2.07383600	H	4.15484800	-4.20772600	-0.69228700
C	4.76661300	2.88632400	-1.50284300	C	3.73270500	-1.40487500	-0.57819400
H	4.12360900	3.67841300	-1.90433500	H	4.58546500	-1.70530400	0.04680200
H	5.67393100	3.36677500	-1.12052700	C	4.85499500	4.37415600	-0.55493400
H	5.05507400	2.24426900	-2.34258000	C	4.67299700	3.39388300	-1.72034500
C	1.58945800	-0.02720200	-0.51741100	C	4.32818200	2.49559500	1.08585600
C	0.88536000	0.25388000	1.49360500	C	3.71156600	2.25434900	-1.35178100
O	0.92729700	-0.79098300	2.10706300	C	4.15909200	1.49601000	-0.07760200
O	0.76883900	1.45709200	1.63556500	H	3.90366300	4.89003500	-0.36408500
10B				H	5.64940800	2.97056300	-1.99693900
Sum of electronic and thermal Free Energies= -3788.632775				H	2.70624500	2.65986800	-1.17342600
C	-3.34286500	2.80283500	1.10902800	H	3.35130100	2.92544000	1.34936200
C	-3.63878900	4.30174300	0.89232800	H	5.58493500	5.14932900	-0.81566900
C	-5.23949300	2.19998600	-0.42936700	H	4.29814600	3.91675000	-2.60792300
C	-5.11425800	4.54629600	0.54920900	H	4.70579400	1.99096400	1.98060800
C	-5.54733700	3.69635800	-0.65240900	H	3.61040500	1.56627400	-2.19610100

H	5.14133200	1.04031600	-0.26377800
C	5.29420300	3.63525100	0.71521900
H	5.37380300	4.33251900	1.55756400
H	6.29864000	3.21545200	0.56208400
C	2.73124100	-2.69803400	3.66742000
C	4.03032900	-2.30439400	2.94934400
C	1.57535100	-0.64557200	2.70949600
C	4.14400000	-0.77966300	2.78196700
C	2.91216000	-0.11797100	2.11861900
H	2.74660100	-2.28785100	4.68753000
H	4.06763300	-2.80075600	1.97172500
H	4.25032300	-0.34035600	3.78429400
H	1.46518100	-0.16739700	3.69322400
H	2.92894500	0.94142500	2.39320800
H	2.67227900	-3.78787200	3.77132400
H	4.90005700	-2.66810700	3.50973600
H	0.73158800	-0.29476500	2.10626300
H	5.06477300	-0.52306100	2.24342500
C	1.49908000	-2.16254500	2.92467000
H	0.58679300	-2.39363300	3.48639400
H	1.39501700	-2.68079900	1.96441000
P	2.93667800	0.08787300	0.24506200
Cu	0.98322100	0.56360200	-0.49616900
Si	-3.46983400	-1.58144000	-1.58393500
C	-4.54345700	-1.89641800	-0.05703900
C	-4.13707700	-1.43732900	1.21388900
C	-5.76205600	-2.59500300	-0.13740600
C	-4.91854000	-1.66983400	2.34706400
H	-3.20760900	-0.88313300	1.32260400
C	-6.54622000	-2.82988500	0.99468000
H	-6.11039200	-2.96653800	-1.09820900
C	-6.12465000	-2.36653900	2.24127600
H	-4.58506900	-1.30484900	3.31521000
H	-7.48314800	-3.37345800	0.90268200
H	-6.73143100	-2.54672400	3.12496400
C	-1.73787700	-2.29587800	-1.28740600
H	-1.78973500	-3.37525000	-1.10656100
H	-1.09645700	-2.12449200	-2.15926200
H	-1.25770400	-1.82864700	-0.42239400
C	-4.22879400	-2.42646000	-3.10206500
H	-3.60892200	-2.23983500	-3.98643200
H	-4.29924800	-3.51205400	-2.97278300
H	-5.23355800	-2.04963300	-3.32235500
C	-2.96127000	1.14372500	-0.76645700
C	-1.52078700	0.94259200	-0.36019300
O	-1.20001500	0.68028500	0.82065200
O	-0.65802300	0.99372600	-1.32493100

11B

Sum of electronic and thermal Free Energies= -4643.444936

C	-1.52055600	0.53083600	-0.27798000
O	-0.50659600	0.17759500	0.37691600
O	-1.46709200	1.33660000	-1.29237900
B	-0.28025400	2.26604800	-1.65461000
O	0.97610500	1.45905400	-1.82100600
O	-0.57951800	2.76826900	-2.97939500
C	1.13537200	1.19819600	-3.22128400
C	0.45155400	2.40661200	-3.87232800
H	1.17202500	3.23146700	-4.00001100
H	0.03841800	2.16456600	-4.86023200
H	2.20127800	1.11245900	-3.45970000
H	0.63412500	0.25908300	-3.49631900
C	-2.44594300	-0.01322900	2.55981100
C	-3.15066000	0.95809200	3.53428900
C	-4.67298000	-0.73858000	1.67273600
C	-4.56443000	0.48746200	3.89582700
C	-5.39529200	0.23230700	2.63254800
H	-2.31214200	-0.98101700	3.06920000
H	-3.20138700	1.95016600	3.06697100
H	-4.50045600	-0.44231100	4.48010500
H	-4.56312300	-1.71001800	2.17773500
H	-6.37985400	-0.17469700	2.89321000
H	-1.45302300	0.35289500	2.31331000
H	-2.54029400	1.06651300	4.43942700
H	-5.28932400	-0.92649000	0.79328700
H	-5.06138700	1.22587800	4.53682700
H	-5.57088900	1.18338400	2.11269900
C	-3.28333300	-0.24540200	1.31681700
C	-2.89885700	0.02395300	0.04219800
C	-3.80151600	-0.10780900	-1.17059900
H	-3.60613600	0.73635100	-1.83939900
H	-4.85694200	-0.04371400	-0.89328200
Si	-3.56613100	-1.69422400	-2.21138700
C	-1.77819600	-1.81046800	-2.82538600
H	-1.50567600	-0.90417700	-3.37575200
H	-1.07073200	-1.92073700	-1.99638200
H	-1.64897000	-2.67113200	-3.49047700
C	-4.73479000	-1.59225400	-3.69750700
H	-4.49405000	-0.71410700	-4.30687400

H	-4.65071200	-2.47510200	-4.34042400
H	-5.78264500	-1.49919400	-3.39181800
C	-3.96631300	-3.23888000	-1.18756900
C	-5.11702100	-4.01072400	-1.43089600
C	-3.11605100	-3.65692900	-0.14422800
C	-5.41136900	-5.14480300	-0.67011100
H	-5.79771200	-3.72651200	-2.22942200
C	-3.40457100	-4.78730700	0.62177300
H	-2.21744400	-3.08740900	0.08007600
C	-4.55499500	-5.53517500	0.35982100
H	-6.30729500	-5.72249100	-0.88196400
H	-2.73213300	-5.08658400	1.42167700
H	-4.78056300	-6.41671000	0.95391600
C	4.12469900	-2.24967000	-1.71216400
C	4.37267500	-3.63913900	-2.32538600
C	2.24075500	-3.20392500	-0.34014800
C	3.09698700	-4.48922200	-2.35460000
C	2.47946900	-4.59249900	-0.95466300
H	3.43208800	-1.69133900	-2.35731100
H	5.14231600	-4.15862100	-1.73692700
H	2.36957100	-4.02905200	-3.03799100
H	1.48736700	-2.66757800	-0.93374600
H	1.53321700	-5.14474500	-0.99109300
H	5.06697000	-1.69465400	-1.70215300
H	4.78054400	-3.52365600	-3.33668100
H	1.81844800	-3.31278200	0.66083100
H	3.31246700	-5.48731200	-2.75357500
H	3.15163200	-5.16742200	-0.30160800
C	3.52708200	-2.35261100	-0.29246600
H	4.26589600	-2.86012300	0.34308100
C	6.20847800	2.87788800	-0.46862600
C	5.79742000	1.91303600	-1.58694800
C	5.17237400	1.30007400	1.24457900
C	4.56145900	1.08906400	-1.19673700
C	4.75931800	0.31511000	0.12973500
H	5.42453700	3.63670700	-0.33722700
H	6.63363200	1.23336800	-1.80658100
H	3.68914300	1.74577900	-1.08658600
H	4.33947100	1.98564400	1.45739700
H	7.12277000	3.41708500	-0.74309600
H	5.59304000	2.46324800	-2.51302800
H	5.38953300	0.76554900	2.17455800
H	4.30954200	0.40025600	-2.00792000
H	5.58155100	-0.40360700	0.00274200
C	6.41134900	2.12329900	0.85042300
H	6.65472800	2.82221100	1.65948600
H	7.27318900	1.44748300	0.75337900
C	2.48739800	-3.27967400	4.04351800
C	3.79584100	-3.23329100	3.24294000
C	1.78411100	-1.06104400	3.01543600
C	4.25798500	-1.78579600	3.00537900
C	3.18479700	-0.86490300	2.37261200
H	2.65486000	-2.83520700	5.03526600
H	3.64937200	-3.75086800	2.28658200
H	4.52566800	-1.35789400	3.98226800
H	1.79865600	-0.51690400	3.97009100
H	3.45653800	0.16305100	2.63259500
H	2.18300000	-4.31891700	4.21465600
H	4.58673600	-3.77973300	3.77062300
H	1.02605600	-0.57450000	2.39408100
H	5.18110800	-1.77492100	2.41286400
C	1.37549300	-2.50924700	3.31946500
H	0.46218500	-2.49706500	3.92596800
H	1.11209600	-3.03671400	2.39548400
P	3.18603600	-0.67583800	0.49344100
Cu	1.41786500	0.28316300	-0.23694900
Si	-0.06727300	3.76703400	-0.24807400
C	0.88122700	5.22600400	-1.02937300
H	0.98409400	6.06854700	-0.33625100
H	1.88872100	4.91777900	-1.33451200
H	0.36266300	5.58547500	-1.92406000
C	0.90992000	3.27716900	1.32286500
H	0.43977100	2.44771400	1.86082300
H	1.92370800	2.96205800	1.04342800
H	1.01934800	4.11629500	2.02010100
C	-1.78022000	4.40200200	0.29805600
C	-2.79766200	4.56852100	-0.66299300
C	-2.10071100	4.70946000	1.63292400
C	-4.06702100	5.02934300	-0.31019100
H	-2.59365000	4.32470200	-1.70349100
C	-3.37149700	5.16590900	1.99584500
H	-1.34783400	4.59312300	2.40917200
C	-4.35883200	5.32837600	1.02282200
H	-4.83159300	5.14981100	-1.07386300
H	-3.58880500	5.39709000	3.03600200
H	-5.34788100	5.68359400	1.30073300

TS8B

Sum of electronic and thermal Free Energies= -4643.425931

C	-1.41536300	0.69747400	-0.14446300	C	-7.54266700	-2.73363800	-0.68555000
O	-0.53384600	0.15342300	0.56203100	H	-6.99232800	-1.24155700	-2.11926900
O	-1.12484300	1.35295800	-1.23418400	C	-5.73274900	-3.75915200	0.53693900
B	0.29212500	1.58420400	-1.71505400	H	-3.75987500	-3.07060200	0.06412200
O	0.89979800	0.33830600	-2.20571500	C	-7.09908400	-3.64575500	0.27359400
O	0.20660800	2.47850100	-2.84403500	H	-8.60420200	-2.64216600	-0.90018500
C	1.00341200	0.43210100	-3.62828900	H	-5.37890300	-4.47036500	1.27886600
C	0.98674400	1.94195400	-3.89681600	H	-7.81256300	-4.26567600	0.80974000
H	2.00807400	2.35398700	-3.87829700	C	3.19296400	-2.69649800	-1.80909300
H	0.53331600	2.19623400	-4.86222100	C	2.91660000	-4.04657900	-2.49332300
H	1.92216500	-0.05864900	-3.97084200	C	1.23576000	-3.07639600	-0.27893900
H	0.14611600	-0.06770500	-4.10320200	C	1.43464600	-4.43334200	-2.41695200
C	-2.49963800	0.49719400	2.69197600	C	0.94384300	-4.42091700	-0.96375900
C	-2.94769600	1.62566600	3.64888900	H	2.65465700	-1.90403600	-2.34435500
C	-4.82235800	0.37859400	1.75720700	H	3.52254500	-4.82628600	-2.00962400
C	-4.44250700	1.54522000	3.98082700	H	0.84257100	-3.71665700	-3.00251100
C	-5.28501900	1.51031600	2.70006600	H	0.66501300	-2.27843200	-0.76941100
H	-2.63133400	-0.46830400	3.20546200	H	-0.13229800	-4.62644900	-0.92184900
H	-2.72764500	2.59206500	3.17660400	H	4.26073900	-2.47306000	-1.88858500
H	-4.63704400	0.63406400	4.56514300	H	3.24738900	-4.00020900	-3.53800900
H	-4.98393400	-0.58380600	2.26587600	H	0.88906400	-3.11105600	0.75609200
H	-6.34688300	1.37663200	2.93934900	H	1.27271600	-5.41923100	-2.86883100
H	-1.44134900	0.59160900	2.46512000	H	1.43813400	-5.22934800	-0.40554000
H	-2.34851700	1.57873900	4.56665800	C	2.73264200	-2.70541100	-0.33419100
H	-5.44564100	0.35065300	0.86369200	H	3.31771400	-3.46963700	0.19655300
H	-4.74048500	2.39128500	4.61221100	C	7.13345200	1.13367500	-0.63634000
H	-5.19544900	2.47135200	2.17650400	C	6.24731300	0.52131700	-1.72815200
C	-3.34434100	0.48293400	1.43265200	C	5.70626300	-0.02179200	1.13763800
C	-2.88040500	0.62244800	0.16264200	C	4.82637300	0.25289400	-1.20810000
C	-3.76722500	0.72257200	-1.06596200	C	4.82646200	-0.65931400	0.04104300
H	-3.31876300	1.43957500	-1.75932300	H	6.75595800	2.13450600	-0.38428600
H	-4.75628400	1.11453100	-0.81496900	H	6.69365400	-0.42158100	-2.07605800
Si	-4.00271100	-0.91384000	-2.03281700	H	4.35574900	1.20680500	-0.93841500
C	-2.35268300	-1.82305900	-2.20481000	H	5.25363900	0.92095900	1.47552500
H	-1.59347900	-1.17241700	-2.65006400	H	8.15807300	1.26890000	-1.00236800
H	-1.96479300	-2.14245900	-1.23174200	H	6.20095800	1.18393400	-2.60054600
H	-2.45830900	-2.71425500	-2.83302100	H	5.77543200	-0.67279500	2.01424900
C	-4.68299700	-0.48485300	-3.74726500	H	4.20913700	-0.17216200	-2.00414800
H	-3.95112900	0.10987100	-4.30502600	H	5.29327600	-1.61716900	-0.22864700
H	-4.89957500	-1.38533100	-4.33186700	C	7.13052700	0.25880700	0.62332600
H	-5.60414500	0.10545900	-3.69077800	H	7.71844800	0.73075900	1.41968700
C	-5.23889500	-2.03152800	-1.12474500	H	7.62236400	-0.69879900	0.40015500
C	-6.62184400	-1.94068600	-1.37302900	C	1.81220600	-3.49585600	4.04139600
C	-4.81887800	-2.96244200	-0.15574400	C	2.98459400	-3.83662500	3.11168900

C	1.84754300	-1.09833500	3.19983200	H	3.79249000	-0.66445500	-2.12972600
C	3.89601600	-2.61867300	2.88360400	H	4.22508400	-3.53298200	-1.15170000
C	3.15570400	-1.34607900	2.40093700	H	3.19760900	-2.56189800	-3.87259000
H	2.20443900	-3.21719500	5.03023100	H	1.25758900	-1.19695700	-2.63430600
H	2.58994400	-4.20282200	2.15614000	H	1.02726700	-3.58198000	-3.24169000
H	4.37742700	-2.37779100	3.84260400	H	4.47369800	-1.12928600	-0.57920200
H	2.14706300	-0.67851600	4.17058600	H	5.17172900	-2.70037100	-2.37879000
H	3.79078900	-0.49057600	2.65244300	H	0.31859700	-2.03132100	-1.41051000
H	1.18003400	-4.37848700	4.19402800	H	3.45698300	-4.23676400	-3.40214000
H	3.58030500	-4.65535600	3.53298200	H	1.67771100	-4.08009800	-1.68521300
H	1.25188400	-0.32780300	2.70005800	C	2.32260600	-1.49432700	-0.76060600
H	4.71039400	-2.87842700	2.19680100	H	2.31992600	-2.26767100	0.01664500
C	0.98262800	-2.33531800	3.47634000	C	2.94317900	4.24038200	-1.67488100
H	0.18566500	-2.05979600	4.17708600	C	3.00362100	2.99824300	-2.57295300
H	0.47610600	-2.65719300	2.55986900	C	2.65958500	2.73581600	0.36409900
P	3.03980100	-1.05973200	0.53601000	C	2.22492500	1.82429300	-1.95829700
Cu	1.43141800	0.33119200	0.01312800	C	2.72434600	1.48167600	-0.53560600
Si	1.33712900	2.91901100	-0.27807500	H	1.90701500	4.60343100	-1.62854800
C	2.62967400	3.85203800	-1.32085800	H	4.05248800	2.70216000	-2.71749300
H	3.06677400	4.68208000	-0.75436200	H	1.16003400	2.08865800	-1.90334400
H	3.44901400	3.19204400	-1.62854900	H	1.61225800	3.02280000	0.52392300
H	2.17621200	4.26235200	-2.22684100	H	3.54067100	5.05251700	-2.10541300
C	2.24516400	2.67263000	1.41160900	H	2.60321100	3.22302600	-3.56856700
H	1.70549600	2.06843100	2.14756100	H	3.07479100	2.52133700	1.35350300
H	3.23727500	2.23157500	1.27684900	H	2.29068200	0.95152800	-2.61697300
H	2.39542200	3.66540700	1.85542300	H	3.77405700	1.16683900	-0.60520300
C	-0.08284200	4.12306200	0.15273500	C	3.42996300	3.91419200	-0.25679100
C	-0.78580200	4.81385200	-0.85512000	H	3.33434700	4.79236000	0.39228500
C	-0.47324900	4.36272300	1.48341400	H	4.50077600	3.66658100	-0.29080000
C	-1.81408700	5.70546500	-0.54724900	C	3.35336300	-2.60622400	3.25596200
H	-0.53532600	4.63309900	-1.89622300	C	4.24213700	-1.77389800	2.32139100
C	-1.50689800	5.24975900	1.79905300	C	1.40312100	-1.05058500	2.80354100
H	0.03648700	3.85401700	2.29706300	C	3.79117500	-0.30382500	2.26105300
C	-2.17925600	5.92818100	0.78243900	C	2.28699200	-0.09417100	1.95748500
H	-2.33469600	6.22581700	-1.34753200	H	3.46485600	-2.23715300	4.28555100
H	-1.77937500	5.41530600	2.83873300	H	4.22667900	-2.22261600	1.32105100
H	-2.97994500	6.62283800	1.02296800	H	3.98035500	0.14264800	3.24796300
TS1B[S]				H	1.42035600	-0.66278100	3.83114400
Sum of electronic and thermal Free Energies= -4002.284741				H	2.01889200	0.91222300	2.29559900
C	3.75058200	-1.42916900	-1.34428800	H	3.68467200	-3.65146000	3.26169100
C	4.16496800	-2.78127900	-1.95169900	H	5.28614900	-1.81309200	2.65523000
C	1.32210300	-1.95237700	-1.84142600	H	0.35680900	-0.98650300	2.49042000
C	3.16607800	-3.25219100	-3.01761400	H	4.41695400	0.25801500	1.55778400
C	1.73817900	-3.29899600	-2.45655000	C	1.87780900	-2.50995400	2.84573100

H	1.25031800	-3.06753500	3.55087100
H	1.73502600	-2.99464300	1.87060700
P	1.73699300	0.04612600	0.16372600
Cu	-0.52655900	0.56608700	0.25253000
B	-2.21221400	0.78811100	1.37524900
O	-3.38014400	1.53964700	1.33854800
O	-2.37643500	-0.42469700	2.05023500
C	-4.29339300	0.92883600	2.26009500
C	-3.74870900	-0.50090600	2.46420100
H	-3.79561700	-0.82410100	3.50963200
H	-4.27420900	-1.23230600	1.84059000
H	-4.29739100	1.50231100	3.19608300
H	-5.29934400	0.93984600	1.83097600
Cl	-0.66507900	1.87940400	2.30065100
Si	-2.28280700	0.69422400	-1.25148700
C	-2.81710100	2.48420200	-1.58604100
H	-3.30940100	2.92596100	-0.71784000
H	-1.94361700	3.09914400	-1.83201200
H	-3.49887100	2.53031300	-2.44409600
C	-1.45614500	0.12248800	-2.88546800
H	-2.15656800	0.30694600	-3.70987400
H	-0.53348900	0.66941400	-3.10594100
H	-1.22565000	-0.94590900	-2.88224600
C	-3.79391700	-0.44780900	-1.10607400
C	-5.11307700	0.03900400	-1.10425500
C	-3.61889500	-1.84162500	-1.02746300
C	-6.20870300	-0.82513400	-1.02698900
H	-5.28941500	1.10985400	-1.15899300
C	-4.70671100	-2.71251800	-0.94647800
H	-2.61260000	-2.25641800	-1.02070500
C	-6.00826500	-2.20440600	-0.94592000
H	-7.21838100	-0.42201000	-1.03050500
H	-4.54128200	-3.78511200	-0.88371300
H	-6.85845600	-2.87848800	-0.88438400

B(Pin)-Cl

Sum of electronic and thermal Free Energies= -714.208325

B	-0.32448400	-0.00013500	-0.00011600
O	0.40500900	-1.15090500	-0.03154600
O	0.40488500	1.15082700	0.03133500
C	1.79390200	-0.77572800	0.03438700
C	1.79375400	0.77586300	-0.03426200
H	2.32687200	1.23781000	0.80134200
H	2.21509100	1.15513800	-0.97067500
H	2.21502300	-1.15488000	0.97098200
H	2.32741300	-1.23760100	-0.80100600
Cl	-2.08629800	0.00000100	0.00005100

TS2B^{S}

Sum of electronic and thermal Free Energies= -3770.489309

C	-3.46819600	-1.93750200	-1.32219500
C	-3.68291800	-2.69706500	-2.64362700
C	-0.95788300	-1.94311100	-1.73694600
C	-2.46368200	-3.55675900	-3.00450000
C	-1.18329300	-2.71120900	-3.04906900
H	-3.38961300	-2.66894400	-0.50901900
H	-3.87028100	-1.97432500	-3.45068100
H	-2.34734600	-4.35150700	-2.25389500
H	-0.74209500	-2.65131300	-0.92814900
H	-0.31301300	-3.34390000	-3.25792300
H	-4.34610100	-1.32189500	-1.10156300
H	-4.58290600	-3.31922200	-2.56844100
H	-0.06609700	-1.31343800	-1.81651000
H	-2.62390400	-4.05786300	-3.96639200
H	-1.25411100	-1.99343000	-3.87913500
C	-2.18753700	-1.07706500	-1.37516700
H	-2.31008200	-0.35180700	-2.19013600
C	-2.20882300	-2.04818700	4.35313200
C	-2.28870900	-2.93837500	3.10743600
C	-2.48172200	0.00619100	2.87705800
C	-1.79390000	-2.20431200	1.85078100
C	-2.55451000	-0.87829100	1.61181500
H	-1.15579700	-1.82285500	4.57208200
H	-3.32988700	-3.25804300	2.95621600
H	-0.72212200	-1.98719000	1.94412000
H	-1.44024100	0.32500800	3.02899500
H	-2.60547100	-2.57630100	5.22817700
H	-1.70063400	-3.85261200	3.24993100
H	-3.07577600	0.91701200	2.74974200
H	-1.89018000	-2.86585100	0.98551300
H	-3.60948400	-1.10885700	1.40961800
C	-2.97188200	-0.73641100	4.13185900
H	-2.87256300	-0.08069900	5.00492000
H	-4.04425800	-0.95358100	4.02520000
C	-4.01419800	2.64053700	-2.58586400
C	-4.70860700	1.51374300	-1.80763400
C	-2.13056800	2.66712200	-0.89364100
C	-4.35357200	1.54425800	-0.31052400
C	-2.83569200	1.60680100	-0.00825400
H	-4.39600500	3.61143900	-2.23907300

H	-4.42563500	0.55043300	-2.24690700
H	-4.80355900	2.44997500	0.12114500
H	-2.42859200	3.65675100	-0.52061200
H	-2.72893800	1.96472100	1.02295500
H	-4.26229500	2.57118000	-3.65147100
H	-5.79705500	1.59041900	-1.91746100
H	-1.04674700	2.60443900	-0.75905200
H	-4.82241700	0.70167500	0.21159300
C	-2.49348300	2.59742900	-2.38302800
H	-2.01336500	3.43070400	-2.90822100
H	-2.08825800	1.68168300	-2.83438500
P	-1.84154300	0.01384000	0.12142000
Cu	0.35434800	0.31689800	0.44406800
B	1.97307000	-0.69051400	1.03283900
O	1.99812100	-2.04548000	0.73305400
O	2.80095600	-0.39908200	2.11052900
C	3.02406300	-2.67578000	1.52000500
C	3.42386200	-1.61324100	2.56490100
H	3.05249200	-1.84781400	3.57010800
H	4.50681300	-1.46521500	2.62288200
H	2.62593900	-3.59072900	1.97133100
H	3.85789500	-2.94051500	0.86124300
O	1.27582200	4.43921600	0.26630200
C	0.96353100	3.52602100	1.01108200
O	1.29745000	2.24030300	0.84600700
C	0.14818900	3.74717600	2.27537400
H	0.78852300	3.57963600	3.14767900
H	-0.23738900	4.76706000	2.29786200
H	-0.67418300	3.02874000	2.34025300
Si	2.61114800	1.50955100	-0.35493000
C	1.81741900	2.17222500	-1.94747900
H	2.55051400	2.15710200	-2.76097500
H	0.95461900	1.58489800	-2.28484300
H	1.48631500	3.19918000	-1.77805200
C	3.97712200	2.59890600	0.37601600
H	4.24420200	2.25358800	1.38092800
H	4.88090200	2.57243600	-0.24029800
H	3.63099900	3.63180100	0.45104400
C	3.65427500	0.01839700	-1.04228100
C	4.91640100	-0.31639300	-0.51753100
C	3.21220700	-0.72263000	-2.15432900
C	5.70054500	-1.33009700	-1.07712900
H	5.30199500	0.22459700	0.34239300
C	3.98671700	-1.73352100	-2.72245000
H	2.23916500	-0.50714800	-2.58996500
C	5.23880700	-2.04262300	-2.18457500
H	6.67570600	-1.55681300	-0.65229900
H	3.61638700	-2.28043900	-3.58620400
H	5.84701700	-2.82804000	-2.62529000

$PhMe_2Si$-OAc

Sum of electronic and thermal Free Energies= -829.383260

O	-3.44034300	-0.34729400	0.00008600
C	-2.78496500	0.67456800	-0.00062100
O	-1.43402000	0.68860600	-0.00069600
C	-3.36728600	2.06770100	-0.00163500
H	-3.01947400	2.61470500	-0.88299100
H	-4.45531200	2.01315300	-0.00101800
H	-3.01849300	2.61648900	0.87821400
Si	-0.49415600	-0.75993800	0.00049600
C	-0.84835500	-1.74039100	1.56240500
H	-0.20230700	-2.62331400	1.62416400
H	-0.66500100	-1.13351900	2.45482200
H	-1.88949200	-2.07311600	1.57747700
C	-0.84812400	-1.74294100	-1.55984500
H	-0.66535400	-1.13730200	-2.45321700
H	-0.20156800	-2.62557200	-1.62042200
H	-1.88906200	-2.07632200	-1.57419500
C	1.26269900	-0.08943300	0.00000200
C	1.54076300	1.28890800	0.00117600
C	2.35485800	-0.97758200	-0.00135700
C	2.85469700	1.76065800	0.00103800
H	0.71830600	1.99772100	0.00214800
C	3.66943100	-0.51173200	-0.00149100
H	2.18415900	-2.05269100	-0.00237700
C	3.92151900	0.86151200	-0.00028400
H	3.04532800	2.83038800	0.00194400
H	4.49560600	-1.21730900	-0.00255500
H	4.94433700	1.22771200	-0.00039500

1B^S

Sum of electronic and thermal Free Energies= -2941.185248

C	-1.59620500	0.38416100	2.48094400
C	-2.49376700	-0.18273400	3.59462000
C	-1.45792000	-1.90149400	1.43593800
C	-2.21845600	-1.66971600	3.84950600
C	-2.34480100	-2.47715500	2.55180900
H	-0.54842800	0.33904500	2.80847900
H	-3.54741200	-0.05045700	3.30982700
H	-1.20202900	-1.78599100	4.25084100

H	-0.40018600	-2.00242700	1.71477300
H	-2.08004100	-3.52686500	2.72524800
H	-1.83727400	1.44093800	2.33394300
H	-2.34516400	0.39765600	4.51307900
H	-1.59129000	-2.49162800	0.52673000
H	-2.90272200	-2.05969200	4.61227500
H	-3.39335300	-2.47108700	2.22043200
C	-1.75265900	-0.41018800	1.16430500
H	-2.79435600	-0.30319800	0.82962600
C	0.09200900	4.94017800	-0.44297900
C	0.15723000	4.22431100	0.91185600
C	-0.92869300	2.84749900	-1.48172500
C	0.27009600	2.70301700	0.73792300
C	-0.87991700	2.12135200	-0.12152900
H	1.04833100	4.80794900	-0.96795800
H	-0.74770500	4.45928600	1.49099300
H	1.22296800	2.45172100	0.25295300
H	-0.01843800	2.62159700	-2.05542700
H	-0.04152900	6.01930900	-0.30214200
H	1.00698000	4.59071300	1.49960900
H	-1.77734500	2.49706200	-2.07833800
H	0.30132900	2.21869800	1.71845300
H	-1.83560100	2.31404500	0.38521200
C	-1.04243500	4.37251100	-1.30525100
H	-1.05314400	4.85306000	-2.29095300
H	-2.00804600	4.60669800	-0.83451500
C	-2.82424800	-2.78693400	-2.56779500
C	-3.51298100	-1.66401800	-1.77797800
C	-0.64524000	-1.48123600	-2.53482200
C	-2.87977300	-0.29387800	-2.07367300
C	-1.34344200	-0.24997600	-1.89491400
H	-2.97795100	-2.61603300	-3.64310100
H	-3.45494600	-1.88738100	-0.70591100
H	-3.09600900	-0.04486200	-3.12285600
H	-0.63802900	-1.31500200	-3.62137900
H	-0.97984200	0.60103700	-2.47846500
H	-3.28925600	-3.75254300	-2.33669500
H	-4.58076200	-1.62637100	-2.02537300
H	0.40361900	-1.50632800	-2.21750500
H	-3.36416800	0.48736400	-1.47502500
C	-1.31787600	-2.83486600	-2.27414100
H	-0.83471800	-3.59786000	-2.89566800
H	-1.15362100	-3.14810900	-1.23663800
P	-0.64217900	0.24374000	-0.21186800
Cu	1.52454000	-0.30214600	-0.06342900
B	3.45899900	-0.75851800	0.02152800
O	3.99966600	-2.00149500	-0.29973600
O	4.46694100	0.12517000	0.40154000
C	5.42703200	-1.96084300	-0.16123700
C	5.73713000	-0.54098400	0.36231200
H	5.74898000	-2.74653700	0.53269100
H	5.89171900	-2.15994200	-1.13508100
H	6.17318900	-0.55055900	1.36913100
H	6.41893200	0.01198100	-0.29489300

2B^{S}

Sum of electronic and thermal Free Energies= -3253.075514

B	-1.43965700	-1.61964300	-0.47572500
O	-1.55897000	-2.22679100	-1.72544400
O	-1.71483400	-2.54281500	0.53264400
C	-1.85334600	-3.62343600	-1.56006100
C	-2.12597000	-3.78929400	-0.05103100
H	-3.18939200	-3.95367000	0.16375400
H	-1.55696000	-4.61050200	0.39796900
H	-2.71564100	-3.89027000	-2.18039000
H	-0.99438800	-4.21723500	-1.89778300
C	3.83911600	-0.62516000	-0.79782100
C	4.55464300	-1.79724800	-1.49315200
C	1.74282300	-1.09758400	-2.12924500
C	3.97876300	-2.05813100	-2.89177100
C	2.45831300	-2.26144500	-2.83614200
H	4.02551600	0.28776500	-1.37768600
H	4.44487300	-2.70280400	-0.87940300
H	4.20520800	-1.19872300	-3.53914100
H	1.86945200	-0.18632800	-2.72899600
H	2.05159800	-2.38351900	-3.84701400
H	4.27833300	-0.45959400	0.19060100
H	5.63026800	-1.59081300	-1.55365200
H	0.67071200	-1.30098800	-2.07946300
H	4.46608400	-2.92819400	-3.34819300
H	2.23637600	-3.19482000	-2.29876600
C	2.31721500	-0.87378900	-0.70994100
H	2.15568000	-1.80789600	-0.15584800
C	2.35700600	4.92481100	-0.60274300
C	2.78323300	3.85565500	-1.61609800
C	1.81277900	3.09018800	1.07857900
C	2.04887200	2.52581500	-1.37980000
C	2.23371100	2.00514900	0.06396000
H	1.29843200	5.17399400	-0.76208000

H	3.86722700	3.69044700	-1.53449800
H	0.97649100	2.66178500	-1.57088100
H	0.73089100	3.25419100	1.00792200
H	2.92378900	5.85010500	-0.76069700
H	2.59776000	4.20079500	-2.64034500
H	2.01771100	2.76207700	2.10254800
H	2.40005000	1.78465700	-2.10398700
H	3.30192700	1.80155200	0.22044300
C	2.54865400	4.41906200	0.83256300
H	2.20011400	5.16848400	1.55338000
H	3.62198800	4.27805500	1.02502000
C	2.43279800	-2.61156700	3.27370100
C	3.43760000	-1.61347900	2.68082900
C	0.52439400	-1.06172600	2.67305400
C	2.91043800	-0.16727600	2.72235100
C	1.49109600	0.02287900	2.13235800
H	2.31313200	-2.41236400	4.34856400
H	3.66140600	-1.90898200	1.64977600
H	2.86157100	0.13921900	3.77752600
H	0.34641600	-0.83023000	3.73366800
H	1.10937500	0.97427400	2.52180800
H	2.82309000	-3.63294800	3.18840200
H	4.38907800	-1.66119600	3.22470500
H	-0.44434200	-1.00539200	2.17118000
H	3.62631000	0.51352100	2.24751600
C	1.06666900	-2.49303100	2.58569700
H	0.34387100	-3.17719100	3.04407300
H	1.14355900	-2.79979500	1.53509800
P	1.30533700	0.37765600	0.28425000
Cu	-0.96050600	0.30211100	-0.14816600
C	-4.57018500	-0.30198900	-0.77462000
C	-5.68432800	-0.64128500	0.23651300
C	-4.94135900	2.17121600	-0.35492900
C	-6.72181400	0.48764000	0.33244200
C	-6.05715300	1.83407800	0.65551200
H	-5.01753900	-0.24838300	-1.77985700
H	-5.22889400	-0.80466000	1.22241700
H	-7.25493500	0.56999100	-0.62607100
H	-5.40119300	2.33011000	-1.34322800
H	-6.80505900	2.63686700	0.66729900
H	-3.81493300	-1.08797900	-0.80400400
H	-6.17178100	-1.58231900	-0.04728300
H	-4.43489600	3.10067300	-0.07968300
H	-7.47858500	0.24704600	1.08933900
H	-5.62180600	1.79149300	1.66305500
C	-3.93608900	1.03172200	-0.45685700
C	-2.64746700	1.25751400	-0.22950400
C	-1.65926900	2.18572800	0.07347700
H	-1.29819400	2.87192600	-0.69346800
H	-1.54324300	2.54667000	1.09648500

3B^S

Sum of electronic and thermal Free Energies= -3253.066652

C	3.73104500	0.65197600	-0.75345800
C	4.92950600	0.57743100	0.21587900
C	4.52055000	-1.46776400	-1.88974600
C	6.12347900	-0.14767200	-0.42210000
C	5.72260300	-1.54126400	-0.92682700
H	4.01537700	1.29670000	-1.60104200
H	4.62124000	0.03707000	1.12182200
H	6.49769600	0.44953400	-1.26644400
H	4.84166300	-0.93872700	-2.80202000
H	6.57274200	-2.02638500	-1.42278000
H	2.87613900	1.12491800	-0.26604400
H	5.22074000	1.58706900	0.53216600
H	4.20715000	-2.47023800	-2.19472400
H	6.94994800	-0.22440300	0.29518700
H	5.45447700	-2.17339100	-0.06928300
C	3.34739800	-0.71732300	-1.27099200
C	2.13460600	-1.26310800	-1.19201000
C	1.46220200	-2.45547300	-1.49479400
H	1.12776200	-2.67214100	-2.51048500
H	1.60199000	-3.34606700	-0.88074300
C	-3.04141000	0.01401500	1.39497000
C	-4.56423800	0.23476900	1.44562500
C	-3.02962500	0.72743700	-1.02167600
C	-5.21901300	0.05134300	0.07100500
C	-4.55021600	0.95239400	-0.97414700
H	-2.82973600	-1.02988700	1.13581800
H	-4.77038400	1.25153800	1.81046300
H	-5.11921400	-0.99786700	-0.24098100
H	-2.82300400	-0.29546300	-1.35774300
H	-4.97859100	0.77133300	-1.96720200
H	-2.63117500	0.18015100	2.39535300
H	-5.00743400	-0.45252900	2.17652100
H	-2.59057900	1.39421900	-1.76704000
H	-6.29411300	0.26047400	0.12856200
H	-4.75839100	2.00487600	-0.73132300
C	-2.37143500	0.94397400	0.35759300

H	-2.55001800	1.98088200	0.67762600
C	1.67162400	0.08038800	4.48991800
C	0.42918700	-0.74138600	4.12458900
C	1.25197200	1.57598900	2.46720400
C	0.13997700	-0.68580800	2.61672800
C	-0.01367400	0.76969500	2.11093900
H	2.55877400	-0.38680200	4.03956300
H	-0.43970400	-0.35356900	4.67610200
H	0.97371200	-1.15122300	2.07257600
H	2.11493800	1.17280700	1.92084900
H	1.83215300	0.07544900	5.57469700
H	0.55344900	-1.78515200	4.43623800
H	1.14587900	2.62412700	2.16996300
H	-0.74536500	-1.28237100	2.38229300
H	-0.85269100	1.23861600	2.64301300
C	1.54464300	1.52069200	3.97802100
H	2.45942200	2.08644000	4.19233800
H	0.73200200	2.02700100	4.51851500
C	-0.98006900	4.19596500	-2.47385100
C	-1.51177100	4.16584700	-1.03370100
C	0.61458100	2.29629200	-1.92711100
C	-0.44030200	3.68131300	-0.04260100
C	0.23566100	2.33962200	-0.42281400
H	-0.16750700	4.93385400	-2.54260900
H	-2.39450100	3.51775100	-0.98790900
H	0.35166500	4.44386700	-0.00921500
H	1.50597300	2.92927600	-2.04246600
H	1.19421800	2.31412800	0.10129500
H	-1.76558000	4.53327300	-3.16043500
H	-1.84956500	5.16529500	-0.73367200
H	0.92891700	1.28296400	-2.19923500
H	-0.85425800	3.63777900	0.97202300
C	-0.44939100	2.82005100	-2.90077100
H	-0.01280100	2.87858400	-3.90504600
H	-1.28184800	2.11118000	-2.97774400
P	-0.49605200	0.73997300	0.27658000
Cu	0.22457500	-1.19061300	-0.65705300
B	-1.32328200	-2.47657100	-0.65360400
O	-2.13638000	-2.76189300	-1.74733700
O	-1.67353300	-3.27739200	0.43370800
C	-3.11902600	-3.74095800	-1.37108700
C	-2.67378700	-4.22564000	0.02301700
H	-4.10956500	-3.26805200	-1.34994100
H	-3.14055800	-4.54343000	-2.11584600
H	-3.49049300	-4.23737300	0.75249600
H	-2.22759500	-5.22756900	-0.00742700

TS3B^{S}

Sum of electronic and thermal Free Energies= -3253.051900

B	1.83492800	-1.40903900	-0.31624800
O	2.22914700	-2.13645200	0.79893300
O	1.91784300	-2.18257400	-1.47345800
C	2.76626800	-3.39546200	0.35500200
C	2.29353800	-3.51776100	-1.10565900
H	3.07740500	-3.87630000	-1.78036300
H	1.42322100	-4.17965700	-1.20436800
H	3.86015500	-3.36645400	0.43459400
H	2.39240000	-4.19800500	0.99823800
C	-3.48353700	-0.13340600	1.80939000
C	-3.99130000	-1.04241900	2.94292800
C	-1.09655200	-0.81126800	2.33257100
C	-2.93854100	-1.20662600	4.04745900
C	-1.60634400	-1.70812800	3.47273900
H	-3.32668700	0.87451500	2.21424300
H	-4.24304900	-2.02960500	2.52961300
H	-2.77900700	-0.23650200	4.53963500
H	-0.84540700	0.17777500	2.73963200
H	-0.84724900	-1.76855000	4.26145300
H	-4.25326400	-0.04037300	1.03583400
H	-4.92070500	-0.63271600	3.35699000
H	-0.17125600	-1.22064400	1.91556600
H	-3.30372800	-1.89180500	4.82181300
H	-1.73915200	-2.73068500	3.09104000
C	-2.15863800	-0.66130900	1.21905200
H	-2.34253400	-1.66852700	0.82375800
C	-1.54204900	4.98910800	-0.09866900
C	-1.69663000	4.20680000	1.21122400
C	-1.93865100	2.83866100	-1.40940900
C	-1.29853000	2.73346400	1.03503600
C	-2.09054700	2.03935800	-0.09749900
H	-0.47854100	5.03117800	-0.37163600
H	-2.74150600	4.26349700	1.54899100
H	-0.22922700	2.67213800	0.78768500
H	-0.89551200	2.76712200	-1.74647900
H	-1.87419900	6.02582800	0.03268200
H	-1.08819100	4.65888300	2.00360000
H	-2.56183300	2.40654800	-2.19897000
H	-1.43171800	2.20160700	1.98304700
H	-3.15423100	2.01661700	0.17443600

C	-2.32977800	4.31586600	-1.22940600
H	-2.17458000	4.85004900	-2.17447900
H	-3.40516900	4.38124000	-1.00885700
C	-3.80341100	-2.95885700	-2.03716900
C	-4.44594000	-1.72149600	-1.39430700
C	-1.65553800	-1.66309400	-2.40164500
C	-3.82886600	-0.41384400	-1.92085600
C	-2.28270800	-0.35563600	-1.85108000
H	-4.03193700	-2.96933500	-3.11262000
H	-4.33140200	-1.78602800	-0.30638600
H	-4.10538500	-0.31652600	-2.98079800
H	-1.81151500	-1.65630900	-3.49016500
H	-1.95836300	0.43636600	-2.53546800
H	-4.24048100	-3.87253700	-1.61691100
H	-5.52563800	-1.71062300	-1.58690300
H	-0.57233400	-1.66872100	-2.24612100
H	-4.27721400	0.44988000	-1.41600400
C	-2.28051000	-2.95174300	-1.84824800
H	-1.83104700	-3.81463700	-2.35398000
H	-2.03897200	-3.06530000	-0.78300900
P	-1.47494600	0.27124200	-0.27309400
Cu	0.70402400	0.23402000	-0.50990300
C	4.00023800	0.29892100	1.35667500
C	5.38750200	-0.36688500	1.46192800
C	4.79544300	1.65099900	-0.63390200
C	6.49349000	0.53806100	0.90207400
C	6.17677100	0.97244800	-0.53563600
H	3.99776400	1.17967400	2.02192800
H	5.37232600	-1.31066800	0.89923300
H	6.58366900	1.43149000	1.53775200
H	4.84098400	2.60572900	-0.08198300
H	6.95360000	1.65126600	-0.91026700
H	3.22651900	-0.37599200	1.72110000
H	5.59844000	-0.62717100	2.50696000
H	4.56074400	1.89790400	-1.67285000
H	7.46456100	0.02842800	0.94280500
H	6.18506000	0.09007400	-1.19012800
C	3.69540100	0.78241400	-0.04300400
C	2.56878900	0.57209200	-0.76254800
C	1.88965700	1.35169900	-1.74668100
H	2.05606900	2.42715300	-1.73483600
H	1.70093100	0.93916800	-2.74017700

TS4B[S]

Sum of electronic and thermal Free Energies= -3253.052770

C	-4.05149300	-0.94969800	-1.15529100
C	-5.25338600	-1.23134400	-0.23057200
C	-4.76848600	1.47034600	-1.36264600
C	-6.41974500	-0.27648500	-0.52637800
C	-5.97553600	1.19141000	-0.44221000
H	-4.34932500	-1.20438600	-2.18676100
H	-4.93619500	-1.10070300	0.81367600
H	-6.80309600	-0.47934900	-1.53741300
H	-5.10322200	1.36007700	-2.40778900
H	-6.81047100	1.85682600	-0.69773800
H	-3.20330800	-1.59252100	-0.89846900
H	-5.58005200	-2.27432800	-0.33468200
H	-4.43348100	2.50648200	-1.24715300
H	-7.25201300	-0.46264000	0.16436400
H	-5.69304500	1.42279900	0.59416400
C	-3.62317500	0.50466400	-1.09424400
C	-2.37235200	0.87194000	-0.80400200
C	-1.78752700	2.23225600	-0.68734000
H	-1.70375800	2.80672800	-1.61413300
H	-2.15171700	2.85298300	0.13630700
C	3.01652800	0.48043000	1.51483700
C	4.50512200	0.85811300	1.61110100
C	3.21542500	0.36239400	-0.99447500
C	5.00017500	1.57341100	0.34842100
C	4.70414900	0.73653300	-0.90169500
H	2.40884200	1.39411800	1.47058900
H	5.09887100	-0.05408900	1.76655500
H	4.49418600	2.54552200	0.26040700
H	2.61541800	1.27188500	-1.12686700
H	5.00190900	1.27992300	-1.80640800
H	2.72769200	-0.04434700	2.43000400
H	4.66515100	1.48603200	2.49602500
H	3.05461300	-0.24623200	-1.88683600
H	6.07334800	1.78550100	0.42482400
H	5.31061200	-0.18054600	-0.87591100
C	2.72360500	-0.38144100	0.26541100
H	3.27909300	-1.32569100	0.36545300
C	-1.33988300	-1.94856800	4.20557200
C	-0.45665500	-0.69641100	4.13957300
C	-0.43100800	-2.68459900	1.93933800
C	-0.16848800	-0.28981300	2.68668400
C	0.47958500	-1.44091500	1.87765600
H	-2.33311500	-1.71144200	3.79964500
H	0.49262800	-0.89125700	4.65961700

H	-1.11235000	-0.01853300	2.19344400
H	-1.37974400	-2.46961000	1.42915200
H	-1.49191600	-2.25844000	5.24637700
H	-0.93367800	0.13854300	4.66618000
H	0.02796600	-3.53325700	1.42225700
H	0.45757400	0.60630000	2.66533400
H	1.43411400	-1.71031400	2.35054500
C	-0.72275900	-3.09468000	3.39427700
H	-1.38520100	-3.96861300	3.39929400
H	0.21545100	-3.41266300	3.87157700
C	2.32931500	-3.07050900	-3.36726300
C	2.86871200	-3.26659400	-1.94232400
C	0.21783900	-2.02240200	-2.42778600
C	1.73174500	-3.43718100	-0.92133100
C	0.65565700	-2.32589600	-0.97170100
H	1.80539700	-3.98487300	-3.68135400
H	3.49717000	-2.41057100	-1.67047900
H	1.22511100	-4.38900000	-1.13763500
H	-0.40943800	-2.86773800	-2.74524400
H	-0.24529800	-2.72207600	-0.49582500
H	3.16001700	-2.93196400	-4.06941100
H	3.52043000	-4.14794900	-1.90355900
H	-0.43722800	-1.14412200	-2.43699600
H	2.14213100	-3.54012700	0.09052400
C	1.35786000	-1.88354100	-3.44466900
H	0.93122900	-1.81084600	-4.45213700
H	1.90216100	-0.94606400	-3.28175700
P	0.89513600	-0.81555700	0.13711900
Cu	-0.51932600	0.76028100	-0.34062800
B	0.12362000	2.65921200	-0.19547600
O	0.84328900	3.29716600	-1.20160400
O	0.26470700	3.31716000	1.02336000
C	1.37980100	4.51784100	-0.67036800
C	1.20962300	4.38333500	0.85729800
H	2.42495100	4.62737800	-0.97704500
H	0.81150000	5.36502800	-1.07580700
H	2.15097600	4.11351100	1.35402600
H	0.82254600	5.29362000	1.32659000

4B^{S}

Sum of electronic and thermal Free Energies= -3253.119996

B	-3.10838900	1.40481400	-0.99827400
O	-4.31773800	2.05460900	-0.82566100
O	-2.08066000	2.30605200	-1.24710100
C	-4.09819500	3.46766400	-0.86939700
C	-2.63504800	3.62212700	-1.34556700
H	-2.57062200	3.96239300	-2.38654900
H	-2.05634700	4.31239700	-0.72252200
H	-4.81856900	3.92839600	-1.55315400
H	-4.25679900	3.88948100	0.13102400
C	2.68996100	-0.34675400	2.47219000
C	2.38435300	-0.17962300	3.97158200
C	0.21182600	-0.66491000	2.00902100
C	1.10639600	-0.92871700	4.37587100
C	-0.08664400	-0.50369700	3.50787000
H	2.91180200	-1.40313800	2.27525700
H	2.26598100	0.88959800	4.19873600
H	1.27082900	-2.00960500	4.26057300
H	0.33069900	-1.73158700	1.77682900
H	-0.97858000	-1.08382500	3.77169400
H	3.59433800	0.21392900	2.21183600
H	3.23779200	-0.53064600	4.56431700
H	-0.63620200	-0.31722100	1.40940600
H	0.88690800	-0.75896700	5.43660500
H	-0.32858700	0.54873900	3.71429000
C	1.49458600	0.10136400	1.60741300
H	1.30533200	1.16009500	1.82419300
C	3.81378800	-3.72147300	-2.13748100
C	3.29881300	-3.81670900	-0.69604600
C	3.53381800	-1.19149900	-2.05414500
C	2.35387400	-2.65363400	-0.35660500
C	3.00331500	-1.27153000	-0.60566900
H	2.97256700	-3.85073400	-2.83264200
H	4.15259500	-3.80725600	-0.00329000
H	1.44707700	-2.72120500	-0.97369900
H	2.68140800	-1.19865500	-2.74866900
H	4.52068300	-4.53313000	-2.34624100
H	2.77902500	-4.76872400	-0.53601300
H	4.06737400	-0.24985700	-2.21910800
H	2.02272600	-2.74181500	0.68333800
H	3.85158500	-1.14831900	0.08126400
C	4.47526200	-2.36082000	-2.38914600
H	4.80119100	-2.27926600	-3.43295100
H	5.38204900	-2.28008700	-1.77269800
C	2.60913800	4.17632900	0.83871700
C	3.58670700	3.02570600	1.11848000
C	1.51107000	2.81678300	-1.00037400
C	3.82922900	2.16260500	-0.13233100
C	2.53979600	1.66790700	-0.83119700

H	3.06400100	4.86985700	0.11675100	H	-4.69087500	-2.14875100	-2.52840700
H	3.19279200	2.41058900	1.93572100	H	-6.57046200	-1.62227500	-1.00352900
H	4.37654600	2.77787500	-0.86143900	H	-1.74039600	-2.56048600	-0.20368800
H	1.89665900	3.48537000	-1.78364500	H	-3.50470600	-3.82796400	1.10177800
H	2.81843600	1.37162000	-1.84964900	H	-4.81898200	-0.40701500	-2.30354400
H	2.43272700	4.75247000	1.75486900	H	-5.88378200	-3.00263800	0.98487200
H	4.54660700	3.42157900	1.47169900	H	-5.48612500	-0.72507700	0.05893000
H	0.55937100	2.41765500	-1.36633300	C	-3.11571500	-1.33267700	-1.30489700
H	4.49209200	1.32225200	0.10626200	C	-2.20588600	-0.34165900	-1.43761200
C	1.28402200	3.65450500	0.26580700	C	-2.54970700	0.97807800	-2.14224800
H	0.61845400	4.49303200	0.02782900	H	-1.71689900	1.27903800	-2.79163700
H	0.75953300	3.06032800	1.02549700	H	-3.44741700	0.92791100	-2.77281400
P	1.73425500	0.06742900	-0.26199100	C	2.01759700	2.46362500	0.23203900
Cu	-0.17353400	-0.28472200	-1.29711200	C	2.82391900	3.65277000	-0.31941200
C	-4.39520600	-0.46243700	1.03279800	C	2.48499300	1.17658000	-1.87566400
C	-5.74959900	-1.20296000	1.02247000	C	2.79900000	3.69658300	-1.85217200
C	-3.28241000	-2.44784700	-0.03049100	C	3.28012100	2.36466700	-2.44017400
C	-5.55722600	-2.72474100	1.07571300	H	0.96079200	2.58622200	-0.04070400
C	-4.62646000	-3.20753700	-0.04531900	H	3.86521300	3.57578400	0.02587300
H	-3.91379000	-0.66123600	2.00722800	H	1.77232200	3.89136900	-2.19126300
H	-6.28985800	-0.93454900	0.10477900	H	1.43300300	1.25672300	-2.18185300
H	-5.12077100	-2.99838600	2.04821900	H	3.19617000	2.37420300	-3.53342500
H	-2.75590300	-2.70875300	0.90467200	H	2.07172700	2.47697000	1.32490800
H	-4.45009000	-4.28752600	0.04377500	H	2.42622000	4.58619800	0.09681500
H	-4.56365200	0.61418700	0.97401100	H	2.86211000	0.24845000	-2.31045900
H	-6.36878500	-0.86826100	1.86509900	H	3.41586300	4.52431900	-2.22190200
H	-2.64810800	-2.79732200	-0.84790600	H	4.34715200	2.22884700	-2.21091900
H	-6.52610300	-3.23694900	1.01554200	C	2.53292700	1.11862300	-0.33336500
H	-5.11351100	-3.04503800	-1.01630300	H	3.57313600	0.98012400	-0.00453500
C	-3.48383400	-0.94632500	-0.07945400	C	0.20365900	-0.19216000	4.89549800
C	-2.88721900	-0.13734700	-1.00106700	C	-0.01505000	1.02895200	3.99185400
C	-1.92089400	-0.59315400	-2.06313100	C	1.63577900	-1.25953100	3.07606900
H	-2.08450400	-1.63297300	-2.36461100	C	0.09319500	0.65421100	2.50621700
H	-2.02992700	0.01967600	-2.96738400	C	1.44549500	-0.02210100	2.17536800

5B[S]

Sum of electronic and thermal Free Energies= -3253.114250

C	-2.77585200	-2.61411900	-0.56321200	H	-0.62301100	-0.90159700	4.75039400
C	-3.74223200	-2.87503600	0.60953300	H	0.73525700	1.79693600	4.22976800
C	-4.55563400	-1.33726300	-1.79334300	H	-0.71368800	-0.04237400	2.24178000
C	-5.20233100	-2.87086800	0.13419200	H	0.86823200	-2.01031400	2.84086600
C	-5.53961200	-1.58069700	-0.62783800	H	0.18085700	0.10240700	5.95133300
H	-2.83128400	-3.47608100	-1.25039200	H	-0.99501300	1.47976500	4.18976800
H	-3.60470600	-2.08435300	1.36115800	H	2.60813400	-1.72977600	2.89732300
H	-5.36515000	-3.73254800	-0.53065300	H	-0.06157300	1.53619800	1.87772700
				H	2.25636400	0.67961800	2.41405200
				C	1.53043400	-0.88758300	4.56641600

H	1.65166300	-1.78989000	5.17771300
H	2.36463600	-0.22065000	4.82714000
C	4.41943200	-2.66443500	-2.04975000
C	4.81525300	-1.68721400	-0.93279800
C	2.06665000	-2.80215600	-1.10047700
C	4.00370800	-1.93593100	0.34925800
C	2.47114800	-1.95522600	0.13627800
H	4.67014000	-3.68827900	-1.73668800
H	4.66745900	-0.65812700	-1.28081100
H	4.29348800	-2.92048600	0.74420400
H	2.16291800	-3.85771900	-0.80969000
H	2.03640200	-2.49024700	0.98636900
H	5.00577000	-2.46349900	-2.95407200
H	5.88373400	-1.78371300	-0.70568100
H	1.00555800	-2.63583400	-1.31931400
H	4.28185900	-1.20889600	1.12188600
C	2.91724900	-2.58339900	-2.35820000
H	2.64370400	-3.33426300	-3.10878000
H	2.68533800	-1.61158700	-2.80843700
P	1.51998500	-0.33404300	0.30670700
Cu	-0.46963100	-0.41111800	-0.63349700
B	-2.74824400	2.05143400	-1.02183300
O	-1.71173900	2.72184300	-0.38609000
O	-3.98158800	2.41536800	-0.52355600
C	-2.28120800	3.65151000	0.54605500
C	-3.78587500	3.29378500	0.58823200
H	-1.79196600	3.54335600	1.51981700
H	-2.10619300	4.67260000	0.18487900
H	-4.06108700	2.77117000	1.51259700
H	-4.43330100	4.17048400	0.48330300

TS5B^{S}

Sum of electronic and thermal Free Energies= -3990.735459

C	-4.32780300	-0.88479900	0.34013500
C	-5.65221800	-1.07928700	-0.42040900
C	-3.18810500	-0.25709800	-1.81032700
C	-5.41910700	-1.46216100	-1.88855600
C	-4.50080100	-0.44913900	-2.58630400
H	-3.77852600	-1.83294600	0.36402200
H	-6.23500600	-0.14801200	-0.37487200
H	-4.95428400	-2.45713200	-1.93149800
H	-2.64117400	-1.20802900	-1.77665700
H	-4.28331800	-0.77422000	-3.61119000
H	-4.54558300	-0.60371300	1.37601100
H	-6.25412600	-1.84641200	0.08149900
H	-2.54770400	0.46437200	-2.32842800
H	-6.37566300	-1.54050200	-2.41860700
H	-5.01797900	0.51743300	-2.67094600
C	-3.44943600	0.17814900	-0.34920700
H	-4.01817800	1.11480500	-0.36383600
C	-1.15178400	-0.55878000	5.07543400
C	-2.14556800	-1.37710700	4.24249500
C	-1.03033500	1.15096700	3.18806800
C	-1.94042300	-1.15149700	2.73616800
C	-2.05209100	0.34303600	2.35410100
H	-0.13421100	-0.93165100	4.89265600
H	-3.17215800	-1.09592000	4.51849500
H	-0.94472200	-1.51256700	2.44742900
H	-0.01337500	0.84477500	2.90366400
H	-1.34525800	-0.68984000	6.14666000
H	-2.04621000	-2.44547500	4.46885800
H	-1.10260700	2.22121400	2.98056600
H	-2.64448700	-1.75800200	2.16709600
H	-3.06039200	0.69841200	2.61091400
C	-1.22027400	0.92584300	4.69896600
H	-0.46353800	1.49748800	5.24956500
H	-2.19638400	1.33237300	4.99998900
C	-3.27509200	4.42929900	-1.19159900
C	-3.74981800	3.87199400	0.15532700
C	-1.22844100	2.92996100	-1.10907700
C	-2.57327800	3.39516400	1.02446400
C	-1.55504000	2.44726000	0.32936400
H	-2.66772900	5.32956900	-1.01986800
H	-4.45583700	3.05116500	-0.02364000
H	-2.01047200	4.28787100	1.33359000
H	-0.55225800	3.78946000	-1.00877800
H	-0.61014900	2.53914500	0.87677400
H	-4.13340400	4.74185800	-1.79809400
H	-4.30993600	4.63518800	0.70938700
H	-0.65371000	2.16712700	-1.64252800
H	-2.95823600	2.95238600	1.94894500
C	-2.43761000	3.38588600	-1.94094000
H	-2.07790800	3.79626600	-2.89199300
H	-3.07901700	2.53450400	-2.19973400
P	-1.80903700	0.58519600	0.49501200
Cu	-0.04288500	-0.64727000	-0.30874400
C	-1.32608100	-3.92588300	-0.41633100
O	-1.23408900	-2.65643500	-0.24341200
C	-1.97639800	-4.73486600	0.69915400

H	-3.05247300	-4.52806700	0.71393800
H	-1.82540000	-5.80381000	0.54397000
H	-1.57394600	-4.43264500	1.66977700
C	6.96436000	-0.32464200	1.24649100
C	6.38350000	0.36931400	0.00515900
C	5.49777000	-0.59044800	-0.81628800
C	4.97420200	-1.90771300	1.29241900
C	5.85716600	-0.94447400	2.11229700
H	5.04624500	-0.06139500	-1.65994100
H	5.77682400	1.22945000	0.31585600
H	7.19255100	0.76186000	-0.62361900
H	7.65906700	-1.11630600	0.92874000
H	7.55437400	0.38652200	1.83797600
H	4.15630300	-2.29925700	1.90606700
H	5.58933400	-2.77027800	0.98934100
H	5.22551200	-0.14280700	2.51823300
H	6.29258000	-1.47192000	2.97069600
H	6.13917100	-1.38345100	-1.23415000
C	4.42329900	-1.22346900	0.04658800
C	3.12501700	-1.15289700	-0.21862500
C	1.85492300	-1.51866300	0.24570800
H	1.53049700	-2.54953400	0.08498400
H	1.50297000	-1.11466300	1.20695400
O	-0.93127600	-4.52192100	-1.45310400
Na	-0.10028300	-2.65252800	-2.28287400
Si	1.75720000	-0.26867100	-1.76922300
C	2.31503100	-1.91563400	-2.72341900
H	1.69969100	-2.11054200	-3.62067400
H	3.31430600	-1.72975500	-3.13015700
H	2.40979200	-2.83025300	-2.12537000
C	1.17183800	0.55590500	-3.46554500
H	0.38705700	-0.06264800	-3.92897700
H	0.76148900	1.56376300	-3.34363500
H	1.97381900	0.62191700	-4.21530800
C	2.39668200	1.37258800	-0.93668900
C	3.11614100	2.28160600	-1.73611800
C	2.19074500	1.75036000	0.40395100
C	3.60822000	3.48818400	-1.22792100
H	3.30134600	2.05011800	-2.78146400
C	2.66577100	2.95634000	0.91895800
H	1.64022400	1.09073000	1.06935200
C	3.38500500	3.83530800	0.10381800
H	4.16622500	4.15706600	-1.87885700
H	2.47776100	3.20919200	1.96003200
H	3.76285100	4.77300100	0.50180200

TS6B^{S}

Sum of electronic and thermal Free Energies= -3476.667602

C	3.19754400	-1.30588300	-0.98141000
C	3.57199700	-2.63422200	-1.66265500
C	0.81977000	-1.53800600	-1.84796300
C	2.69569300	-2.90423700	-2.89367200
C	1.20460500	-2.85905900	-2.53300800
H	3.42040900	-0.48323100	-1.67140400
H	3.45298900	-3.45722800	-0.94334700
H	2.90706900	-2.14456000	-3.65960000
H	0.93224000	-0.71372500	-2.56374000
H	0.58744700	-3.00147600	-3.42746700
H	3.82844000	-1.15034200	-0.10049800
H	4.63212900	-2.61749700	-1.94263700
H	-0.23501600	-1.56205300	-1.56165200
H	2.95263600	-3.87350600	-3.33698700
H	0.96706900	-3.69279700	-1.85745700
C	1.69999700	-1.27499000	-0.60589800
H	1.51227100	-2.09968600	0.09342400
C	2.38566600	4.44649500	-1.36781000
C	2.67291300	3.20600100	-2.22169800
C	1.90550300	2.94325100	0.62318200
C	1.89010500	1.98285700	-1.71676100
C	2.18186000	1.68032000	-0.22664000
H	1.32778900	4.72019000	-1.47472500
H	3.75049700	2.98641900	-2.19958400
H	0.81507100	2.17248100	-1.82631000
H	0.83107800	3.16429500	0.58396800
H	2.97563000	5.30035600	-1.72139300
H	2.41363100	3.39301800	-3.27040500
H	2.16536400	2.77216300	1.67322900
H	2.12917200	1.11741200	-2.34244300
H	3.23891900	1.40139800	-0.11568100
C	2.68643000	4.16444100	0.10907500
H	2.43782800	5.03624000	0.72532700
H	3.76441100	3.98722100	0.23639600
C	2.06297100	-2.63257000	3.45934300
C	3.14925300	-1.92297300	2.63830700
C	0.43262900	-0.76856400	2.93864400
C	2.93360400	-0.39964400	2.58954700
C	1.50869500	0.03946000	2.17090800
H	2.14299700	-2.32479600	4.51167000
H	3.16064600	-2.34150700	1.62550600

H	3.10438800	-0.00449900	3.60113700
H	0.44546800	-0.41949600	3.98063800
H	1.38643300	1.07926800	2.49579000
H	2.22317100	-3.71689000	3.43937800
H	4.13918900	-2.12873900	3.06278200
H	-0.56087000	-0.52676100	2.54598100
H	3.69022200	0.07471000	1.95426800
C	0.65970100	-2.28618200	2.94278100
H	-0.10277700	-2.76406800	3.56938400
H	0.52127300	-2.69323600	1.93246100
P	1.11839400	0.24204800	0.34027100
Cu	-0.98326300	0.86667800	0.06730800
Si	-3.36994600	0.63133800	0.37713800
C	-3.78394900	0.43937500	2.20997000
H	-3.00287000	-0.08199600	2.77244700
H	-3.89334600	1.43861300	2.63934800
H	-4.72339000	-0.10706600	2.35136700
C	-4.86444200	1.27603100	-0.59046600
H	-5.22951100	2.20049800	-0.13527500
H	-4.60111800	1.50343700	-1.62798700
H	-5.67682100	0.54098600	-0.59718900
C	-2.96447800	-1.08354800	-0.37020400
C	-2.57820000	-2.17763000	0.43133600
C	-3.09899800	-1.31895800	-1.75449600
C	-2.34043800	-3.43937100	-0.11660100
H	-2.47701700	-2.04661600	1.50567000
C	-2.86062900	-2.57737900	-2.30971700
H	-3.40474900	-0.50712100	-2.40986700
C	-2.48148100	-3.64440400	-1.49153700
H	-2.05829700	-4.26618500	0.53043700
H	-2.98121100	-2.72842400	-3.37935100
H	-2.30476300	-4.62714100	-1.91973100
C	-2.24500600	2.53359900	0.11241500
O	-2.79446700	3.22447300	0.95979300
O	-1.49728900	2.76597400	-0.87124700

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Sum of electronic and thermal Free Energies= -3476.700932

C	3.50538500	-1.38602800	-0.84613700
C	3.92628200	-2.55374900	-1.75580100
C	1.41608500	-1.05075600	-2.25705800
C	3.37700300	-2.38583300	-3.17915000
C	1.85194000	-2.20848800	-3.16870900
H	3.97078500	-0.46580100	-1.21999300
H	3.55422100	-3.49670300	-1.33042400
H	3.84181300	-1.50485000	-3.64410300
H	1.76710600	-0.10043700	-2.68062900
H	1.47954100	-2.03774000	-4.18536800
H	3.89568100	-1.54280400	0.16498700
H	5.01991900	-2.63057300	-1.77359600
H	0.32340000	-0.98713500	-2.22200500
H	3.65518700	-3.24715700	-3.79745300
H	1.38186500	-3.13753400	-2.81590800
C	1.97123200	-1.22235400	-0.82398000
H	1.54162700	-2.15045200	-0.42829500
C	3.51132200	4.26888600	0.39846400
C	3.82547100	3.29808000	-0.74683900
C	2.32776900	2.38995200	1.64796500
C	2.77984200	2.17643100	-0.83501600
C	2.63422400	1.40465800	0.49810300
H	2.57342600	4.79713600	0.17845700
H	4.82013500	2.85677200	-0.58990800
H	1.80241300	2.60544900	-1.09585600
H	1.33084900	2.82580700	1.48910700
H	4.29175100	5.03472200	0.47563900
H	3.86836400	3.83268700	-1.70270100
H	2.29472100	1.86635900	2.60890800
H	3.04108600	1.49358200	-1.64983100
H	3.58238800	0.89720100	0.71819000
C	3.37134900	3.51747600	1.72821000
H	3.09715200	4.20922600	2.53320400
H	4.34355200	3.08584000	2.00597700
C	1.11479600	-3.52027500	2.70616000
C	2.40972500	-2.72436700	2.48931700
C	-0.25390200	-1.45811000	2.15267100
C	2.21534400	-1.22605000	2.77909900
C	1.01807000	-0.57734800	2.04140000
H	0.83739400	-3.47807900	3.76925400
H	2.75230700	-2.87238100	1.45843400
H	2.02450100	-1.11510300	3.85616000
H	-0.61312300	-1.36700400	3.18741200
H	0.78105500	0.35648100	2.56625200
H	1.27723300	-4.57814300	2.46864200
H	3.20770800	-3.11162900	3.13403900
H	-1.05106400	-1.05959500	1.51783600
H	3.14301400	-0.67552000	2.58302000
C	-0.03279000	-2.94955200	1.86264600
H	-0.96451700	-3.49006100	2.06173400
H	0.17677500	-3.10527000	0.79672900

P	1.29001900	0.11199300	0.31810500
Cu	-0.45954500	1.06169000	-0.50805400
Si	-3.82209800	1.21302600	0.23578900
C	-3.01430800	1.60600600	1.91081600
H	-1.92452300	1.53015900	1.81750400
H	-3.24873800	2.62797500	2.22766200
H	-3.33416500	0.92297200	2.70532700
C	-5.67568300	1.55214700	0.30454600
H	-5.85107500	2.61426400	0.50235500
H	-6.14355600	1.31717500	-0.65618100
H	-6.17779400	0.96738600	1.08320600
C	-3.50858900	-0.62350400	-0.15733700
C	-3.98689100	-1.63915700	0.69238000
C	-2.83023100	-1.02440400	-1.32510800
C	-3.80276900	-2.99119200	0.39392200
H	-4.52073700	-1.37555600	1.60357600
C	-2.64872300	-2.37537200	-1.63444300
H	-2.44848600	-0.26446800	-2.00109600
C	-3.13296100	-3.36284400	-0.77435500
H	-4.18946100	-3.75361400	1.06549400
H	-2.13613000	-2.65645500	-2.55120600
H	-2.99691700	-4.41384700	-1.01515600
C	-2.98426400	2.30369300	-1.11640900
O	-3.64752500	3.16641100	-1.68500900
O	-1.71486800	2.07081200	-1.37381600

TS7B[S]

Sum of electronic and thermal Free Energies=-3788.458633

C	4.58393900	-1.33265800	-0.76717300
C	5.20347800	-2.64787200	-1.27240100
C	2.38752600	-1.94671500	-1.88224200
C	4.52903200	-3.13390700	-2.56341000
C	3.00895100	-3.25855300	-2.38596300
H	4.78874300	-0.54194500	-1.50013100
H	5.09860800	-3.41811500	-0.49510400
H	4.74102000	-2.42021100	-3.37222600
H	2.49666900	-1.17440000	-2.65510100
H	2.53666300	-3.55418300	-3.33004000
H	5.07146600	-1.02712900	0.16496700
H	6.27983900	-2.51163500	-1.43145200
H	1.31024000	-2.06626200	-1.72207600
H	4.95592800	-4.09403700	-2.87587800
H	2.79185000	-4.05900900	-1.66442700
C	3.06062400	-1.47466400	-0.57240300
H	2.89093300	-2.26424700	0.16979800
C	3.19422900	4.27913500	-1.55259400
C	3.61764800	3.05126400	-2.36770900
C	2.73200300	2.77735100	0.45133900
C	2.91372900	1.77807100	-1.87321200
C	3.13657100	1.52865400	-0.36264400
H	2.12600600	4.47489400	-1.71880100
H	4.70628600	2.91919500	-2.28891800
H	1.83262200	1.86291000	-2.05159500
H	1.64481600	2.92165200	0.39134400
H	3.73552900	5.16944300	-1.89358900
H	3.39797800	3.19960500	-3.43158700
H	2.97446000	2.63929800	1.50996800
H	3.25609300	0.91840600	-2.45917600
H	4.20321200	1.33321100	-0.19049400
C	3.43807900	4.04617800	-0.05652600
H	3.09371600	4.90819200	0.52666000
H	4.51892400	3.95758900	0.12531400
C	2.87415700	-2.53679900	3.56355200
C	3.99500500	-1.71827000	2.90439100
C	1.14022000	-0.92861200	2.65490800
C	3.60138600	-0.24126500	2.72287800
C	2.23477900	-0.02448800	2.03116300
H	2.72603300	-2.18194700	4.59346000
H	4.24567800	-2.16797600	1.93648900
H	3.52975400	0.21261000	3.72170700
H	0.93980800	-0.53682800	3.66220300
H	1.91992800	1.00477300	2.23986000
H	3.17154400	-3.58964000	3.63750200
H	4.90856600	-1.77295100	3.50873000
H	0.20105300	-0.82818700	2.10037000
H	4.39719600	0.30555800	2.20287600
C	1.55136100	-2.40026600	2.79546500
H	0.75506400	-2.95013400	3.31005000
H	1.64814400	-2.86616900	1.80500800
P	2.16258700	0.01341300	0.15445500
Cu	0.10205000	0.10847600	-0.47000600
C	-2.45374900	0.09494600	-0.06151100
O	-2.08137100	-0.26944600	1.06756400
O	-1.66587000	0.25033600	-1.08430200
C	-3.21945600	-4.98427200	0.15369500
C	-2.22024800	-3.86765900	0.48844700
C	-2.18682800	-2.78550100	-0.60933700
C	-4.57205500	-3.32707100	-1.22826300
C	-4.61549400	-4.41763400	-0.13996600

H	-1.47191900	-2.00415600	-0.35991600
H	-2.49281600	-3.38641800	1.43578900
H	-1.21446200	-4.28549300	0.62021900
H	-2.86190100	-5.53560900	-0.72819300
H	-3.27066700	-5.70972400	0.97461000
H	-5.56502800	-2.90314000	-1.39251100
H	-4.24099600	-3.77156600	-2.17851800
H	-5.03534600	-3.98376400	0.77684300
H	-5.29685600	-5.21828500	-0.45382000
H	-1.85623200	-3.24856000	-1.55174100
C	-3.56994900	-2.22974000	-0.84034500
C	-4.11118200	-1.02702500	-0.72097800
C	-5.28580100	-0.27021000	-0.83453800
H	-6.08966400	-0.53136500	-0.14304200
H	-5.63861400	-0.11262500	-1.85568300
Si	-4.16262900	1.43905000	-0.11588200
C	-4.88590000	2.43899400	-1.58412900
H	-5.96272600	2.25554300	-1.64285100
H	-4.71071400	3.51308600	-1.47344200
H	-4.45088100	2.12264900	-2.53928700
C	-5.12462500	1.38603900	1.52490100
H	-4.91475900	2.25987900	2.14766100
H	-6.19965900	1.34245500	1.32791300
H	-4.84830300	0.49112500	2.09188200
C	-2.70676000	2.72636500	0.36148300
C	-2.23652900	2.85798800	1.68172200
C	-2.11351400	3.56493900	-0.60073800
C	-1.26388000	3.79709000	2.03373600
H	-2.62325500	2.20038700	2.45558600
C	-1.13578400	4.50601200	-0.26560800
H	-2.41422600	3.48678500	-1.64233500
C	-0.71141900	4.63247400	1.05945300
H	-0.93883100	3.87954400	3.06870800
H	-0.71353600	5.14776700	-1.03630700
H	0.03620800	5.37443800	1.32965700

TS8B[S]

Sum of electronic and thermal Free Energies=-3788.488161

C	-5.09116000	-0.14284200	1.79116000
C	-5.44559000	-0.92522900	3.06855400
C	-2.61908200	-0.44036100	2.29835100
C	-4.34566200	-0.80204200	4.13289600
C	-2.97750300	-1.21858400	3.57360600
H	-5.05132800	0.92654000	2.03345700
H	-5.58845600	-1.98502800	2.81329300
H	-4.29397000	0.24067100	4.47743900
H	-2.49706100	0.62125600	2.55078200
H	-2.19389900	-1.07060100	4.32497700
H	-5.88683500	-0.26430900	1.04845000
H	-6.40428400	-0.56908800	3.46440700
H	-1.65020400	-0.77135500	1.90924900
H	-4.60023300	-1.40696700	5.01108000
H	-2.98949900	-2.29403200	3.34582100
C	-3.72758000	-0.59517600	1.22879400
H	-3.79772700	-1.66662900	1.00046400
C	-3.56393000	4.83605200	-0.88622800
C	-3.72242600	4.23605800	0.51585100
C	-3.77758400	2.50498500	-1.89029100
C	-3.22517000	2.78276500	0.56774400
C	-3.92227700	1.88593400	-0.48232800
H	-2.49525200	4.90966000	-1.13113000
H	-4.78141400	4.26859700	0.80920000
H	-2.14237900	2.75990600	0.38101200
H	-2.72113800	2.46606600	-2.19294600
H	-3.96250500	5.85676400	-0.91291000
H	-3.17610300	4.83394500	1.25440600
H	-4.33907100	1.92385100	-2.62860500
H	-3.37179400	2.38179600	1.57515000
H	-4.99153900	1.82300500	-0.23824100
C	-4.26657900	3.96296800	-1.93286000
H	-4.11130600	4.36829700	-2.93952600
H	-5.35089000	3.98289600	-1.75287900
C	-5.14428700	-3.53213300	-1.60084800
C	-5.93096000	-2.30581700	-1.11587500
C	-3.18978900	-2.04966000	-2.22717400
C	-5.50091000	-1.02156500	-1.84636400
C	-3.97422900	-0.76617600	-1.85030000
H	-5.38914500	-3.72742300	-2.65467300
H	-5.78986700	-2.19539800	-0.03472100
H	-5.81402700	-1.11153800	-2.89644000
H	-3.34775300	-2.22463600	-3.30050600
H	-3.76826600	-0.04904600	-2.65377300
H	-5.45053600	-4.42263900	-1.03989700
H	-7.00576800	-2.45998800	-1.26840700
H	-2.11564500	-1.87285200	-2.09781100
H	-6.04094800	-0.15439000	-1.44817000
C	-3.63090400	-3.30977600	-1.47027200
H	-3.08396100	-4.17533400	-1.86140700
H	-3.35803400	-3.23406600	-0.40941100

P	-3.19889900	0.15905000	-0.40992600
Cu	-1.05047400	0.12719200	-0.56895300
C	4.02162600	-2.75207400	-1.78392800
C	5.29135900	-3.54907800	-1.40168400
C	3.38125400	-2.54194600	0.62876600
C	5.10300400	-4.29479800	-0.07449500
C	4.64448600	-3.34094300	1.03553700
H	3.20339800	-3.46966200	-1.95246200
H	6.13156400	-2.84784500	-1.31684700
H	4.34869500	-5.08405300	-0.20681900
H	2.55964400	-3.25973100	0.48587100
H	4.43692500	-3.89550800	1.95870300
H	4.18763900	-2.20651200	-2.71436600
H	5.54197300	-4.24940800	-2.20764500
H	3.06270800	-1.88096300	1.42919000
H	6.03396100	-4.79835800	0.21413500
H	5.45341900	-2.63495400	1.26736500
C	3.60390600	-1.81222000	-0.67163000
C	3.67050500	-0.43919700	-0.86819700
C	3.73204100	0.21506100	-2.07883000
H	3.23559400	-0.17235800	-2.96497800
H	4.14567700	1.21400100	-2.15991300
C	1.38266500	-0.25370700	0.37466900
O	0.89494100	-0.73907100	1.39134400
O	0.81313700	0.12652400	-0.70419900
Si	3.61487800	0.85861300	0.61960000
C	3.73365100	0.35286200	2.44986500
H	3.99870400	1.24582800	3.02872700
H	2.78421200	-0.03875700	2.82151200
H	4.51630800	-0.38906600	2.63670100
C	2.51516000	2.40647400	0.42890800
H	2.12146400	2.49213700	-0.58670100
H	1.66491400	2.34788600	1.11408000
H	3.07835700	3.31419300	0.66949900
C	5.41172700	1.53379000	0.29380400
C	5.67183600	2.77246500	-0.31901200
C	6.53236500	0.77523500	0.68203400
C	6.97507700	3.23462200	-0.52876300
H	4.84466500	3.39832500	-0.64514800
C	7.83773600	1.22672100	0.48397700
H	6.38732600	-0.19552900	1.15276100
C	8.06442700	2.46329100	-0.12489500
H	7.13731100	4.19782200	-1.00689100
H	8.67844300	0.61475400	0.80239200
H	9.07902500	2.81955500	-0.28318600

TS9B^{S}

Sum of electronic and thermal Free Energies= -3828.435538

C	-5.28803500	1.95566700	-0.84991500
C	-6.12328000	2.11333500	0.43733400
C	-3.38593600	3.24105300	0.22153500
C	-5.72934800	3.38531200	1.20367400
C	-4.22343500	3.41007100	1.50692700
H	-5.57423300	2.77643600	-1.53544100
H	-5.94939100	1.23816400	1.07810100
H	-5.98728800	4.26567900	0.59385300
H	-3.52772800	4.14858800	-0.39466000
H	-3.95723300	4.34271400	2.02647400
H	-5.52893000	1.01531600	-1.35431300
H	-7.19862700	2.13010000	0.20586300
H	-2.32026000	3.20025600	0.47514700
H	-6.30911300	3.47202500	2.13373300
H	-3.98405000	2.58653600	2.19335200
C	-3.79205700	1.99820900	-0.57260900
C	-2.95761600	1.03918000	-0.99243600
C	-1.54658500	0.92253500	-0.79758200
H	-0.95941500	1.43042600	-1.57074400
H	-1.12718500	1.16603300	0.20729400
C	3.35999800	1.31196700	2.05158500
C	3.85453200	2.63847300	2.65727300
C	1.62240400	2.56247200	0.73934000
C	2.73132300	3.68289000	2.72373900
C	2.09792600	3.89379100	1.34162700
H	2.57628600	0.89588600	2.69363800
H	4.68394800	3.03315500	2.04998100
H	1.95811700	3.32937000	3.41821900
H	0.84507800	2.12626400	1.37637700
H	1.25227100	4.58905300	1.41267000
H	4.19296000	0.59999800	2.02148300
H	4.26290200	2.45499900	3.65983500
H	1.17017500	2.73879000	-0.24259200
H	3.11299200	4.63197600	3.12330400
H	2.83431500	4.36384500	0.67094500
C	2.77307000	1.53546700	0.64316600
H	3.57114200	1.95661400	0.02006300
C	3.76245700	-4.27442200	1.16540600
C	3.70184900	-3.12533300	2.17896500
C	3.30221400	-2.59883500	-0.69943900
C	2.79948000	-1.98336200	1.68492400

C	3.26382100	-1.43270300	0.31588600
H	2.76765600	-4.73400500	1.08425800
H	4.71907400	-2.74331400	2.35576000
H	1.76798200	-2.33991400	1.58656300
H	2.28075000	-2.96690400	-0.85989000
H	4.44652800	-5.06170700	1.50886800
H	3.33494100	-3.48981700	3.14669500
H	3.67110200	-2.26851300	-1.67428400
H	2.76440100	-1.19174500	2.43394600
H	4.28595700	-1.03771800	0.42183400
C	4.19135400	-3.75704200	-0.21276900
H	4.17138700	-4.56916600	-0.95103700
H	5.23459700	-3.41072900	-0.15934700
C	3.98216700	2.63146200	-3.34989600
C	4.81677200	1.70727700	-2.45431800
C	1.91222100	1.24705700	-2.87284300
C	4.22820800	0.28629200	-2.38682900
C	2.71011900	0.19333100	-2.06400700
H	4.02765100	2.27027600	-4.38821900
H	4.87899600	2.14336600	-1.45014600
H	4.37512200	-0.17541900	-3.37554000
H	1.87464500	0.89841500	-3.91575700
H	2.37002300	-0.77443100	-2.44989800
H	4.40573500	3.64388300	-3.35184400
H	5.84896900	1.64713800	-2.82407900
H	0.87337700	1.27414300	-2.53212100
H	4.81525700	-0.31743300	-1.68696800
C	2.52021400	2.65802200	-2.88536500
H	1.92217700	3.30070200	-3.54316700
H	2.47003900	3.10801800	-1.88738800
P	2.14903000	-0.01240400	-0.26070500
Cu	-0.05545800	-0.42608700	0.03198500
C	-0.26296300	-0.74530300	2.82760400
O	-0.46941800	-1.41007700	1.74753500
O	0.27969500	0.37382300	2.91054400
C	-0.74244600	-1.44398900	4.10452900
H	-0.49044200	-0.85641700	4.98992300
H	-1.82710400	-1.58680900	4.05648900
H	-0.29229400	-2.43988600	4.17902900
Si	-1.62120300	-1.19581300	-1.57518100
C	-1.81635400	-0.66593300	-3.39182000
H	-0.83070500	-0.60646500	-3.87179300
H	-2.39833200	-1.41217000	-3.94715600
H	-2.33082800	0.29319900	-3.47889100
C	-0.51870600	-2.80089600	-1.85154900
H	0.41915300	-2.54969900	-2.36309600
H	-0.26964600	-3.31191200	-0.91512400
H	-1.05335400	-3.52246700	-2.48658600
C	-3.19348300	-1.97197700	-0.83865600
C	-4.42926000	-1.92085300	-1.50997200
C	-3.13662000	-2.71773700	0.35368300
C	-5.55619900	-2.58667100	-1.02309800
H	-4.51109100	-1.33299400	-2.41913000
C	-4.26690600	-3.37036800	0.85714800
H	-2.20764500	-2.75486100	0.91662600
C	-5.47902000	-3.31305200	0.16804500
H	-6.49854700	-2.52623800	-1.56419600
H	-4.19864300	-3.92436300	1.79153300
H	-6.35743400	-3.82456700	0.55675200

TS10B^{S}

Sum of electronic and thermal Free Energies=-3828.468160

C	-0.95183300	3.76233100	1.29933300
C	-0.23546600	5.06286900	0.88042800
C	-2.40975000	3.88308700	-0.75855900
C	-1.14792100	5.94985400	0.01963700
C	-1.69602300	5.18085000	-1.19244200
H	-1.77471200	4.03924200	1.98324200
H	0.66309800	4.80478900	0.30166400
H	-1.99372800	6.29522100	0.63413500
H	-3.31264000	4.17163800	-0.19126400
H	-2.37518100	5.82306400	-1.77209000
H	-0.27914000	3.11012200	1.86287200
H	0.10753100	5.62024500	1.76385700
H	-2.75784700	3.33393300	-1.64013200
H	-0.61334800	6.85270900	-0.30790100
H	-0.86117300	4.92046100	-1.85864600
C	-1.51380800	3.00465300	0.10834500
C	-1.22197800	1.71568700	-0.12993300
C	-1.79154400	0.88170400	-1.20442900
H	-2.86837100	0.99536800	-1.38011600
H	-1.26143000	0.89860400	-2.16234500
C	3.59433400	-0.66628000	1.80329900
C	4.65805800	0.11230900	2.59884200
C	2.23331200	1.43854300	1.57009100
C	4.04349200	1.30445200	3.34548300
C	3.28126200	2.21987900	2.37745200
H	2.85692500	-1.07728200	2.49791000
H	5.43935200	0.47691300	1.91320700

H	3.34409900	0.92592700	4.10299700
H	1.47276400	1.02517700	2.24056300
H	2.79286700	3.03413200	2.92821700
H	4.07882900	-1.50229200	1.28517000
H	5.15722500	-0.56349200	3.30651500
H	1.70754200	2.10819800	0.88432200
H	4.82216700	1.86597100	3.88005500
H	3.99972300	2.69651800	1.69145400
C	2.87030500	0.26021100	0.80340000
H	3.64114800	0.66196400	0.13550700
C	1.65883400	-5.26667800	-0.83388400
C	2.14603600	-4.64659700	0.48225800
C	1.67939900	-2.94393900	-1.89340100
C	1.70221500	-3.18187200	0.61758000
C	2.18098600	-2.31844100	-0.57257600
H	0.56195700	-5.32476600	-0.81763000
H	3.24470800	-4.70337500	0.52414800
H	0.60924900	-3.12922600	0.66422400
H	0.58543800	-2.86879600	-1.92952600
H	2.02683100	-6.29618300	-0.93976300
H	1.77311600	-5.22622000	1.33634400
H	2.05427900	-2.39299100	-2.76027900
H	2.04845600	-2.77078900	1.56579700
H	3.28177500	-2.32468400	-0.59240600
C	2.10157900	-4.41763900	-2.03277200
H	1.69593300	-4.83158100	-2.96563300
H	3.19733900	-4.46741400	-2.12262300
C	4.03602200	2.38095600	-2.72359100
C	4.50144500	0.94627500	-2.44785500
C	1.63708700	1.71809100	-2.20522500
C	3.38551400	-0.08233200	-2.70740600
C	2.00162200	0.21493200	-2.05756400
H	3.81242100	2.49109000	-3.79570100
H	4.85326000	0.87656600	-1.41172500
H	3.22568100	-0.11638200	-3.79662100
H	1.33236800	1.87934400	-3.25110100
H	1.26308800	-0.31969700	-2.66744100
H	4.84071300	3.09273000	-2.49708200
H	5.36569100	0.69655500	-3.07848100
H	0.76950300	1.96137700	-1.58471400
H	3.74592300	-1.07766400	-2.42902300
C	2.77882300	2.70293500	-1.90745700
H	2.43334100	3.72152000	-2.12530200
H	3.02688200	2.68754600	-0.84020500
P	1.58128700	-0.53438300	-0.35437900
Cu	-0.63106700	-0.12155500	0.21029700
C	-0.53378600	-1.32530600	2.91801200
O	0.67328600	-1.06249300	3.06134200
O	-1.24721900	-1.13644500	1.86790800
C	-1.30397000	-1.94307200	4.09589600
H	-2.06654300	-1.23761500	4.44486900
H	-1.82893600	-2.84829700	3.77325000
H	-0.62810900	-2.17963500	4.92085800
Si	-2.37922900	-1.29633100	-1.08859200
C	-4.14293600	-0.99646100	-0.40882300
C	-5.25358200	-0.79187200	-1.24798200
C	-4.37295900	-0.97751100	0.98212600
C	-6.53696800	-0.58527700	-0.73303600
H	-5.12018000	-0.79531000	-2.32783800
C	-5.65227000	-0.76947100	1.50181100
H	-3.52857900	-1.11424000	1.65428600
C	-6.74065200	-0.57494300	0.64729700
H	-7.37579600	-0.43142500	-1.40934500
H	-5.80049900	-0.75520200	2.57968600
H	-7.73679200	-0.41286000	1.05363300
C	-2.05189500	-3.09899600	-0.49899200
H	-1.16266000	-3.53643300	-0.96041400
H	-1.92386500	-3.11271100	0.58542300
H	-2.91428100	-3.72472900	-0.76499400
C	-2.52294900	-1.48915400	-2.98811500
H	-3.23639700	-2.27932600	-3.25213100
H	-2.83804600	-0.57055100	-3.49478700
H	-1.55087600	-1.77743900	-3.40706400

TS11B[S]

Sum of electronic and thermal Free Energies= -3476.661084

C	-3.75214900	-0.44246200	1.62698800
C	-4.30535600	-1.41042500	2.68750100
C	-1.38338700	-1.03217700	2.33183500
C	-3.33929100	-1.56477700	3.87043800
C	-1.94310000	-1.99073500	3.39565900
H	-3.68542600	0.56011400	2.06540900
H	-4.47630300	-2.39372300	2.22630900
H	-3.26468200	-0.60620000	4.40317600
H	-1.20289900	-0.05028900	2.78669000
H	-1.25058100	-2.04457200	4.24364700
H	-4.45344000	-0.36821200	0.79027100
H	-5.28301100	-1.05593300	3.03499200
H	-0.41239900	-1.39258900	1.97755900

H	-3.73372300	-2.29099400	4.59063400
H	-1.99713500	-3.00419900	2.97316100
C	-2.35651000	-0.88819100	1.13898500
H	-2.45995300	-1.88704800	0.69598200
C	-1.58258700	4.80893800	0.27091800
C	-2.03637500	3.95882700	1.46346700
C	-1.77052700	2.76957400	-1.23226400
C	-1.65123300	2.48221800	1.27815100
C	-2.21777500	1.89434100	-0.03749600
H	-0.48572600	4.80407300	0.22184600
H	-3.12674100	4.04231400	1.58104900
H	-0.55796500	2.39496700	1.25372700
H	-0.67983200	2.68857300	-1.33290600
H	-1.89258100	5.85207700	0.40395400
H	-1.59205800	4.33361600	2.39286000
H	-2.21073700	2.40934400	-2.16809500
H	-1.99914100	1.90619300	2.14096900
H	-3.31534100	1.88892100	0.01250600
C	-2.14905300	4.24725800	-1.03855100
H	-1.78615600	4.82738400	-1.89484900
H	-3.24454200	4.34358200	-1.03599100
C	-3.64381500	-3.10082500	-2.33457700
C	-4.40264900	-1.93714000	-1.68065500
C	-1.55560500	-1.67947800	-2.47340600
C	-3.82351100	-0.56962200	-2.08517900
C	-2.29009100	-0.43763600	-1.90706100
H	-3.78832800	-3.06451400	-3.42366900
H	-4.37151700	-2.05937200	-0.59197300
H	-4.03377800	-0.41964800	-3.15366400
H	-1.62726100	-1.62632900	-3.56872800
H	-1.96808100	0.40600100	-2.52882400
H	-4.05781600	-4.05811200	-1.99722600
H	-5.46249800	-1.97122400	-1.95969100
H	-0.48806600	-1.62131400	-2.23423600
H	-4.34840400	0.23866400	-1.56320100
C	-2.14199200	-3.02556900	-2.02661900
H	-1.60785700	-3.83828700	-2.53219800
H	-1.97762400	-3.17628000	-0.95113700
P	-1.60669900	0.13271900	-0.25005600
Cu	0.58642200	0.28616200	-0.31454800
Si	2.76947500	-0.82273900	-0.65442700
C	2.95400800	-1.37261800	-2.45471800
H	1.99902400	-1.72377800	-2.86186400
H	3.29963100	-0.53546600	-3.06445800
H	3.67585700	-2.19279100	-2.53974600
C	2.31026200	1.35725600	-0.74656200
O	2.98384500	1.66125000	-1.72393100
O	1.72722200	2.01789000	0.15271000
C	1.93676900	-2.28256400	0.28510600
H	1.72266400	-2.05536400	1.33470900
H	1.00142700	-2.59446500	-0.19024300
H	2.61055200	-3.14959500	0.27436800
C	4.46393800	-0.58982900	0.17377600
C	5.43213400	0.28480400	-0.35870200
C	4.81663600	-1.32204900	1.32257100
C	6.69284500	0.41156600	0.22401700
H	5.18260800	0.88976800	-1.22472900
C	6.07545700	-1.19236000	1.91452200
H	4.10388200	-2.00762500	1.77166100
C	7.01990900	-0.32674500	1.36370700
H	7.41981800	1.09379400	-0.20900800
H	6.31658000	-1.76881000	2.80409600
H	8.00088100	-0.22437500	1.82022700

TS12B[S]

Sum of electronic and thermal Free Energies= -3990.791657

C	-1.73842100	3.51704400	0.95826600
C	-1.00055500	4.84760100	0.70018300
C	-2.54032300	3.48538400	-1.44364800
C	-1.67422300	5.64951700	-0.42255200
C	-1.80153600	4.81539500	-1.70531000
H	-2.73489000	3.76686400	1.36634100
H	0.03687200	4.62594400	0.41462200
H	-2.67695400	5.95930500	-0.09291600
H	-3.58220800	3.72645700	-1.17429100
H	-2.32101200	5.38967200	-2.48301600
H	-1.20752400	2.93380400	1.72023400
H	-0.95590500	5.44173600	1.62152200
H	-2.58143800	2.88786100	-2.36016300
H	-1.11438500	6.57180600	-0.62163600
H	-0.79770500	4.59479300	-2.09376900
C	-1.89041200	2.69255200	-0.31422100
C	-1.43085800	1.42914600	-0.41641100
C	-1.58105100	0.52977300	-1.57498600
H	-2.59541000	0.44981200	-1.97682700
H	-0.87002400	0.63226800	-2.39986500
C	3.37300900	-0.36063200	2.16328300
C	4.15907000	0.47649800	3.18792400
C	1.82358300	1.57916900	1.76090100

C	3.27665400	1.54550200	3.84687700
C	2.59167500	2.42352800	2.79080100
H	2.58222300	-0.91138800	2.68838800
H	5.00507000	0.96327400	2.68141600
H	2.50762000	1.05135700	4.45749400
H	0.99973700	1.05203100	2.25799500
H	1.90759900	3.13351700	3.27118100
H	4.04145400	-1.10429300	1.71713600
H	4.59193500	-0.18423200	3.94917300
H	1.35004700	2.22678000	1.01782900
H	3.87078600	2.16148300	4.53276200
H	3.35185300	3.02654600	2.27254800
C	2.74138000	0.53754300	1.08160200
H	3.56635400	1.07372200	0.59995200
C	2.63187100	-4.98193400	-1.03082700
C	2.88064500	-4.39073400	0.36212100
C	2.38083800	-2.61393600	-1.94639300
C	2.19857900	-3.02312200	0.53201800
C	2.65746000	-2.01427300	-0.54735400
H	1.56357100	-5.21549800	-1.13798400
H	3.96343000	-4.28103100	0.52181000
H	1.11213900	-3.13813700	0.47178800
H	1.29533500	-2.71159400	-2.08228000
H	3.17215300	-5.92887100	-1.15070300
H	2.52163600	-5.07820600	1.13770400
H	2.73322300	-1.95074500	-2.74047000
H	2.39826800	-2.64279800	1.53380400
H	3.74315900	-1.86722200	-0.44683500
C	3.04670000	-3.99013200	-2.12440900
H	2.80311400	-4.38864400	-3.11698800
H	4.13859100	-3.86224200	-2.10129100
C	4.13714700	3.01510100	-2.12811700
C	4.73629100	1.62568000	-1.88104200
C	1.79234700	2.03921800	-2.00202300
C	3.80757200	0.50665800	-2.38255800
C	2.32813300	0.58421100	-1.90807800
H	4.05179700	3.18623300	-3.21108500
H	4.94226600	1.50456300	-0.81028500
H	3.79003600	0.56450100	-3.48117900
H	1.60817700	2.24625600	-3.06653700
H	1.74343200	0.01026100	-2.63821100
H	4.80501800	3.79356000	-1.74011600
H	5.70547900	1.53237000	-2.38658700
H	0.82431000	2.12091400	-1.49960900
H	4.24784000	-0.46616500	-2.14470400
C	2.74957100	3.12601700	-1.48531200
H	2.31148800	4.10999300	-1.69292500
H	2.85253700	3.06305800	-0.39590300
P	1.81227600	-0.33868900	-0.32970300
Cu	-0.57293800	-0.34305900	-0.03695800
C	-1.03717400	-1.26264500	2.88819400
O	-0.63803000	-1.44212100	1.68347600
C	-0.39970600	-2.16805300	3.93751900
H	-1.02009700	-2.21869500	4.83384200
H	-0.22805300	-3.16809100	3.53282300
H	0.57541200	-1.75328900	4.21842100
Si	-1.99090300	-1.77063300	-1.38466200
C	-3.73944400	-1.51878700	-0.64904300
C	-4.78843600	-0.90351600	-1.36257300
C	-4.00811500	-1.87751100	0.68990700
C	-6.02881500	-0.64374300	-0.77311800
H	-4.64216200	-0.62891000	-2.40468400
C	-5.24440900	-1.61344400	1.29154100
H	-3.23504500	-2.36845800	1.27457700
C	-6.25982100	-0.99069300	0.55993700
H	-6.81668100	-0.17403600	-1.35625400
H	-5.41526000	-1.90593900	2.32448400
H	-7.22364500	-0.79103900	1.01974700
C	-1.45777800	-3.49923800	-0.75857800
H	-0.53908500	-3.82721300	-1.25308200
H	-1.28140100	-3.50716800	0.31909300
H	-2.24346900	-4.22765000	-0.99581600
C	-2.10778000	-1.98238400	-3.27187200
H	-2.76223500	-2.82470100	-3.52284900
H	-2.48058900	-1.09877200	-3.79856500
H	-1.11485500	-2.21067900	-3.67705800
O	-1.88157100	-0.41131000	3.26294800
Na	-2.75594700	0.52143300	1.49028000