Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic insight into the C7-selective C–H functionalization of N-acyl indole catalyzed by rhodium complex: a theoretical study

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Table S1. The relative free energies and relative enthalpic energies (in kcal/mol) calculated by using DFT and DFT-D3 methods.

	ΔG	ΔH
TS1(C2)-DFT	0.0	0.0
TS1(C2)-DFT-D3	0.9	0.7
TS1(C7)-DFT	0.0	0.0
TS1(C7)-DFT-D3	-0.4	-0.8

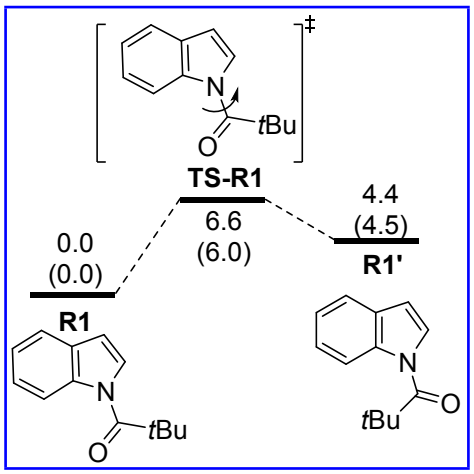

Fig. S1 The transformation from **R1** to **R1'**. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

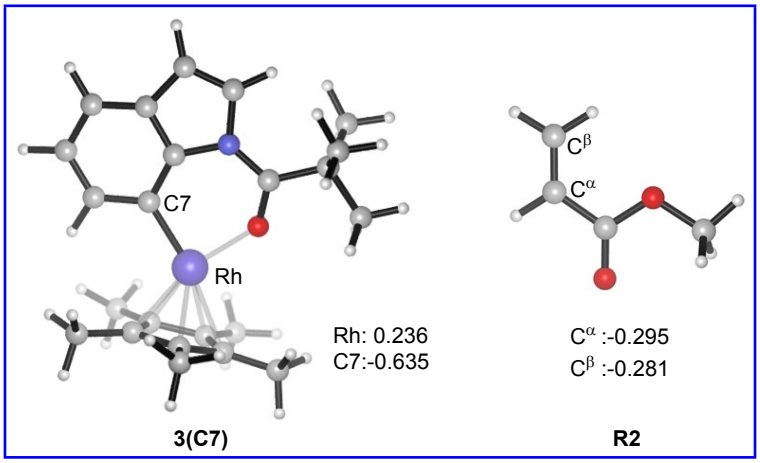

Fig. S2 NBO charges (in *e*) of the intermediate **3(C7)** and substrate **R2**.

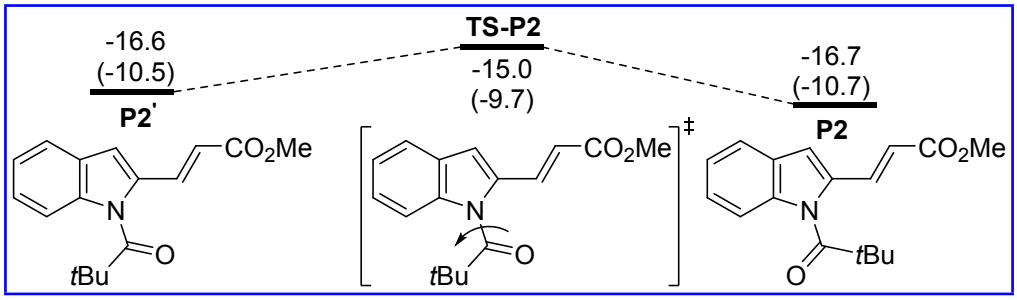

Fig. S3 The transformation from **P2'** to **P2**. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

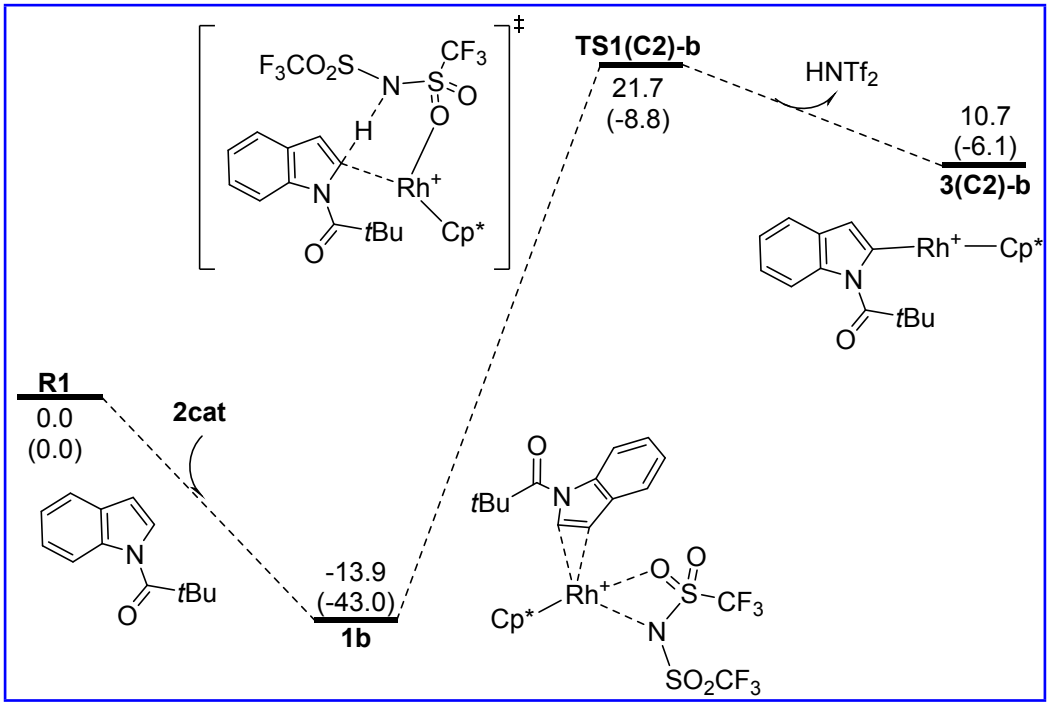

Fig. S4 The C−H activation step in the unfavorable pathway to produce **P2'** catalyzed by **2cat**. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

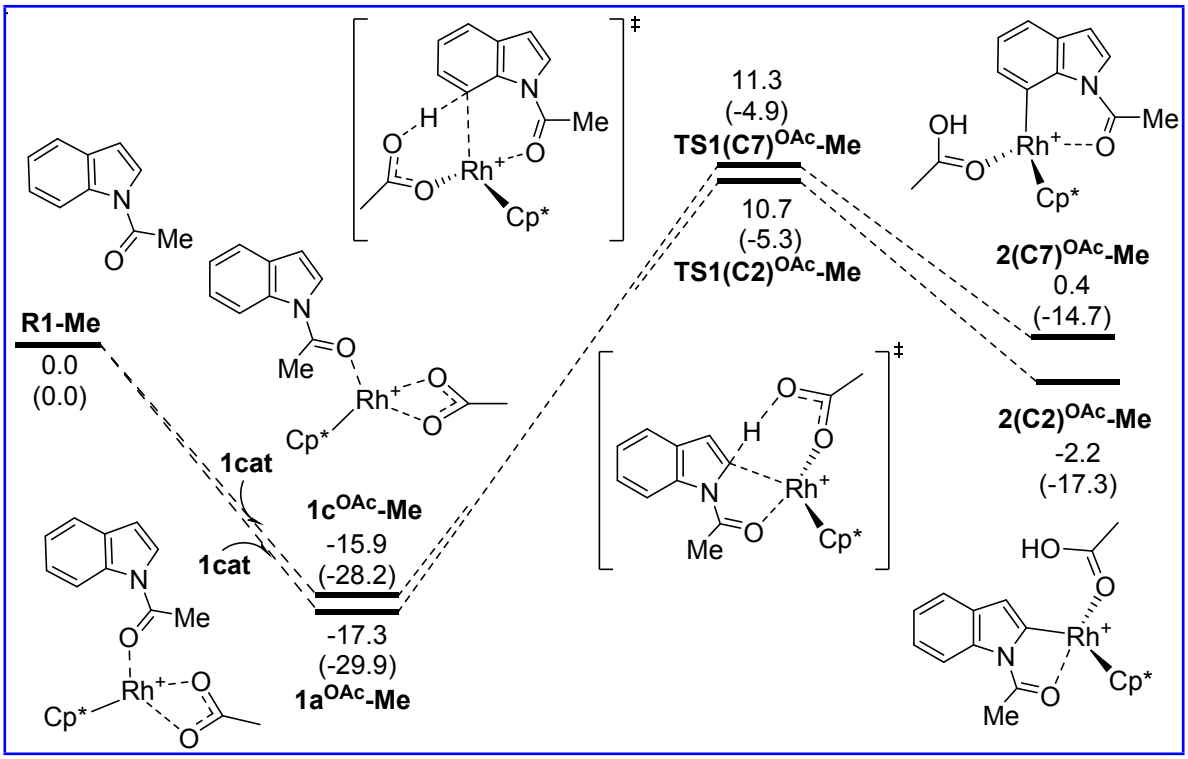

Fig. S5 The free energy diagrams for the C7– and C2–H bond activation processes of **R1-Me** catalyzed by **1cat**. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

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

1cat

Sum of electronic and thermal Free Energies= -727.716021

C	1.62158900	-0.73349200	-0.79054900
C	1.62047900	0.73701300	-0.78889900
C	1.35792700	1.18359500	0.53665800
C	1.14529600	-0.00108700	1.36045000
C	1.35980100	-1.18347500	0.53401300
C	1.29823500	-2.59908400	1.01124400
H	1.07531500	-3.29066100	0.19731900
H	2.26581900	-2.88610700	1.44127500
H	0.53832500	-2.73126100	1.78442400
C	1.88658200	-1.58551000	-1.98772000
H	1.47251000	-1.14610500	-2.89820000
H	2.97033100	-1.68154200	-2.13449800
H	1.47539300	-2.58944800	-1.87164800
C	1.88416900	1.59214100	-1.98414300
H	1.47314300	2.59577100	-1.86495800
H	2.96775100	1.68849200	-2.13192700
H	1.46901700	1.15514200	-2.89530200
C	1.29411100	2.59798800	1.01717000
H	0.53454300	2.72693400	1.79122100
H	2.26148200	2.88582800	1.44714500
H	1.06927600	3.29102200	0.20500700
C	0.87506600	-0.00283700	2.82593900
H	1.83362300	-0.00064400	3.36341600
H	0.32002600	0.88339900	3.13903800
H	0.32467200	-0.89235800	3.13784000
C	-2.84053700	-0.00180700	-0.18741900
O	-2.16583800	-1.09457500	-0.14212900
O	-2.16590700	1.09157400	-0.14158700
C	-4.32851000	-0.00045900	-0.26288500
H	-4.67688100	0.86852300	-0.82423100
H	-4.68738800	-0.92900300	-0.70918700
H	-4.72848200	0.07216900	0.75540000
Rh	-0.36332800	-0.00031300	-0.16367900

2cat

Sum of electronic and thermal Free Energies= -2326.329025

C	2.23778900	-1.61974400	0.39996000
C	2.80163700	-1.08625100	-0.83696900
C	3.31262800	0.23980400	-0.57617200
C	3.03040800	0.54955100	0.79486800
C	2.37130400	-0.60881900	1.40592300
C	1.95203000	-0.73266900	2.83281000
H	0.99812300	-1.25673800	2.91877100
H	2.70995500	-1.30574800	3.38279700
H	1.85815800	0.24127700	3.31538500
C	1.68659100	-2.99361600	0.59597700
H	1.27963300	-3.40355700	-0.32961300
H	2.49255500	-3.65918500	0.93119000
H	0.89807800	-3.00270800	1.34958600
C	2.87475900	-1.81220200	-2.13616400
H	2.87516900	-1.12835300	-2.98691800
H	3.81101000	-2.38629200	-2.17134600
H	2.05187200	-2.51993100	-2.25347400
C	4.00192300	1.12632700	-1.56482200
H	3.84578700	2.18302100	-1.34047400
H	5.08188700	0.93521600	-1.53853900
H	3.65757700	0.94244000	-2.58429100
C	3.36952300	1.81814900	1.50215700
H	4.33681200	1.70098100	2.00890300
H	3.45581600	2.65878400	0.81180100
H	2.62899700	2.06764000	2.26512000
Rh	1.12790600	0.15718700	-0.21484800
N	-0.92590100	-0.00773900	-0.08196000
S	-1.32979700	1.36029400	-0.92781000
O	0.08582200	1.70720700	-1.36704200
O	-2.39012300	1.27683700	-1.90863100
S	-1.99223500	-0.95746600	0.82777500
O	-1.16251100	-1.65214700	1.80742600
O	-3.16236600	-0.17279000	1.18913700
C	-1.76180100	2.72064000	0.32693700
C	-2.50950800	-2.24312100	-0.44171900
F	-3.04519000	2.66931000	0.60526900
F	-1.02796800	2.52431100	1.42346700
F	-1.44152900	3.87510100	-0.23685500

F	-3.33178800	-3.09685900	0.14574400
F	-1.41395300	-2.88227800	-0.86833700
F	-3.10330900	-1.63986200	-1.46043300

1a

Sum of electronic and thermal Free Energies= -2960.530190

C	-1.57993400	3.15583400	-1.11220500
C	-0.50037400	2.84892600	-1.99705400
C	-0.79460700	1.58372500	-2.65062100
C	-2.10950200	1.15483100	-2.21978700
C	-2.57476800	2.09032900	-1.22984900
C	-3.89504700	2.05895300	-0.53049500
H	-3.83436000	2.50874900	0.46243600
H	-4.63003800	2.62972300	-1.11224000
H	-4.27005400	1.04080500	-0.42120600
C	-1.72334600	4.36549000	-0.24686100
H	-0.76131700	4.83133100	-0.03115400
H	-2.35059600	5.10634000	-0.75886700
H	-2.20716100	4.12432000	0.70237100
C	0.73235300	3.65693800	-2.23941700
H	1.63036800	3.03660400	-2.18042300
H	0.69108100	4.08603600	-3.24796300
H	0.83129800	4.47868200	-1.52989200
C	0.03084300	0.92513900	-3.70719700
H	-0.00425100	-0.16118000	-3.61052600
H	-0.35808400	1.19751500	-4.69702100
H	1.07332100	1.24487200	-3.66048400
C	-2.83985300	-0.03605300	-2.74046900
H	-3.31548400	0.23465100	-3.69234500
H	-2.16007300	-0.86879100	-2.92496700
H	-3.62180400	-0.36831700	-2.05743000
Rh	-0.73379500	1.20951600	-0.51767900
C	3.61292200	-0.67008900	-0.34152000
C	4.74504300	-1.45800200	-0.03466800
C	5.26002000	-2.34853500	-0.98049300
C	4.64027800	-2.43431000	-2.22482100
C	3.52543800	-1.63923400	-2.52051400
C	2.99520500	-0.74411900	-1.58807300
C	4.33786200	-0.15757200	1.77238900
C	5.16170600	-1.11955100	1.30702900
H	6.12838900	-2.95640600	-0.74655600
H	5.02235100	-3.12268100	-2.97191800
H	3.04974900	-1.72684800	-3.49227200
H	2.12255300	-0.15718100	-1.82327100
N	3.35265200	0.16201100	0.79415600
C	2.33833500	1.08012400	0.90404400
O	1.43687700	1.05583500	0.03324500
H	5.97998300	-1.56211200	1.85779700
H	4.32290900	0.30496200	2.74018600
C	2.37607700	2.16955500	2.00744200
C	3.73804900	2.91296400	1.98555500
H	3.70770200	3.71943900	2.72384900
H	4.59501500	2.28302700	2.22000300
H	3.91876200	3.36636100	1.00525800
C	2.06440500	1.57980600	3.40789600
H	2.81003300	0.87079100	3.76851400
H	2.02036200	2.40212400	4.12849500
H	1.09739300	1.07274500	3.41195800
C	1.29116000	3.22126100	1.69898700
H	1.36874700	4.02814700	2.43314000
H	1.43221300	3.65481200	0.70504500
H	0.28868400	2.79920000	1.76890100
N	-1.01349100	-0.86498300	0.19600200
S	-1.16033500	-0.53962100	1.79940300
O	-0.27921800	-1.20652800	2.74364400
O	-1.18270800	0.96643100	1.73755000
S	-0.30912000	-2.22980700	-0.48822100
O	-0.09032800	-1.86032600	-1.88769300
O	0.72923500	-2.82312500	0.33736400
C	-2.93454300	-0.97658300	2.30326000
C	-1.74148500	-3.43760100	-0.50623800
F	-2.96181200	-2.18137000	2.84444600
F	-3.33194700	-0.06599100	3.18414700
F	-3.72733500	-0.93852200	1.22690600
F	-1.32383900	-4.58227800	-1.02469400
F	-2.74073300	-2.94367400	-1.24219300
F	-2.16634300	-3.62660000	0.74531000

1b

Sum of electronic and thermal Free Energies= -2960.527937

C	3.24943600	-0.12204200	1.34247500
C	2.20411500	-0.87423400	1.92050400
C	2.50693000	-1.97419100	2.73607500
C	3.84479100	-2.29505200	2.94488100
C	4.87219800	-1.53406800	2.35531700
C	4.59534700	-0.43564100	1.54452400
C	1.29978500	0.88107600	0.77309900
C	0.95206600	-0.25522300	1.51688600

H	1.71446300	-2.54868500	3.20620300
H	4.10364100	-3.13559700	3.58083500
H	5.90691600	-1.80431000	2.54025600
H	5.38871000	0.14007900	1.08579400
N	2.65871300	0.96197600	0.64033700
C	3.41394600	1.88228200	-0.19122400
O	4.37299900	1.42409400	-0.77238700
H	0.01091500	-0.36345600	2.03709700
H	0.64924900	1.64368200	0.38042400
C	3.01018100	3.36544600	-0.25060600
C	2.45021600	3.87781200	1.09384300
H	2.32834400	4.96282100	1.03247000
H	1.47370800	3.45932000	1.34640800
H	3.13609800	3.66926600	1.92079000
C	1.98079100	3.56689000	-1.39403700
H	1.02960300	3.05688700	-1.22461400
H	1.76588600	4.63569400	-1.48601200
H	2.38927400	3.22630500	-2.35013800
C	4.29024800	4.15788900	-0.59954800
H	4.03872400	5.21737900	-0.69790000
H	5.04610300	4.05870000	0.18495800
H	4.72933500	3.81384000	-1.53719200
C	1.66273400	-2.11038500	-1.55683200
C	0.78279400	-3.12723900	-1.06125300
C	-0.52095900	-2.95074900	-1.70400000
C	-0.44397600	-1.80522700	-2.55280700
C	0.88905200	-1.23488100	-2.41370400
C	1.41376200	-0.07821700	-3.19968300
H	2.34910400	0.30181800	-2.78590800
H	1.61510500	-0.40288300	-4.22910000
H	0.68511500	0.73319500	-3.23766400
C	3.13333100	-2.02972900	-1.32204500
H	3.42424500	-2.48020800	-0.37297200
H	3.63504800	-2.58907500	-2.12361900
H	3.51309400	-1.00770500	-1.35240300
C	1.15051500	-4.25540100	-0.15312800
H	0.29559500	-4.58520000	0.44092700
H	1.48973300	-5.11174400	-0.75048600
H	1.95894800	-3.97983200	0.52687400
C	-1.69876000	-3.85224300	-1.53285800
H	-2.63610700	-3.34624000	-1.76933600
H	-1.59702900	-4.71156400	-2.20837200
H	-1.76774000	-4.23433000	-0.51269900
C	-1.52080500	-1.29869000	-3.45468600
H	-1.46120500	-1.83242100	-4.41240300
H	-2.51696900	-1.47195300	-3.04194500
H	-1.41015200	-0.23281400	-3.65143300
Rh	-0.04717300	-1.21069700	-0.42516500
N	-1.75409600	0.23817400	-0.03175500
S	-2.72125100	-0.84518500	0.75908900
O	-3.92946200	-1.29396800	0.08517000
O	-1.67561600	-1.84975400	1.15353800
S	-2.29429200	1.41029100	-1.09999000
O	-1.16330800	1.64993000	-2.00182100
O	-3.64187700	1.17783700	-1.59789600
C	-3.24316200	-0.09145700	2.40613100
C	-2.36094900	2.94080400	-0.01925100
F	-4.30478500	0.67722700	2.22815600
F	-3.52779000	-1.09372200	3.22545800
F	-2.22897100	0.62519500	2.89811900
F	-2.72980100	3.96839500	-0.76786800
F	-1.14226800	3.17578600	0.49528700
F	-3.22552700	2.75904700	0.97492200

1c

Sum of electronic and thermal Free Energies= -1361.907721

C	1.10150200	2.01847200	-2.31524800
C	0.70297400	3.11771000	-1.44760700
C	1.72541100	3.30622200	-0.46694500
C	2.78449500	2.33330600	-0.72690600
C	2.41747600	1.57983800	-1.89903100
C	3.23753200	0.53113600	-2.57123200
H	2.61197000	-0.25621900	-2.99302100
H	3.80236200	0.99568400	-3.39004200
H	3.95232600	0.07495900	-1.88575000
C	0.35369000	1.53124800	-3.51305600
H	-0.71994000	1.69925000	-3.41045800
H	0.69402400	2.07692600	-4.40274100
H	0.51796000	0.46564000	-3.67774900
C	-0.56416200	3.89664300	-1.58498000
H	-0.81198000	4.43975600	-0.67211200
H	-0.45259100	4.63087400	-2.39266400
H	-1.40481000	3.24851600	-1.84140300
C	1.75024200	4.32214400	0.62835900
H	2.15091800	3.90282000	1.55425100
H	2.39752300	5.15861100	0.33579500
H	0.75770400	4.72353800	0.83651600
C	4.07235900	2.24131100	0.02540900
H	4.79264400	2.95405700	-0.39598800

H	3.93710500	2.48834600	1.08012900
H	4.50987700	1.24461000	-0.03810200
Rh	0.96847700	1.25000300	-0.29518100
C	-4.61072900	-0.44590800	-0.03315100
C	-4.95715700	-1.23281200	-1.16113800
C	-6.22744200	-1.80326200	-1.27921600
C	-7.15734200	-1.59638800	-0.26577800
C	-6.81243100	-0.82960300	0.85204000
C	-5.54802800	-0.24971700	0.98591900
C	-2.81200100	-0.59786600	-1.46193000
C	-3.80832200	-1.30151000	-2.03122300
H	-6.47334900	-2.40323500	-2.14988700
H	-8.14818100	-2.03301800	-0.33734800
H	-7.53784500	-0.67613700	1.64457100
H	-5.34570100	0.32417300	1.87471500
N	-3.24341900	-0.02635200	-0.22710800
C	-2.34051000	0.74655400	0.48367400
O	-1.18401500	0.81590200	0.01120200
H	-3.74625600	-1.83642100	-2.96860400
H	-1.79923900	-0.44555300	-1.78632800
C	-2.70830000	1.50869900	1.76669200
C	-2.95130400	0.48170400	2.90796800
H	-3.30973900	1.00862800	3.79765900
H	-3.66759800	-0.30003500	2.66270200
H	-2.01006600	-0.01282800	3.16434300
C	-3.89048900	2.47863600	1.49750000
H	-4.74300600	2.03548900	0.98862800
H	-4.24018200	2.89282900	2.44799200
H	-3.54498400	3.31622000	0.88260400
C	-1.52098700	2.38931400	2.20803100
H	-1.82091200	2.95107800	3.09779800
H	-0.63915100	1.80065200	2.45838700
H	-1.25150100	3.11421000	1.43391600
N	1.33036400	-0.89917000	0.10140100
S	0.65719000	-2.12700900	-0.82580900
O	-0.36750400	-2.89205700	-0.13401800
O	0.41624400	-1.50737600	-2.13223900
S	1.33518900	-0.82064300	1.74686800
O	1.31469600	0.67588600	1.91769200
O	0.40681900	-1.64700700	2.49951300
C	2.11923700	-3.27141100	-1.07514600
C	3.07446700	-1.29275100	2.30600000
F	2.53531000	-3.71072800	0.11244500
F	1.73346600	-4.28780700	-1.83200700
F	3.11238400	-2.60967600	-1.67626900
F	3.30339100	-0.67031800	3.45565300
F	3.96003400	-0.88825000	1.38917300
F	3.15580100	-2.60272100	2.46623900

2(C2)

Sum of electronic and thermal Free Energies= -2960.510559

C	-2.86336100	2.31321300	-0.86469300
C	-3.16528400	1.85756100	0.47215600
C	-2.28232000	2.56378200	1.38800100
C	-1.40968400	3.40355700	0.61372100
C	-1.74072700	3.21517600	-0.79094300
C	-1.08206300	3.93163600	-1.92625800
H	-1.28247100	3.44794000	-2.88376600
H	-1.45311500	4.96221000	-1.98508400
H	0.00037800	3.97036000	-1.78536500
C	-3.61726600	1.94526600	-2.10029900
H	-4.00529300	0.92586300	-2.05860300
H	-4.47512400	2.62294800	-2.20246600
H	-3.00596600	2.05187700	-2.99759700
C	-4.30063600	0.96222100	0.86043400
H	-4.09802700	0.44183900	1.79851400
H	-5.21366700	1.55361700	1.00304600
H	-4.50691500	0.21372200	0.09215100
C	-2.28413900	2.43015100	2.87501200
H	-1.30120000	2.63826100	3.30073100
H	-2.99775300	3.14422600	3.30561100
H	-2.58522100	1.42863200	3.18739700
C	-0.33788500	4.30577100	1.12822500
H	-0.70166400	5.34124100	1.13153500
H	-0.04067900	4.04712000	2.14530000
H	0.55004500	4.26030300	0.49427500
Rh	-1.09172200	1.30607300	0.04043800
C	-2.57355000	-2.29844500	-0.74598600
C	-2.61619100	-1.84141800	-2.10009700
C	-3.61560300	-2.30098900	-2.98245200
C	-4.56557600	-3.18617100	-2.50604300
C	-4.53256700	-3.60695600	-1.16032800
C	-3.55796200	-3.17137500	-0.26678300
C	-0.86687200	-0.79439600	-1.08315700
C	-1.53313700	-0.94081800	-2.28643100
H	-3.62622700	-1.96619900	-4.01499500
H	-5.34071500	-3.56305200	-3.16459600
H	-5.28767900	-4.30135800	-0.80547200

H	-3.56967000	-3.53098900	0.75102900
N	-1.48446900	-1.66343800	-0.12498700
C	-1.09591800	-1.47300900	1.21188000
O	-0.70714500	-0.32320700	1.49195600
H	-1.22180600	-0.48979100	-3.21979700
H	0.20455800	-0.60586100	-0.96753100
C	-1.08654500	-2.56393900	2.28223000
C	-0.85296700	-3.96775300	1.68728000
H	-0.81469500	-4.68843900	2.50896600
H	-1.63486200	-4.29587700	1.00171000
H	0.10512800	-4.00106300	1.16416500
C	-2.42217200	-2.46345200	3.07255300
H	-3.31580400	-2.58238800	2.45520500
H	-2.43564400	-3.25104100	3.83079600
H	-2.49099600	-1.50083400	3.58850200
C	0.06735500	-2.25481200	3.26907900
H	0.02878300	-2.98860500	4.07894400
H	1.03686100	-2.34136400	2.77627400
H	-0.02175900	-1.25682000	3.70098000
N	2.15680500	-0.42951000	-0.24851700
S	3.02584200	-1.68651600	0.39125200
O	3.89663000	-1.32312900	1.50396600
O	2.10372100	-2.82186800	0.49718400
S	2.17034700	1.05457200	0.31003200
O	0.99471200	1.71823300	-0.40032400
O	2.26439200	1.28949100	1.74728000
C	4.13052100	-2.06207200	-1.06984200
C	3.58263200	1.99753800	-0.49119200
F	4.84913900	-0.97718600	-1.37003100
F	4.94212800	-3.06256200	-0.74283700
F	3.38963200	-2.40863500	-2.12312200
F	3.43958100	3.29435100	-0.20474000
F	3.54841400	1.82675500	-1.81075600
F	4.73069800	1.54774800	-0.00322900

2(C7)

Sum of electronic and thermal Free Energies= -2960.516568

C	2.69184200	-1.49434200	-1.76449900
C	3.51637600	-0.77142100	-0.80686600
C	3.51846800	-1.51791700	0.42333200
C	2.63275800	-2.65343800	0.26438300
C	2.16675300	-2.66325700	-1.11013100
C	1.27871900	-3.69730600	-1.71585100
H	0.79841400	-3.33586300	-2.62585300
H	1.87526100	-4.58288900	-1.96979000
H	0.49602300	-4.00244200	-1.01863700
C	2.44230100	-1.11019000	-3.18550000
H	1.41428500	-1.32857300	-3.48370500
H	2.63043500	-0.04975900	-3.35688900
H	3.11244900	-1.67952100	-3.84212200
C	4.33675900	0.44745500	-1.09184800
H	4.47736000	1.05589500	-0.19609700
H	5.32881200	0.15225000	-1.45582600
H	3.87862300	1.07236500	-1.86078000
C	4.32628700	-1.19114500	1.63328200
H	3.94793500	-1.69002200	2.52537500
H	5.35793700	-1.52929800	1.46971800
H	4.35818700	-0.11645100	1.82640900
C	2.34481800	-3.71458200	1.27791400
H	3.02644700	-4.56250700	1.13612400
H	2.47392400	-3.34737500	2.29747400
H	1.32264900	-4.08499000	1.17685100
Rh	1.44888500	-0.86585300	-0.07391800
C	1.48006700	1.72978300	1.42736700
C	2.43941200	2.29457200	2.29678900
C	2.71837900	1.65359200	3.51228000
C	2.04151900	0.47339600	3.84025700
C	1.05092100	-0.03838500	2.99693700
C	0.73251200	0.58311500	1.76756800
C	2.22590100	3.67214100	0.51619400
C	2.89086600	3.52589800	1.68830300
H	3.43758300	2.08215000	4.20421700
H	2.24827100	-0.01491800	4.78714900
H	0.46171300	-0.89633600	3.30482900
H	-0.23738900	0.38700400	1.31029700
N	1.36424600	2.56512100	0.30581900
C	0.77440100	2.15425500	-0.89279400
O	0.59129200	0.93825100	-1.07132000
H	3.61123400	4.22271700	2.09294500
H	2.29391500	4.45987400	-0.21200800
C	0.40144300	3.15657000	-1.99643400
C	1.68862600	3.51801000	-2.79165800
H	1.40813000	4.18532500	-3.61110100
H	2.45096200	4.02933100	-2.19960500
H	2.14077800	2.62522100	-3.23692400
C	-0.28091100	4.41941500	-1.42230800
H	0.37451000	5.03008300	-0.79809800
H	-0.60541800	5.04414600	-2.25930600

H	-1.16181400	4.14620200	-0.83796800
C	-0.57472900	2.46620500	-2.97474100
H	-0.79595100	3.16335900	-3.78752700
H	-0.14590700	1.56014800	-3.40717800
H	-1.51575000	2.19956700	-2.49207100
N	-2.14729900	-0.07564600	0.39936900
S	-1.73336200	-1.34798400	-0.44177700
O	-1.67574700	-1.28864400	-1.90082100
O	-0.46557500	-1.85519900	0.24188800
S	-3.08762100	1.17258600	-0.13575100
O	-2.38995400	2.40953700	0.23360700
O	-3.62634500	1.00581500	-1.48342500
C	-2.90407700	-2.74506800	0.00065100
C	-4.52449000	1.01437900	1.05010800
F	-4.10426400	-2.46383600	-0.49058900
F	-2.44149600	-3.87455500	-0.54325500
F	-2.97106100	-2.88245600	1.32212000
F	-5.41861400	1.95279700	0.75424800
F	-4.10093000	1.17294000	2.30283600
F	-5.07532700	-0.19375000	0.91405500

3(C2)

Sum of electronic and thermal Free Energies= -1132.868637

C	-2.76626000	-0.48989200	1.28408100
C	-3.25978200	0.69964700	0.58593800
C	-3.33223900	0.39305400	-0.78271300
C	-2.90771700	-1.00716400	-0.96170600
C	-2.63024500	-1.56702300	0.32312200
C	-2.35485800	-3.00472600	0.64318900
H	-1.66884100	-3.10722800	1.48677000
H	-3.28846200	-3.51483500	0.90953700
H	-1.92650400	-3.53281700	-0.21129800
C	-2.61394700	-0.61346500	2.76427600
H	-2.28535900	0.32461900	3.21671600
H	-3.58436100	-0.87139300	3.21009300
H	-1.90467000	-1.39759100	3.03498600
C	-3.58704100	2.00192800	1.24916300
H	-3.60678500	2.82592900	0.53390600
H	-4.57389000	1.94814800	1.72482000
H	-2.86104500	2.24978100	2.02793400
C	-3.76334600	1.29208700	-1.89838000
H	-3.13333400	1.16654900	-2.78306000
H	-4.79281400	1.05597600	-2.19618700
H	-3.73449300	2.34342300	-1.60742800
C	-2.91650100	-1.72967700	-2.26997900
H	-3.94336900	-2.02754100	-2.52002300
H	-2.55440700	-1.09510500	-3.08255600
H	-2.30413300	-2.63233800	-2.24078700
Rh	-1.16683400	0.00577100	-0.09125500
C	2.95653900	-0.68123300	-0.01345600
C	2.58178400	-2.05044400	-0.02777700
C	3.55098800	-3.06075600	-0.02575300
C	4.89506000	-2.70288100	-0.00813100
C	5.25909700	-1.35166300	0.00736900
C	4.30465000	-0.32710400	0.00505800
C	0.62207600	-0.85976500	-0.03625100
C	1.14604800	-2.12188600	-0.03639100
H	3.25059000	-4.10387500	-0.03813300
H	5.66338800	-3.46883800	-0.00639700
H	6.30956300	-1.07935500	0.02210000
H	4.64748800	0.69525600	0.01844900
N	1.73327900	0.07031900	-0.02223800
C	1.38341100	1.39246700	-0.04087200
O	0.14077600	1.63854500	-0.06051800
H	0.56907200	-3.03672300	-0.04128100
C	2.33680700	2.58928800	-0.03891000
C	3.20306100	2.56842900	-1.32563300
H	3.93286700	3.38187100	-1.27685000
H	3.74424900	1.63756200	-1.48861500
H	2.57247900	2.74068100	-2.20317000
C	3.16497800	2.59176500	1.27284600
H	3.69787300	1.66262800	1.46981100
H	3.89859100	3.40212600	1.22989300
H	2.50966200	2.78266700	2.12815500
C	1.50705600	3.89158100	-0.06311600
H	2.19538600	4.74155800	-0.06165700
H	0.88320200	3.95807400	-0.95703100
H	0.85869600	3.97509800	0.81174000

3(C7)

Sum of electronic and thermal Free Energies= -1132.870055

C	-2.67742700	-1.13052100	-0.97228200
C	-2.46261900	-1.70273000	0.29536300
C	-2.49432000	-0.62377200	1.26656000
C	-2.88165800	0.60882200	0.59009700
C	-2.92344700	0.31744600	-0.80132000
C	-3.32919700	1.24050100	-1.90714900
H	-2.78406200	1.02730600	-2.82956500

H	-4.39902400	1.11933100	-2.12072800
H	-3.15718300	2.28652400	-1.64798300
C	-2.68824100	-1.82597700	-2.29543700
H	-2.23214900	-2.81563300	-2.24100200
H	-3.72147600	-1.95149500	-2.64364900
H	-2.15955300	-1.24553000	-3.05683300
C	-2.17262900	-3.13823500	0.61246000
H	-1.38700300	-3.23149800	1.36696000
H	-3.06827800	-3.63247700	1.00719500
H	-1.85207500	-3.69104900	-0.27236800
C	-2.34560500	-0.78063000	2.74429500
H	-1.98543400	0.13743400	3.21298300
H	-3.32269300	-1.01865400	3.18654300
H	-1.66340100	-1.59426600	2.99958800
C	-3.30414800	1.87070100	1.27876000
H	-4.29833600	1.72840800	1.72006000
H	-2.62172900	2.15206600	2.08426900
H	-3.37781500	2.70949400	0.58475000
Rh	-0.87792100	-0.02842500	-0.07034500
C	1.67484200	1.52943700	-0.01601000
C	2.51858700	2.66888700	-0.01556700
C	1.96431600	3.94673300	-0.03800100
C	0.57200100	4.06757800	-0.06024000
C	-0.24055000	2.93338300	-0.04744800
C	0.27263300	1.61466900	-0.02541100
C	3.87306600	0.85928100	0.01510800
C	3.88768400	2.20810600	0.00686700
H	2.60128700	4.82572000	-0.03940500
H	0.11749700	5.05325500	-0.08449200
H	-1.31389400	3.07892700	-0.06061400
N	2.52885900	0.38817300	-0.00307700
C	2.10059600	-0.90777300	-0.03618100
O	0.87067500	-1.15469200	-0.07889500
H	4.77463100	2.82626900	0.01407100
H	4.69748200	0.17264600	0.02972000
C	3.06695900	-2.11307600	-0.02921700
C	3.90973000	-2.13521800	1.27202200
H	4.52833800	-3.03721500	1.27257600
H	4.57636100	-1.28038200	1.38988500
H	3.26192300	-2.17683100	2.15329200
C	3.95635500	-2.10759800	-1.29987300
H	4.63256900	-1.25522100	-1.37046900
H	4.56839600	-3.01406400	-1.30174900
H	3.34044600	-2.12120000	-2.20448300
C	2.22435000	-3.40657400	-0.05931000
H	2.90135700	-4.26501300	-0.05399400
H	1.57020900	-3.48295900	0.81230200
H	1.60499700	-3.46506100	-0.95711700

4(C2)

Sum of electronic and thermal Free Energies= -1439.264332

C	1.95833800	-0.63852400	2.01006500
C	0.93725200	-1.66550400	1.80010000
C	1.36555700	-2.48574500	0.69797700
C	2.57514900	-1.89993100	0.17706000
C	2.96378900	-0.78687900	1.02785300
C	4.26697100	-0.05437000	0.94347500
H	4.24992200	0.86893900	1.52656800
H	5.07075900	-0.68274900	1.34737900
H	4.52534300	0.19448400	-0.08781100
C	1.91411600	0.37485400	3.10811500
H	2.63312000	1.17956600	2.94968200
H	0.91964200	0.82013000	3.19669900
H	2.14718100	-0.10377200	4.06725100
C	-0.19238700	-1.96555100	2.73946000
H	-1.03285600	-2.43193200	2.22168600
H	0.14349400	-2.65523000	3.52378000
H	-0.55625100	-1.06230800	3.23456900
C	0.75831200	-3.78716800	0.27341900
H	0.90435500	-3.97911100	-0.79196600
H	1.23248400	-4.61029900	0.82242800
H	-0.31154400	-3.82051200	0.48410100
C	3.43162900	-2.45490600	-0.91626400
H	4.23861100	-3.05189500	-0.47170000
H	2.87151100	-3.11015100	-1.58638900
H	3.89488000	-1.65544400	-1.49971100
Rh	0.82309400	-0.42950900	-0.02654300
C	-3.36265500	-0.19992700	-0.44488500
C	-3.22032400	-1.47014400	-1.05358200
C	-4.33983000	-2.16141800	-1.52564600
C	-5.59811500	-1.58163100	-1.38887500
C	-5.73366300	-0.32634000	-0.78623500
C	-4.62617400	0.37961600	-0.30799100
C	-1.10815000	-0.82167200	-0.48303500
C	-1.81490800	-1.81857600	-1.06343500
H	-4.22292700	-3.13437000	-1.99294500
H	-6.47804700	-2.10337800	-1.75107200
H	-6.71785500	0.11903900	-0.68373100

H	-4.78792900	1.34402000	0.14634100
N	-2.03518100	0.22156300	-0.08440200
C	-1.47156800	1.31651300	0.50088500
O	-0.21351400	1.29790100	0.63026400
H	-1.40445400	-2.72797800	-1.47979400
C	-2.20668400	2.56321400	1.00581100
C	-3.17535000	2.16968300	2.15106900
H	-3.75913100	3.04755500	2.44332700
H	-3.87037900	1.37086900	1.89679100
H	-2.60617400	1.84552900	3.02804700
C	-2.90276600	3.26857400	-0.18761000
H	-3.56642600	2.62534400	-0.76331400
H	-3.48892900	4.11168900	0.18972000
H	-2.15113400	3.66980900	-0.87441600
C	-1.17787000	3.55581800	1.58965000
H	-1.71315600	4.44364200	1.93820500
H	-0.63817000	3.12965600	2.43829800
H	-0.44480500	3.86755400	0.84269000
C	2.64694000	1.47568000	-1.83062100
O	3.67301600	0.84614500	-2.02452200
O	2.60282800	2.79332900	-1.58741800
C	1.27286700	0.90002000	-1.88301300
C	1.07163100	-0.39133300	-2.32908500
H	0.45825900	1.61488100	-1.85291200
H	0.10806300	-0.70839700	-2.70327700
H	1.93151600	-1.00244200	-2.57889500
C	3.87043200	3.48481700	-1.60888800
H	4.37155000	3.32602500	-2.56580100
H	3.62920600	4.53704100	-1.46806800
H	4.51345600	3.12716400	-0.80172000

4(C7)

Sum of electronic and thermal Free Energies= -1439.262093

C	-2.25114000	-1.70476700	1.06765300
C	-1.56402400	-0.80919800	1.95439700
C	-2.10210400	0.53869200	1.74126300
C	-3.01416400	0.48392400	0.67476200
C	-3.04237900	-0.90165400	0.17960800
C	-3.98013500	-1.41386000	-0.87245800
H	-3.64122000	-2.36434300	-1.28999000
H	-4.97749400	-1.57760000	-0.44521400
H	-4.09470500	-0.70546500	-1.69702300
C	-2.21973800	-3.19817700	1.14533900
H	-1.22222200	-3.58010000	1.36893200
H	-2.89222500	-3.52018300	1.95075200
H	-2.56566600	-3.66966700	0.22483700
C	-0.66480900	-1.20479900	3.08506400
H	0.05102300	-0.41386300	3.32004300
H	-1.25441600	-1.39402600	3.99107700
H	-0.10655300	-2.11458900	2.85489000
C	-1.73582600	1.73779900	2.55702300
H	-2.09178200	2.66213400	2.09881400
H	-2.17817300	1.66627000	3.55808600
H	-0.65260300	1.81452900	2.68060300
C	-3.88019000	1.60379200	0.18088900
H	-4.75703500	1.70645500	0.83213800
H	-3.35356800	2.56054500	0.17448600
H	-4.25518700	1.41758900	-0.82782900
Rh	-0.90760400	-0.26942500	-0.09695000
C	1.76295200	-1.68303000	-0.41119400
C	2.65785300	-2.73988500	-0.71616500
C	2.18335100	-3.93113400	-1.26924900
C	0.82019900	-4.03532300	-1.52303300
C	-0.05052100	-2.97842100	-1.21468400
C	0.38874200	-1.78258700	-0.63008400
C	3.90687000	-1.03229600	0.08732800
C	3.99026000	-2.29522300	-0.38086400
H	2.86469000	-4.74121200	-1.50805200
H	0.41875300	-4.93850800	-1.97299500
H	-1.10178200	-3.09860600	-1.45546900
N	2.55269400	-0.60103000	0.09240800
C	2.06528400	0.61596000	0.48030800
O	0.83773200	0.84963300	0.43353500
H	4.90337100	-2.86306900	-0.49326200
H	4.69453800	-0.38270400	0.41638100
C	2.99039500	1.75078000	0.98113700
C	3.95175400	2.18828200	-0.15595300
H	4.53534400	3.04579000	0.19194100
H	4.65605000	1.41648000	-0.46761100
H	3.37966400	2.49990200	-1.03435700
C	3.74271200	1.33393200	2.27081900
H	4.42988500	0.49719000	2.14560200
H	4.32642600	2.18823700	2.62558100
H	3.03547100	1.06689300	3.06311700
C	2.11853600	2.97416500	1.33302600
H	2.77334600	3.78561900	1.66241400
H	1.55179100	3.31397600	0.46557800
H	1.41922700	2.75630300	2.14385700

C	-0.38729600	2.37216400	-1.85033300
O	0.81364700	2.44202100	-2.01501700
O	-1.18517600	3.42395500	-1.58229000
C	-1.20531600	1.12742700	-1.96708600
C	-0.65182100	-0.04863300	-2.41771200
H	-2.27830900	1.27506900	-1.97321000
H	-1.26905300	-0.84680500	-2.81047800
H	0.40806900	-0.08748500	-2.63935000
C	-0.54654200	4.71819600	-1.56925200
H	-1.35751300	5.44377600	-1.52699800
H	0.09729000	4.81624900	-0.69206600
H	0.05086800	4.85490700	-2.47245700

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Sum of electronic and thermal Free Energies= -1439.267214

C	-1.81305200	-0.77468500	2.14674700
C	-0.63795700	-0.02273600	2.62601800
C	-0.71565500	1.27884200	2.11642700
C	-1.93545900	1.36703500	1.29199900
C	-2.66863600	0.13923300	1.44055600
C	-4.08600500	-0.10919100	1.03175900
H	-4.23232600	-1.10411600	0.60828200
H	-4.73081300	-0.01837300	1.91510400
H	-4.42618800	0.62486200	0.30045000
C	-2.16206100	-2.17028800	2.55938300
H	-2.89004500	-2.61799800	1.87988400
H	-1.27928300	-2.81378600	2.58725600
H	-2.60070800	-2.16831300	3.56591500
C	0.42888900	-0.61027400	3.49619400
H	1.31722100	0.02265000	3.53724200
H	0.05862600	-0.73480100	4.52109700
H	0.72965700	-1.59944500	3.13887300
C	0.23201300	2.41300700	2.35408300
H	0.51799000	2.91346400	1.42496700
H	-0.23883200	3.16618500	2.99786400
H	1.14630600	2.07996700	2.84840900
C	-2.44173100	2.61170000	0.63066700
H	-3.16065700	3.12202900	1.28438200
H	-1.62876700	3.31118100	0.42532100
H	-2.93794200	2.38434100	-0.31571000
Rh	-0.79505900	-0.22212200	0.30889700
C	2.64427200	0.99683900	-0.73776100
C	1.82708500	2.10631500	-1.08524500
C	2.29345600	3.41699900	-0.89671900
C	3.55401200	3.60498200	-0.34416800
C	4.33770300	2.50031000	0.02824300
C	3.89721800	1.18846900	-0.15306900
C	0.64532700	0.21975500	-1.58428300
C	0.59447000	1.59404800	-1.61195600
H	1.67792500	4.26305900	-1.18680500
H	3.93908800	4.60863400	-0.19784700
H	5.31905000	2.66519000	0.46169600
H	4.53370900	0.36608000	0.14080100
N	1.91523400	-0.18198100	-1.05327300
C	1.92934500	-1.42515000	-0.38732900
O	0.85241800	-1.79337000	0.10621200
H	-0.21700800	2.15161500	-2.06136700
C	3.15045400	-2.34798900	-0.35377900
C	3.79391700	-2.27018800	1.05557900
H	4.64041300	-2.96134500	1.09728300
H	4.16547300	-1.27327900	1.30407700
H	3.07519500	-2.56675900	1.82465100
C	4.16492700	-2.02445700	-1.46776700
H	4.59500600	-1.02520200	-1.39364800
H	4.98807200	-2.74245700	-1.41520900
H	3.70606100	-2.11797700	-2.45642400
C	2.62981200	-3.79293700	-0.56576700
H	3.47805500	-4.48180700	-0.52896100
H	1.91361700	-4.07911600	0.20589800
H	2.14880600	-3.90523900	-1.54231100
C	-2.67994800	-0.20525700	-2.03562500
O	-2.60820900	0.94336500	-2.45153100
O	-3.83589100	-0.90489800	-2.01382000
C	-1.53035400	-0.99690500	-1.52335200
C	-0.25264100	-0.75543400	-2.33744300
H	-1.78510600	-2.04659200	-1.37956500
H	0.28139300	-1.69368600	-2.49784300
H	-0.47066400	-0.32740700	-3.32011600
C	-4.98442800	-0.23830300	-2.57507000
H	-4.79818200	0.02303900	-3.61883200
H	-5.80322100	-0.95247700	-2.49854600
H	-5.21729500	0.67404200	-2.02052000

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Sum of electronic and thermal Free Energies= -1439.270875

C	-1.50628400	-1.86601200	1.60401800
C	-1.38568700	-0.65496300	2.29523100
C	-2.22310900	0.34541600	1.60738400

C	-2.96317800	-0.32752400	0.56361000
C	-2.43648900	-1.65514000	0.47783900
C	-2.92736900	-2.74786800	-0.42119100
H	-2.12929000	-3.44709900	-0.67935900
H	-3.71592500	-3.31741900	0.08752700
H	-3.35036800	-2.35360600	-1.34707700
C	-0.83637700	-3.17107700	1.90084300
H	-0.05596100	-3.06528600	2.65639300
H	-1.56819500	-3.89746300	2.27496100
H	-0.38276800	-3.60084200	1.00234400
C	-0.55092500	-0.36156200	3.50287400
H	0.00246500	0.57496900	3.38666900
H	-1.18885800	-0.25275400	4.38839900
H	0.16709900	-1.15839000	3.70530300
C	-2.45951400	1.74374700	2.08272500
H	-2.76403000	2.39056400	1.25819200
H	-3.25737900	1.75485300	2.83697800
H	-1.56450200	2.16867500	2.54275400
C	-4.09515700	0.24785700	-0.22881100
H	-5.01381600	0.21531100	0.37012100
H	-3.90354300	1.28463600	-0.50994200
H	-4.27932200	-0.32250100	-1.14160900
Rh	-0.81685300	-0.21984800	0.07551600
C	1.77193200	-1.27965700	-0.90405500
C	2.31666900	-2.57108300	-0.67727200
C	1.72016300	-3.69653500	-1.25064800
C	0.59664300	-3.51833500	-2.06010100
C	0.12439700	-2.23526200	-2.34590800
C	0.70982800	-1.06393100	-1.81428000
C	3.67537600	-1.08038100	0.34292500
C	3.51700400	-2.40219500	0.10886700
H	2.14209900	-4.68438800	-1.09390800
H	0.12506100	-4.37764600	-2.52647300
H	-0.68516900	-2.11711700	-3.06093300
N	2.59981200	-0.34652800	-0.23082300
C	2.14572100	0.86829300	0.29229300
O	0.92732600	1.06208200	0.40437800
H	4.18696800	-3.18468400	0.43626400
H	4.43991000	-0.57311900	0.90325500
C	3.12975700	1.97223200	0.72217300
C	4.33372400	2.06119400	-0.24138000
H	4.96740500	2.89811500	0.06500000
H	4.95719300	1.16505800	-0.25194500
H	4.00290300	2.25471600	-1.26611500
C	3.59210600	1.72683200	2.18423900
H	4.23055600	0.84908300	2.30602300
H	4.16629100	2.59659400	2.51573700
H	2.73355200	1.62039100	2.85460600
C	2.36766300	3.31735900	0.68732500
H	3.06772100	4.11966800	0.93652500
H	1.93747900	3.51266000	-0.29668000
H	1.55505100	3.33395600	1.41664200
C	-0.97973700	2.30055600	-1.61696900
O	-0.01123900	3.03380200	-1.69943300
O	-2.23366200	2.77523300	-1.39270500
C	-0.95473100	0.81618800	-1.76598100
C	0.32300200	0.29126300	-2.41497000
H	-1.87016500	0.46207700	-2.24220000
H	0.20471000	0.16468300	-3.49779100
H	1.12239700	1.01976600	-2.27124400
C	-2.34374600	4.21182200	-1.31958400
H	-3.40622600	4.41886500	-1.19482900
H	-1.77294200	4.60110900	-0.47315700
H	-1.97018000	4.66906800	-2.23798700

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Sum of electronic and thermal Free Energies= -1439.256585

C	3.64059300	-0.68565800	-0.10657500
C	3.94093000	-1.13673500	-1.41164800
C	5.23174200	-1.56105800	-1.74933400
C	6.21301600	-1.56520400	-0.76622100
C	5.89722800	-1.17504100	0.54305900
C	4.61669500	-0.74564900	0.89194000
C	1.71018000	-0.70238000	-1.35890500
C	2.71616700	-1.13381400	-2.15888400
H	5.44812900	-1.89875400	-2.75806700
H	7.21990600	-1.89335100	-1.00267100
H	6.66042600	-1.21428900	1.31370200
H	4.41941900	-0.48122800	1.91816600
N	2.24526900	-0.35949200	-0.06992400
C	1.49172600	0.28420900	0.90500500
O	0.25866100	0.10836200	0.94349600
H	2.59597600	-1.45151900	-3.18604600
C	2.06531200	1.25423700	1.97141300
C	3.26190200	2.09331200	1.46945800
H	3.48364700	2.85543000	2.22232600
H	4.17518500	1.52972500	1.29985100
H	2.99665200	2.60288300	0.53985800
C	2.35943000	0.46823600	3.27676600

H	3.07825000	-0.34370700	3.16292800
H	2.75284700	1.15936300	4.02790600
H	1.43591900	0.03226100	3.66997200
C	0.93997800	2.26692600	2.30767800
H	1.31726000	2.96717100	3.05809600
H	0.64994400	2.83304500	1.41997600
H	0.05681600	1.77274800	2.71504400
C	-2.94779600	-0.94019600	1.63339700
C	-3.14121000	-1.95311500	0.68451900
C	-3.49466100	-1.31221900	-0.59497700
C	-3.63173900	0.10070900	-0.37679300
C	-3.17524100	0.35693300	0.96617800
C	-3.18001600	1.68424600	1.65600000
H	-2.38286300	1.75562700	2.39895800
H	-4.13440100	1.82721000	2.17979600
H	-3.06310400	2.50553100	0.94618800
C	-2.56013900	-1.08723200	3.07108300
H	-1.75436500	-0.39770400	3.33770300
H	-2.22910600	-2.10113800	3.30184800
H	-3.41498800	-0.85728500	3.71876200
C	-3.02921000	-3.43267700	0.89003200
H	-2.55891600	-3.92628100	0.03562100
H	-4.02690200	-3.87326500	1.00933200
H	-2.44982600	-3.67677300	1.78212100
C	-3.87115600	-2.06014100	-1.83717100
H	-3.79450100	-1.43560500	-2.72934300
H	-4.90995900	-2.40609400	-1.76319600
H	-3.24472200	-2.94382200	-1.98191100
C	-4.15003200	1.12418600	-1.34084900
H	-5.16565600	1.42237400	-1.05403300
H	-4.19808700	0.73126600	-2.35820300
H	-3.52249500	2.01835600	-1.35702800
Rh	-1.52340800	-0.47138500	-0.13397500
C	-0.64023300	0.47788500	-1.77498300
C	0.27227100	-0.73310600	-1.77687700
H	0.23541400	-1.21713100	-2.75780200
H	-0.21047700	-1.56090300	-1.12853800
C	-0.11774500	1.84765300	-1.56275900
O	0.96077400	2.15448900	-1.08375200
O	-1.02441100	2.76393400	-1.97934300
C	-0.62137300	4.14287800	-1.85525900
H	-1.42578100	4.72346100	-2.30498200
H	-0.49411900	4.41488700	-0.80442600
H	0.31860500	4.31431000	-2.38348600
H	-1.36755900	0.46456400	-2.58504200

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Sum of electronic and thermal Free Energies= -1439.253154

C	2.67340600	-1.72238600	-1.16394900
C	2.82605700	-0.53849900	-1.89715700
C	3.08275700	0.55188800	-0.93898200
C	3.21824500	-0.01842600	0.37693500
C	2.84212100	-1.39961800	0.26635400
C	2.91930000	-2.40068000	1.37484900
H	2.24759600	-3.24489000	1.21435800
H	3.94105000	-2.79966200	1.43306600
H	2.68568200	-1.94839600	2.34115200
C	2.40150400	-3.09369800	-1.69725900
H	1.70982000	-3.64628200	-1.05684000
H	1.98289100	-3.06461000	-2.70486200
H	3.33392400	-3.67069600	-1.73903400
C	2.75054700	-0.37179200	-3.38388200
H	2.25254100	0.55952900	-3.66473300
H	3.76059000	-0.34088500	-3.81116900
H	2.21504000	-1.19643800	-3.85793200
C	3.37749500	1.97200000	-1.30860900
H	3.02894100	2.65977100	-0.53553400
H	4.45942200	2.11035000	-1.43007400
H	2.90370900	2.24919700	-2.25282700
C	3.72959900	0.65761600	1.61030800
H	4.71733400	0.25230700	1.86108300
H	3.84329500	1.73153800	1.45630100
H	3.07415500	0.50889400	2.47249700
Rh	1.13591200	-0.18514700	-0.33494500
C	-3.01710800	0.75373400	-0.49983300
C	-4.38176500	1.09659200	-0.70356900
C	-4.76823200	2.35868700	-1.15950600
C	-3.77994900	3.30013900	-1.40101700
C	-2.44144700	2.97937400	-1.15863500
C	-2.01102400	1.72696600	-0.68859100
C	-4.37462700	-1.01343600	0.08577400
C	-5.19575800	-0.03380100	-0.33594900
H	-5.81835000	2.58756900	-1.30951400
H	-4.03671600	4.29175200	-1.75895600
H	-1.68956400	3.74435600	-1.32776900
N	-3.01793600	-0.60061200	-0.00840000
C	-1.94538600	-1.46169000	0.13549200
O	-0.86946700	-1.18508800	-0.41807600

H	-6.27379600	-0.09005400	-0.38882600
H	-4.62099100	-2.00678100	0.40580600
C	-2.07490700	-2.76068600	0.97432800
C	-2.76656400	-3.87698900	0.14516300
H	-2.71834300	-4.81247900	0.71030100
H	-3.81689600	-3.68563900	-0.07802500
H	-2.24663800	-4.03237700	-0.80528100
C	-2.77936400	-2.51994400	2.33182700
H	-3.82578800	-2.22681000	2.25223600
H	-2.74244000	-3.44509200	2.91415600
H	-2.26104900	-1.74707500	2.90856000
C	-0.64585200	-3.25241600	1.28424900
H	-0.70691100	-4.15984800	1.89120300
H	-0.10126500	-3.48890100	0.36831500
H	-0.07857500	-2.50520400	1.84497500
C	0.73136800	1.96982600	1.82609900
O	0.92288800	1.67775800	2.99233300
O	1.18449700	3.12530600	1.27356400
C	0.00181300	1.09257600	0.87714900
C	-0.51457900	1.63179600	-0.44095100
H	-0.69300200	0.48013000	1.44585400
H	-0.06229900	2.60589800	-0.62507900
H	-0.12001500	0.99979500	-1.31390600
C	1.79674800	4.05064300	2.19684200
H	2.06001100	4.92559900	1.60358100
H	1.09103400	4.31933600	2.98545300
H	2.68539900	3.61154700	2.65531300

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Sum of electronic and thermal Free Energies=-1439.256244

C	3.52588500	-0.64308500	-0.10898300
C	3.69035400	-1.53202100	-1.19904500
C	4.90963100	-2.18380400	-1.42971700
C	5.96111900	-1.96509200	-0.55152500
C	5.78545900	-1.11626200	0.55078400
C	4.57956100	-0.45724600	0.79180700
C	1.53119100	-0.82010600	-1.24574000
C	2.43535200	-1.62420200	-1.87375900
H	5.01466300	-2.85562100	-2.27581600
H	6.91499100	-2.45817600	-0.70682700
H	6.60591500	-0.96180000	1.24427400
H	4.50712100	0.17582000	1.65950900
N	2.17120200	-0.16875300	-0.13927700
C	1.48371400	0.65196000	0.75130000
O	0.25408800	0.51219900	0.89922100
H	2.22362300	-2.21967600	-2.75179600
C	2.13599700	1.77689800	1.59004400
C	3.28204500	2.49834300	0.84536600
H	3.63779200	3.31986700	1.47434100
H	4.13998300	1.87616900	0.60459400
H	2.90327900	2.92350000	-0.08682300
C	2.53413700	1.19941100	2.97772600
H	3.17364000	0.31779200	2.93774500
H	3.05825100	1.97160800	3.54855300
H	1.63507000	0.92080600	3.53542100
C	1.05200100	2.85184500	1.85996700
H	1.49766500	3.64305300	2.46946000
H	0.69947600	3.29250400	0.92562000
H	0.19869400	2.44312500	2.40253200
C	-2.70229900	-1.05351100	1.69307000
C	-2.94075000	-2.01384800	0.64878300
C	-3.36760800	-1.27937100	-0.51424200
C	-3.57704500	0.12037000	-0.11976900
C	-3.15664100	0.25471700	1.21606300
C	-3.16150100	1.49838500	2.04877600
H	-2.20992000	1.63064000	2.57155400
H	-3.94729700	1.44126400	2.81188300
H	-3.34650800	2.38907700	1.44612200
C	-2.30110400	-1.35073900	3.10604600
H	-1.69565000	-0.54390700	3.52582200
H	-1.72710200	-2.27652700	3.17662000
H	-3.19130800	-1.45896100	3.73851400
C	-2.85201100	-3.50664100	0.76830900
H	-2.56855100	-3.97532100	-0.17586000
H	-3.83231200	-3.90620300	1.05643800
H	-2.13108500	-3.81200800	1.52835900
C	-3.81349800	-1.88136800	-1.81280300
H	-3.64971400	-1.20473000	-2.65520100
H	-4.88880600	-2.09751500	-1.77680700
H	-3.29610400	-2.81963700	-2.02323800
C	-4.18309300	1.18299600	-0.98466600
H	-5.26625700	1.22983200	-0.81554800
H	-4.02875600	0.98223200	-2.04647100
H	-3.76587200	2.16876700	-0.77178800
Rh	-1.31732900	-0.62735000	0.01406200
C	-0.69581700	0.38668700	-1.89620600
C	0.14884200	-0.71986600	-1.71648200
H	-0.11582700	-1.59400300	-2.30360500

H	-0.41487300	-1.88339800	0.18445000
C	-0.29112000	1.80952200	-1.76402200
O	0.79584800	2.21528200	-1.39528700
O	-1.28943300	2.61547400	-2.17655900
C	-0.98337000	4.02562300	-2.21408800
H	-1.85891800	4.50169900	-2.65290300
H	-0.80507600	4.40548700	-1.20532700
H	-0.09785500	4.20550100	-2.82677900
H	-1.55158000	0.23958100	-2.54581300

7(C7)

Sum of electronic and thermal Free Energies=-1439.256542

C	-0.51682200	0.12337200	-2.57505700
C	-1.03763900	-1.24043800	-2.31597400
C	-2.35939900	-1.12505000	-1.79158000
C	-2.56978000	0.27382500	-1.51284000
C	-1.45513800	1.03900600	-2.10940800
C	-1.40297400	2.53234900	-2.19068600
H	-0.41552400	2.88823800	-2.48885500
H	-2.12818300	2.89853800	-2.92787300
H	-1.65004600	3.00441100	-1.23512200
C	0.78528100	0.41072300	-3.25831200
H	1.15724300	1.40954700	-3.02188800
H	1.55600800	-0.31270000	-2.97906700
H	0.66708100	0.34656800	-4.34733400
C	-0.37598000	-2.50014100	-2.78419600
H	-0.79907600	-3.38132600	-2.29850300
H	-0.50910800	-2.61704700	-3.86726500
H	0.69891700	-2.48803700	-2.58705900
C	-3.36557200	-2.22389500	-1.61328500
H	-4.04891300	-2.01486600	-0.78822500
H	-3.96590800	-2.32233300	-2.52635900
H	-2.88921300	-3.18717600	-1.42230600
C	-3.86386500	0.87625600	-1.05395100
H	-4.56794800	0.92154300	-1.89471700
H	-4.32524900	0.29125100	-0.25626000
H	-3.73005100	1.89689300	-0.68869100
Rh	-0.90796900	-0.44492400	-0.23469400
C	2.02125600	1.48082300	0.47153300
C	2.90960300	2.49923800	0.04777000
C	2.51427400	3.84232100	0.04618100
C	1.23438900	4.16059200	0.48411000
C	0.37080100	3.15704400	0.93611200
C	0.73319100	1.79772400	0.95691000
C	4.04144700	0.55293300	-0.06741300
C	4.16521200	1.87848700	-0.29128000
H	3.20652100	4.61613200	-0.26986400
H	0.90949300	5.19559600	0.51142700
H	-0.59667500	3.43730900	1.33921300
N	2.72953500	0.24532600	0.38266800
C	2.24076700	-1.05750900	0.47615000
O	1.04061400	-1.31518200	0.30888100
H	5.05178500	2.37694000	-0.65674700
H	4.75618300	-0.23063200	-0.23464200
C	3.18052300	-2.23896300	0.83355200
C	4.19114200	-1.86144500	1.94199400
H	4.74168900	-2.76062300	2.23269100
H	4.92468300	-1.11185100	1.64450900
H	3.67448100	-1.49021500	2.83251100
C	3.89194900	-2.76967500	-0.43932000
H	4.59933500	-2.06639800	-0.88368900
H	4.45193000	-3.67133200	-0.17560900
H	3.16208000	-3.04623900	-1.20678200
C	2.29085700	-3.38253100	1.37687600
H	2.93287100	-4.22321300	1.65315600
H	1.73483100	-3.07202900	2.26548300
H	1.57226200	-3.72728500	0.63190400
C	-2.32787800	0.06264600	2.55070200
O	-1.83333300	-0.70014600	3.35210400
O	-3.64426500	0.33029500	2.45964800
C	-1.56090900	0.86506200	1.54272000
C	-0.17636100	0.80019700	1.53473300
H	-2.09672500	1.68580000	1.07923200
H	0.25173900	0.04420700	2.18742100
H	-1.46311100	-1.55948000	0.66849100
C	-4.48133700	-0.35375900	3.41864700
H	-5.49382700	-0.00342800	3.22423800
H	-4.41050600	-1.43497500	3.28044200
H	-4.17356600	-0.10238400	4.43549700

8(C2)

Sum of electronic and thermal Free Energies= -1667.115588

C	-1.71511600	-1.15905200	2.10863800
C	-0.98553600	0.08926200	2.34821000
C	-1.76019500	1.15775700	1.83510800
C	-2.95948400	0.58863800	1.21416800
C	-2.96262400	-0.83077200	1.47643400
C	-4.06776400	-1.78709000	1.17250400

H	-3.67550800	-2.76998900	0.91307000
H	-4.70692600	-1.88121600	2.06031800
H	-4.69334800	-1.43477900	0.35040100
C	-1.29587400	-2.52500200	2.54045100
H	-0.23818700	-2.55439100	2.80687200
H	-1.87414300	-2.82861400	3.42226100
H	-1.47738200	-3.23925000	1.73432400
C	0.31564600	0.20957900	3.07608300
H	0.83818100	1.13192600	2.81470700
H	0.13831300	0.21941400	4.15877100
H	0.97422100	-0.63415000	2.86012600
C	-1.44402300	2.61275500	1.97443200
H	-2.10646200	3.23313200	1.37197400
H	-1.57368700	2.90718000	3.02321900
H	-0.41703900	2.84523300	1.68423500
C	-4.09550600	1.37030000	0.63407400
H	-4.71028200	0.75025500	-0.02044600
H	-4.73741500	1.74452000	1.44187600
H	-3.74678200	2.22539200	0.05329900
Rh	-1.25737800	-0.27963700	0.15670200
C	3.53611400	0.60774800	0.00174800
C	3.41718300	2.01091400	-0.17009500
C	4.45147900	2.87030000	0.23656000
C	5.57272900	2.32448500	0.84254300
C	5.65511700	0.93801300	1.06304500
C	4.64350500	0.06721100	0.66313700
C	1.47031600	1.09151800	-0.89420200
C	2.12895900	2.28080900	-0.72550500
H	4.35843300	3.94157400	0.08875600
H	6.38461400	2.96746600	1.16585400
H	6.52783800	0.52828700	1.56159100
H	4.74033100	-0.98796400	0.87076700
N	2.34063400	0.02039400	-0.48376000
C	1.86933600	-1.29364100	-0.36646400
O	0.67285500	-1.47982800	-0.10381200
H	1.72800400	3.24422500	-0.99643900
C	2.72883400	-2.54166700	-0.67323300
C	3.11521500	-3.23003400	0.66024800
H	3.67833800	-4.14149600	0.44071400
H	3.73364500	-2.60784500	1.31148100
H	2.21630300	-3.51349500	1.21497800
C	3.95033000	-2.25178200	-1.56796800
H	4.71968700	-1.63987400	-1.10097700
H	4.41206500	-3.20521600	-1.83967400
H	3.64634700	-1.75964100	-2.49694700
C	1.80414800	-3.51721900	-1.45272400
H	2.35813200	-4.44004200	-1.64548100
H	0.89717600	-3.75534700	-0.89665200
H	1.51482400	-3.09555100	-2.42101400
C	-1.20722600	2.89188100	-1.40192500
O	-0.45058300	3.66917800	-0.84797600
O	-2.42982100	3.24461000	-1.85176500
C	-0.94789400	1.46727300	-1.72515500
C	0.22307600	0.76197400	-1.54921200
H	-1.70133900	0.99319700	-2.34351400
H	0.20630800	-0.20062800	-2.05129400
C	-2.75704800	4.64733400	-1.74806800
H	-3.73767800	4.75087400	-2.20941300
H	-2.78625000	4.96125900	-0.70205500
H	-2.01432200	5.24685500	-2.27834400
C	-1.99665700	-2.59245300	-1.53232600
O	-1.88280100	-3.29697900	-0.53169500
O	-1.83474600	-1.28599200	-1.56221700
C	-2.34921100	-3.16964900	-2.89519200
H	-3.26438400	-2.70620500	-3.27521100
H	-1.55426800	-2.95028200	-3.61434900
H	-2.48600800	-4.24814300	-2.81520200

8(C7)

Sum of electronic and thermal Free Energies= -1667.116552

C	-0.13463500	-0.97862500	2.39033300
C	-0.83656800	0.28951300	2.62080500
C	-2.19764700	0.12668200	2.21035800
C	-2.31694100	-1.17914900	1.60116700
C	-1.04958000	-1.88525900	1.80578200
C	-0.80605100	-3.33204400	1.51727200
H	0.21575700	-3.52280600	1.18357700
H	-0.97120000	-3.91242100	2.43399200
H	-1.49475100	-3.72129400	0.76459100
C	1.27178000	-1.27518700	2.80690700
H	1.69641500	-2.10528500	2.24015500
H	1.92290100	-0.40744300	2.68114300
H	1.29318000	-1.54751000	3.86959500
C	-0.27115400	1.50741900	3.27486500
H	-0.57153200	2.39704700	2.71597300
H	-0.65069200	1.58940400	4.30103600
H	0.81854000	1.46912300	3.32558400
C	-3.30103500	1.11462400	2.39965000

H	-4.08993700	0.98336500	1.65682500
H	-3.74820400	0.95867000	3.39026200
H	-2.92982600	2.13671500	2.33442600
C	-3.59155500	-1.79231300	1.11278000
H	-4.12310600	-2.25682800	1.95328000
H	-4.24862700	-1.04212800	0.67074600
H	-3.41657100	-2.56093500	0.35901800
Rh	-0.85469500	-0.07592500	0.43214500
C	2.57693900	-1.15143100	-0.63756800
C	3.70933900	-1.96009700	-0.36091100
C	3.66374700	-3.34847600	-0.53449100
C	2.48624900	-3.92400000	-0.99621600
C	1.37959200	-3.12249500	-1.29541800
C	1.38374800	-1.72213700	-1.13849800
C	4.32017500	0.17516700	0.01422800
C	4.78206200	-1.09370000	0.05426500
H	4.54147800	-3.95411600	-0.33252300
H	2.42973400	-4.99483400	-1.16220800
H	0.49795100	-3.58745900	-1.72267000
N	2.96140200	0.19408800	-0.38792700
C	2.14168300	1.32733600	-0.31996500
O	0.92797500	1.21359400	-0.13412500
H	5.77837900	-1.39592800	0.34377000
H	4.82079800	1.08742600	0.27986100
C	2.73109800	2.74641500	-0.51396300
C	3.79009800	2.79323300	-1.64001000
H	4.06439800	3.83761100	-1.81310800
H	4.70860500	2.24820100	-1.42066200
H	3.38333000	2.40166700	-2.57762800
C	3.29672300	3.27017400	0.83378600
H	4.16259700	2.71453000	1.20104300
H	3.60983700	4.30946400	0.69962800
H	2.52491500	3.25408400	1.60923900
C	1.56408300	3.67616400	-0.92027500
H	1.95768700	4.68748000	-1.05479100
H	1.11846900	3.35894800	-1.86783800
H	0.77704900	3.70030300	-0.16613200
C	-2.08562300	-0.75923300	-2.50680300
O	-1.81014600	0.02985700	-3.38216900
O	-3.32080700	-1.23093600	-2.25310000
C	-1.08094800	-1.40331800	-1.60173400
C	0.21863900	-0.95869800	-1.60293800
H	-1.35481200	-2.36495600	-1.18200000
H	0.39029500	-0.03190600	-2.14219800
C	-4.36205400	-0.71198300	-3.10831400
H	-5.27371900	-1.22416500	-2.80400500
H	-4.45786100	0.36701200	-2.97035700
H	-4.13165000	-0.92125100	-4.15492800
C	-1.89255000	2.55965300	-0.37171700
O	-1.82758300	1.29997400	-0.73941700
O	-1.47718700	3.01658300	0.69283700
C	-2.58229800	3.43252800	-1.40999700
H	-3.64959000	3.49164500	-1.16891200
H	-2.17313200	4.44337000	-1.36436200
H	-2.47754100	3.01603100	-2.41290900

Cat1-H

Sum of electronic and thermal Free Energies= -499.799292

C	-1.23267300	0.69766800	-0.53815400
C	0.17331400	1.15432100	-0.65104400
C	1.01866800	-0.00171100	-0.87220700
C	0.16976600	-1.15513700	-0.65074800
C	-1.23480300	-0.69427100	-0.53810300
C	-2.40188200	-1.61895600	-0.40446400
H	-3.31527400	-1.08940000	-0.13105800
H	-2.58376000	-2.13396800	-1.35583400
H	-2.21857800	-2.39422400	0.34618400
C	-2.39689100	1.62591300	-0.40434000
H	-3.31112500	1.09975000	-0.12720100
H	-2.20954600	2.40281700	0.34359400
H	-2.57962700	2.13872500	-1.35675400
C	0.59048400	2.58163600	-0.77425000
H	1.65127300	2.71639000	-0.55702700
H	0.41311300	2.92033700	-1.80462900
H	0.01171400	3.23312900	-0.11510000
C	2.43985100	-0.00390100	-1.33812900
H	2.97815400	-0.88824500	-0.99419600
H	2.45563300	-0.00428000	-2.43568300
H	2.98056900	0.87919900	-0.99481100
C	0.58266000	-2.58373500	-0.77332000
H	0.40466400	-2.92220400	-1.80367200
H	1.64296800	-2.72159100	-0.55568100
H	0.00167200	-3.23328000	-0.11419000
Rh	0.34677900	-0.00028600	1.14749900
H	1.82210800	-0.00124400	1.68715900

CuOAc

Sum of electronic and thermal Free Energies= -424.625717

Cu	1.30440100	-0.00058100	0.00381800
C	-1.06310900	0.00186600	-0.01473300
O	-0.44660200	1.11573400	-0.00907800
O	-0.44508300	-1.11199700	-0.00923000
C	-2.57839600	-0.00125800	0.00530900
H	-2.96220600	-0.87398900	-0.52502800
H	-2.91499300	-0.06239500	1.04617300
H	-2.96791500	0.91968200	-0.42885000

$Cu(OAc)_2$

Sum of electronic and thermal Free Energies= -653.109975

Cu	0.00003800	0.00078800	-0.00265000
C	2.34176900	-0.00222700	-0.01245500
O	1.67800600	-1.09276000	-0.01091900
O	1.67709300	1.08828900	-0.01029400
C	-2.34171800	0.00560100	0.00684100
O	-1.67801200	1.09542800	0.00441900
O	-1.67696800	-1.08559100	0.00518400
C	3.84103000	0.00021700	0.01292100
H	4.22517300	0.91218800	-0.44648600
H	4.17526400	-0.02847800	1.05576500
H	4.22831400	-0.88534000	-0.49368500
C	-3.84119300	-0.00281200	0.00316300
H	-4.19483900	-0.46084700	-0.92566000
H	-4.20398500	-0.61949900	0.82997100
H	-4.23130200	1.01151900	0.08701200

HOAc

Sum of electronic and thermal Free Energies= -229.052718

H	1.72028800	-0.80326600	-0.00003400
O	0.64440900	1.20231000	-0.00000300
C	0.09246400	0.12507600	0.00001300
O	0.77910100	-1.04572800	-0.00000700
C	-1.39686800	-0.11032500	-0.00006200
H	-1.91635100	0.84692200	-0.00407900
H	-1.68241700	-0.69608000	-0.87887200
H	-1.68318000	-0.68874800	0.88335800

P1

Sum of electronic and thermal Free Energies= -939.403832

C	1.54741000	-0.88809700	-0.01440500
C	2.89422100	-1.27165900	0.22078000
C	3.27533200	-2.61917400	0.16681200
C	2.31093300	-3.57102600	-0.13787700
C	0.97573900	-3.19139200	-0.32001600
C	0.53628000	-1.86005900	-0.20939300
C	2.78735500	0.97221400	0.39265800
C	3.64663900	-0.07285100	0.48342300
H	4.30718200	-2.90479200	0.34887300
H	2.58265700	-4.61966700	-0.21078700
H	0.22891600	-3.95821100	-0.50615400
N	1.49010200	0.52066300	0.07854700
C	0.52956900	1.34543800	-0.59394400
O	-0.10055200	0.88196400	-1.51923000
H	4.70315800	-0.00884300	0.70271800
H	2.98910000	2.02583500	0.47775500
C	0.28849800	2.79150600	-0.09046900
C	1.21017900	3.76114500	-0.87211300
H	0.95722400	4.79309000	-0.60797900
H	2.27221800	3.61626900	-0.65479300
H	1.06729400	3.64222900	-1.95032100
C	0.47661900	2.95024500	1.43252600
H	1.50286300	2.79295700	1.76964600
H	0.18881600	3.96607300	1.72223700
H	-0.16646200	2.25809100	1.98499200
C	-1.17824800	3.13804300	-0.43759600
H	-1.38212200	4.17319400	-0.14566400
H	-1.36293500	3.03082600	-1.50761500
H	-1.88082600	2.48810400	0.09246500
C	-3.04099100	-0.53937700	0.49582200
O	-3.60735900	0.39928300	1.03020100
O	-3.70172800	-1.51947100	-0.16743500
C	-1.57930400	-0.71099900	0.49843100
C	-0.91346500	-1.65001900	-0.19591600
H	-1.06436400	0.02149300	1.10919300
H	-1.49882400	-2.38174300	-0.74794000
C	-5.12590000	-1.36258600	-0.22493500
H	-5.49467700	-2.22047800	-0.78765700
H	-5.55536200	-1.35085000	0.78027800
H	-5.39264200	-0.43054200	-0.73010000

P2'

Sum of electronic and thermal Free Energies= -939.403874

C	-1.42094100	1.15442500	-0.17329200
C	-0.37991500	2.10177700	0.01923800
C	-0.69478500	3.46598500	0.16297100
C	-2.02106800	3.86134500	0.08521500
C	-3.03867100	2.91561200	-0.15605800
C	-2.75562600	1.56183600	-0.29994500

C	0.58834500	0.06127500	-0.25580700
C	0.85544800	1.39399700	-0.02140300
H	0.09731200	4.19278100	0.31690700
H	-2.28219000	4.90995600	0.19036900
H	-4.06777000	3.25084900	-0.24522300
H	-3.54939100	0.85955200	-0.52350600
N	-0.83361300	-0.10288500	-0.30674000
C	-1.49865600	-1.34005100	-0.59334800
O	-1.12863500	-2.00340700	-1.54116800
H	1.85047000	1.78885200	0.10695600
C	-2.56999800	-1.89859700	0.37929600
C	-3.90775300	-2.04166900	-0.38047800
H	-4.62555200	-2.58899200	0.23898500
H	-4.35461500	-1.07287300	-0.62376600
H	-3.76189400	-2.59434500	-1.31218300
C	-2.74789000	-1.10533900	1.68503800
H	-3.18638300	-0.11863300	1.53352800
H	-3.41406800	-1.66449700	2.35019700
H	-1.79378300	-0.97378700	2.20440600
C	-2.06416800	-3.32088400	0.74279700
H	-2.79785000	-3.81178400	1.38980700
H	-1.92082200	-3.92438800	-0.15513300
H	-1.11380700	-3.27805900	1.28581000
C	3.85275900	-0.25873100	0.02157900
O	3.74492100	0.94110200	0.21864500
O	5.05991400	-0.88576800	0.05228400
C	2.80181400	-1.24358400	-0.27022700
C	1.45671300	-1.08737900	-0.37401900
H	3.18525000	-2.24763200	-0.41905500
H	0.93327200	-2.00655200	-0.61340600
C	6.18137900	-0.03798900	0.32790200
H	7.05518500	-0.68979400	0.31202300
H	6.27324500	0.74372600	-0.43109500
H	6.07715600	0.43822300	1.30671600

R1'

Sum of electronic and thermal Free Energies= -634.195699

C	1.01671800	-0.00281700	0.00011900
C	2.20037000	0.78995300	-0.00008500
C	3.46559500	0.18962100	-0.00028500
C	3.55974300	-1.19646300	-0.00021800
C	2.39565700	-1.97682800	0.00008300
C	1.12515200	-1.40020000	0.00028700
C	0.45046900	2.20512200	0.00038200
C	1.80233900	2.17245700	0.00005700
H	4.35764400	0.80955800	-0.00044500
H	4.53320900	-1.67746800	-0.00038500
H	2.47391800	-3.05993600	0.00017100
H	0.26748500	-2.05349700	0.00053100
N	-0.08494700	0.89906100	0.00029300
C	-1.51158100	0.79962300	-0.00015000
O	-2.14108600	1.84344100	-0.00048400
H	2.45816300	3.03182700	0.00004800
H	-0.23717600	3.03334800	0.00050400
C	-2.25194500	-0.55197900	-0.00000900
C	-1.94154600	-1.33480800	1.30046900
H	-2.40870100	-2.32434600	1.25352300
H	-0.87987100	-1.47084800	1.50119500
H	-2.36953700	-0.80664000	2.15845800
C	-1.94129000	-1.33520300	-1.30022900
H	-0.87956800	-1.47124000	-1.50071000
H	-2.40844800	-2.32471800	-1.25310600
H	-2.36910500	-0.80728000	-2.15847000
C	-3.76609700	-0.25246500	-0.00020800
H	-4.31700300	-1.19902600	-0.00016000
H	-4.05970200	0.32172000	0.88108800
H	-4.05949600	0.32153400	-0.88168600

R1

Sum of electronic and thermal Free Energies= -634.203443

C	-1.27455300	-0.17854500	-0.00006700
C	-2.09766200	0.97534700	-0.00006600
C	-3.49253400	0.84114200	0.00004700
C	-4.04239200	-0.43583000	0.00015900
C	-3.21404200	-1.57058500	0.00015300
C	-1.82377000	-1.46507900	0.00004100
C	0.05128900	1.66931700	-0.00016000
C	-1.22666000	2.12349300	-0.00013800
H	-4.12800100	1.72224400	0.00005200
H	-5.12148300	-0.55952000	0.00024900
H	-3.66386600	-2.55921800	0.00023700
H	-1.18973400	-2.33866400	-0.00000300
N	0.07433700	0.25996600	-0.00010500
C	1.18623000	-0.60681500	-0.00022100
O	0.99717800	-1.81170300	-0.00053600
H	-1.52528800	3.16267200	-0.00018000
H	0.96287300	2.23724900	-0.00024100
C	2.63119500	-0.03862500	0.00011400

C	2.91281300	0.78192700	1.28264400
H	3.96477200	1.08608500	1.29099200
H	2.30784800	1.68503400	1.37504900
H	2.73615200	0.17268800	2.17492100
C	2.91329500	0.78195000	-1.28230400
H	2.30853300	1.68518700	-1.37481100
H	3.96531400	1.08591600	-1.29032500
H	2.73677600	0.17278600	-2.17465700
C	3.58684000	-1.24972800	0.00026600
H	4.62173200	-0.89256600	0.00045500
H	3.43299300	-1.87692500	0.88094300
H	3.43330000	-1.87691400	-0.88046700

R2

Sum of electronic and thermal Free Energies= -306.404603

C	0.01081800	0.48529500	-0.00005500
O	-0.58863500	1.54274300	0.00004300
O	-0.60462000	-0.72055400	-0.00000600
C	1.49082300	0.38273000	-0.00002800
C	2.17326700	-0.76480600	0.00002900
H	1.98965300	1.34707900	-0.00006400
H	3.25898500	-0.77281200	0.00003900
H	1.66586100	-1.72364400	0.00005900
C	-2.03878300	-0.67197800	-0.00000500
H	-2.36911300	-1.71081800	-0.00099100
H	-2.40806500	-0.15325100	0.88852600
H	-2.40803100	-0.15150300	-0.88751200

TSc(C2)

Sum of electronic and thermal Free Energies= -2960.512453

C	-3.37327000	-1.74993900	-0.58409800
C	-2.74212600	-2.18681900	-1.78108200
C	-3.50679800	-2.75942900	-2.81035700
C	-4.88133200	-2.86220900	-2.64577600
C	-5.49767800	-2.38465900	-1.47576100
C	-4.76151100	-1.81446200	-0.43793600
C	-1.12953400	-1.28933600	-0.46915400
C	-1.33836500	-1.90189800	-1.66973500
H	-3.02436800	-3.11022600	-3.71730600
H	-5.48963700	-3.30550300	-3.42719600
H	-6.57530200	-2.46081700	-1.37143500
H	-5.27163300	-1.45113100	0.44334200
N	-2.35794900	-1.20595700	0.24263500
C	-2.38680500	-0.47307200	1.42306300
O	-1.61526100	0.50398500	1.50713200
H	-0.54941200	-2.16817300	-2.36008500
H	-0.18554700	-1.16650800	0.04918400
C	-3.20293400	-0.86511300	2.66371700
C	-3.56118300	-2.36424000	2.68721000
H	-4.06258200	-2.58845600	3.63270500
H	-4.22748600	-2.67164900	1.88200100
H	-2.66065700	-2.98330100	2.63618300
C	-4.46130000	0.03495200	2.75410600
H	-5.15372400	-0.10450300	1.92033100
H	-5.00148800	-0.20324300	3.67465900
H	-4.17975800	1.09126200	2.79286300
C	-2.30466700	-0.56267500	3.89298200
H	-2.84113100	-0.86021700	4.79785600
H	-1.36752800	-1.12498900	3.85046300
H	-2.06094100	0.49819400	3.96386200
C	-0.03851100	2.22133100	-2.09048600
C	-1.45812900	2.20849000	-1.75977500
C	-1.64464200	3.03570200	-0.59832300
C	-0.33980200	3.51003500	-0.16783600
C	0.64812700	3.02222600	-1.11797300
C	2.10706000	3.34172800	-1.09874900
H	2.71100900	2.52975700	-1.50884500
H	2.28039300	4.23959100	-1.70668300
H	2.46035300	3.54759300	-0.08737300
C	0.57094200	1.55794300	-3.27925400
H	1.65555500	1.48833400	-3.20037400
H	0.17854300	0.55048300	-3.42966400
H	0.32543900	2.15148700	-4.17046100
C	-2.53487500	1.58391700	-2.58776400
H	-3.39804100	1.29297200	-1.98597300
H	-2.88095100	2.30535000	-3.33903400
H	-2.17453100	0.69951900	-3.11435000
C	-2.94420300	3.36661800	0.05744300
H	-2.84813900	3.40885900	1.14455500
H	-3.27861800	4.35438100	-0.28460800
H	-3.72289100	2.64629100	-0.19726800
C	-0.05867300	4.40956100	0.98907200
H	0.05869500	5.44044400	0.63061500
H	-0.86925800	4.39715000	1.71942100
H	0.86620800	4.12356700	1.49456900
Rh	-0.35005300	1.36042100	-0.06566700
N	1.92121700	-0.57999100	-0.05269000
S	2.38615400	0.33246700	1.18128300

O	3.65852400	1.04316000	1.13667800
O	1.15953400	1.15521600	1.53015800
S	2.77180600	-0.85357700	-1.43815000
O	1.82574200	-1.51455600	-2.34025700
O	3.51744500	0.32102700	-1.90023900
C	2.44501400	-0.87767200	2.61085800
C	4.04369500	-2.14603100	-0.96625900
F	3.39750200	-1.77518000	2.38659500
F	2.69515700	-0.20940300	3.73000100
F	1.26132900	-1.49535900	2.70962200
F	4.73449300	-2.47559100	-2.05087400
F	3.42075500	-3.21767700	-0.47964400
F	4.85861900	-1.64305800	-0.03939600

TSc(C7)

Sum of electronic and thermal Free Energies= -2960.513600

C	1.00358400	-1.71736500	-2.72095000
C	2.02918300	-2.11447300	-1.76695300
C	1.38763800	-2.80193300	-0.68274100
C	-0.03689500	-2.87394300	-0.98062100
C	-0.27208900	-2.22551200	-2.24026700
C	-1.57888100	-2.11024700	-2.95192000
H	-1.61589900	-1.22049200	-3.58231100
H	-1.70511400	-2.98822500	-3.59953600
H	-2.42398800	-2.07430300	-2.26114700
C	1.21505200	-1.00306200	-4.01395600
H	0.40813600	-0.29250300	-4.20597100
H	2.16249500	-0.46225200	-4.03138800
H	1.22591100	-1.73032600	-4.83600400
C	3.49354300	-1.86337600	-1.91047800
H	3.99140400	-1.81235300	-0.94068200
H	3.94667700	-2.68797300	-2.47555000
H	3.69372400	-0.94023900	-2.45751700
C	2.05395900	-3.46681500	0.47681600
H	1.45131600	-3.39468600	1.38381400
H	2.19029000	-4.53190400	0.24860400
H	3.03665200	-3.04214800	0.68498500
C	-1.04907200	-3.58007500	-0.14427100
H	-0.91401000	-4.66206400	-0.27824600
H	-0.92869900	-3.35690300	0.91750100
H	-2.06903100	-3.32372100	-0.42877200
Rh	0.58361400	-0.75462300	-0.85233700
C	2.28243400	-0.09702400	2.04849700
C	3.02484000	-0.77501300	3.04062300
C	2.36666400	-1.64185100	3.92407600
C	0.98621300	-1.79968600	3.80868100
C	0.25374800	-1.08117300	2.84997800
C	0.88911100	-0.20618800	1.95834600
C	4.46116600	0.58053100	1.93077600
C	4.39704100	-0.33168700	2.92938400
H	2.92185600	-2.16164700	4.69896900
H	0.46166700	-2.45772600	4.49426200
H	-0.82571100	-1.17705700	2.80339300
H	0.28375800	0.45332600	1.34297900
N	3.17944200	0.73946400	1.34148000
C	2.87637600	1.38893200	0.15749200
O	1.93045800	0.98512100	-0.53984800
H	5.23018200	-0.65397300	3.53820900
H	5.31234700	1.11198700	1.54391100
C	3.65284600	2.63906000	-0.30209000
C	4.94989700	2.21047800	-1.03726900
H	5.43799900	3.10447800	-1.43573100
H	5.67201600	1.70317200	-0.39326500
H	4.72399800	1.55274600	-1.88280600
C	3.96493200	3.57985100	0.88390000
H	4.64764900	3.15105600	1.61887900
H	4.43000000	4.49006400	0.49532200
H	3.04887700	3.87270300	1.40560600
C	2.75735100	3.39975000	-1.30664900
H	3.27776100	4.30713000	-1.62451600
H	2.53818200	2.79912200	-2.19111800
H	1.80570700	3.68847900	-0.85335500
N	-1.98710300	0.21954000	0.27215400
S	-3.26839100	-0.74042500	0.69380400
O	-3.86852400	-1.42512600	-0.45512000
O	-2.80307700	-1.52347500	1.84055100
S	-1.95691700	1.15597600	-1.03351700
O	-0.58720000	0.92900200	-1.64419800
O	-3.08325300	1.17534600	-1.95813000
C	-4.56740500	0.43417600	1.36709500
C	-1.76930400	2.88077700	-0.32547500
F	-4.95607400	1.27126700	0.40650000
F	-5.60018500	-0.28368900	1.79133700
F	-4.04668400	1.12638500	2.37889800
F	-1.63511800	3.74369500	-1.32627600
F	-0.67449100	2.92301200	0.44765100
F	-2.83845200	3.18162600	0.40171600

TS1(C2)

Sum of electronic and thermal Free Energies= -2960.500830

C	2.74475400	-1.20680600	-2.02625200
C	3.59217000	-0.63377200	-0.99720900
C	3.72352900	-1.62618000	0.07229000
C	2.89337800	-2.72891400	-0.24336300
C	2.24504700	-2.45148600	-1.52881800
C	1.32041200	-3.39940700	-2.22580100
H	0.83412600	-2.93645400	-3.08613000
H	1.88127800	-4.27030500	-2.58670800
H	0.54279200	-3.76161900	-1.54859300
C	2.50277200	-0.63466000	-3.38768100
H	2.58416700	0.45303300	-3.39475200
H	3.25659100	-1.03028500	-4.07999300
H	1.52199600	-0.91256700	-3.77856700
C	4.40868500	0.61502700	-1.12308700
H	4.62208600	1.05612700	-0.14708000
H	5.37123800	0.38611900	-1.59796800
H	3.90668300	1.36652500	-1.73550200
C	4.57389300	-1.45613700	1.29076700
H	4.27673700	-2.13459800	2.09150900
H	5.62223400	-1.66339400	1.04314700
H	4.52247800	-0.43465900	1.67542300
C	2.66779300	-3.96909200	0.56060300
H	3.14628800	-4.82550700	0.06994700
H	3.08136400	-3.88418800	1.56633000
H	1.60063300	-4.18879100	0.64986700
Rh	1.62104700	-0.85329600	-0.15168200
C	0.55512100	3.17553800	-0.39000800
C	0.21725000	2.89356600	-1.74445000
C	-0.01130900	3.93114000	-2.66616100
C	0.12212800	5.24119700	-2.23795000
C	0.47868300	5.51323700	-0.90474000
C	0.69905200	4.50203200	0.02921700
C	0.47107200	0.85790600	-0.69726000
C	0.18199100	1.47998900	-1.89982700
H	-0.28226700	3.69930600	-3.69137300
H	-0.04656800	6.06220200	-2.92652400
H	0.58359000	6.54487800	-0.58395800
H	0.96224100	4.77164700	1.03965200
N	0.71955200	1.93118200	0.26084900
C	1.06941900	1.51565100	1.52959200
O	1.46683800	0.32725100	1.62315100
H	-0.10972400	0.95783600	-2.80212200
H	-0.62722900	0.19155600	-0.32547600
C	0.97673100	2.33799100	2.81973500
C	-0.35460500	3.12038900	2.90146200
H	-0.35969900	3.69908700	3.82955900
H	-0.52974100	3.80742800	2.07614200
H	-1.20223000	2.43140500	2.93280900
C	2.23071400	3.24904700	2.91764100
H	2.36402400	3.92040300	2.06827700
H	2.15180100	3.86106200	3.82064100
H	3.13573800	2.64009600	3.00553000
C	1.01542000	1.35896200	4.01720500
H	0.93579300	1.94005500	4.94014600
H	0.18181300	0.65301600	3.98452600
H	1.94526100	0.78832300	4.04932300
N	-1.75973800	-0.35845000	0.18512100
S	-3.07918300	0.67471200	0.37892400
O	-4.00578500	0.20449200	1.39587800
O	-2.54837600	2.03468900	0.35910800
S	-1.47013900	-1.67263600	1.11284000
O	-0.09231800	-2.08529300	0.69706800
O	-1.77063300	-1.54884900	2.52884100
C	-3.88666400	0.41688500	-1.29065600
C	-2.53443400	-3.05823400	0.41437600
F	-4.24540700	-0.85816800	-1.42641200
F	-4.95132800	1.20278100	-1.37281100
F	-3.01326800	0.73627700	-2.25404000
F	-2.20728400	-4.18045900	1.04573300
F	-2.27540400	-3.18432100	-0.88945600
F	-3.81464100	-2.77758300	0.59781500

TS1(C7)

Sum of electronic and thermal Free Energies= -2960.501874

C	3.63949500	-1.24800600	-0.70715900
C	3.69716200	-0.39887000	0.48509000
C	3.16069400	-1.15072200	1.59541900
C	2.62476300	-2.37387400	1.06752900
C	2.98507500	-2.45101100	-0.35239000
C	2.66289900	-3.60996800	-1.23893900
H	2.84562100	-3.38290200	-2.28986200
H	3.28417200	-4.47115400	-0.96435900
H	1.61594300	-3.90603500	-1.13359600
C	4.17244900	-0.86753100	-2.05219800
H	3.75125800	-1.48653700	-2.84560600
H	3.95233100	0.17686900	-2.28774400

H	5.26253800	-0.98740900	-2.07296800
C	4.40669100	0.91599700	0.57400100
H	4.02427100	1.52700900	1.39400000
H	5.47747200	0.75193800	0.74985900
H	4.31124300	1.48504900	-0.35323700
C	3.23411400	-0.74994400	3.03391400
H	2.48215200	-1.25562600	3.63994200
H	4.22086600	-1.02862800	3.42555500
H	3.11437600	0.32634600	3.16782000
C	1.98755400	-3.48328200	1.84475700
H	2.74117300	-4.23111700	2.12199000
H	1.52715500	-3.11920600	2.76530900
H	1.21908700	-3.98953500	1.25615100
Rh	1.58966000	-0.71603300	0.08609100
C	0.55992700	1.89310800	1.18943800
C	0.49366300	2.83075900	2.24353200
C	0.21314500	2.38333900	3.53955900
C	-0.01667700	1.02143700	3.75592400
C	0.04888800	0.11570500	2.69536100
C	0.33301500	0.50852800	1.36100800
C	0.87163600	3.99224200	0.34468700
C	0.71346900	4.14226700	1.67911100
H	0.15154900	3.09023300	4.36161200
H	-0.26093000	0.67004200	4.75356400
H	-0.16355000	-0.93304100	2.88629700
H	-0.70135600	0.08370500	0.58476600
N	0.79379500	2.61861500	-0.00192200
C	0.88908800	2.04791000	-1.25764200
O	1.10019600	0.82342600	-1.35921400
H	0.73984300	5.08099800	2.21417000
H	1.06655600	4.73749400	-0.40381600
C	0.74354700	2.86995600	-2.55439100
C	2.04338800	3.68388000	-2.79558400
H	1.95356200	4.20462300	-3.75310100
H	2.24366900	4.43713500	-2.03072200
H	2.91505300	3.02416300	-2.85905100
C	-0.50306400	3.78800200	-2.51846600
H	-0.42369000	4.61438600	-1.81172100
H	-0.63789600	4.22134500	-3.51328900
H	-1.40483700	3.22458600	-2.26788100
C	0.57692200	1.87750800	-3.72685900
H	0.46456400	2.44865100	-4.65215000
H	1.44473200	1.22319900	-3.83189800
H	-0.30714000	1.24792100	-3.60169700
N	-1.77175800	-0.24217500	-0.13905700
S	-1.45939800	-1.43616900	-1.21006300
O	-1.67268900	-1.12756200	-2.61376400
O	-0.11898800	-1.93656700	-0.76610600
S	-3.02736100	0.87366700	-0.28413000
O	-2.44454500	2.18750300	-0.02311300
O	-3.86685500	0.60651900	-1.44103600
C	-2.60225700	-2.85922200	-0.75333800
C	-4.00777700	0.42254400	1.24709500
F	-3.85213300	-2.52607300	-1.03655200
F	-2.23163300	-3.92337700	-1.45723700
F	-2.47853700	-3.11188700	0.54913600
F	-5.04018100	1.24930300	1.34320100
F	-3.22491200	0.54413100	2.32169100
F	-4.43420500	-0.83533100	1.14649900

TS2(C2)

Sum of electronic and thermal Free Energies= -1439.241489

C	2.19551500	0.19772100	2.04433100
C	1.02412900	-0.59848900	2.44254400
C	1.05877300	-1.82306800	1.73058100
C	2.19115700	-1.77048900	0.81792400
C	2.94550200	-0.56397000	1.11156800
C	4.30532100	-0.23983000	0.57970100
H	4.45900800	0.83566100	0.47185100
H	5.06183200	-0.61747000	1.27922700
H	4.48036500	-0.71746000	-0.38521400
C	2.57901100	1.51367300	2.64777300
H	3.28517800	2.05475700	2.01518600
H	1.70580800	2.15237500	2.80232800
H	3.05303700	1.35999200	3.62538300
C	0.04398700	-0.19100500	3.49873300
H	-0.89263900	-0.74652800	3.42040600
H	0.46155800	-0.38150100	4.49521800
H	-0.18409600	0.87633800	3.44083700
C	0.12343300	-2.98002100	1.89149400
H	-0.06843600	-3.48348800	0.94197300
H	0.56412300	-3.71786700	2.57310800
H	-0.83757900	-2.67421700	2.30917600
C	2.65777100	-2.87928800	-0.07493900
H	3.43896300	-3.46381000	0.42768800
H	1.84443800	-3.56529400	-0.32138900
H	3.07025300	-2.48737200	-1.00764500
Rh	0.87826900	-0.07154300	0.25379600

C	-3.22339100	-0.52296200	-0.57319800
C	-2.84761200	-1.82551500	-0.99598500
C	-3.81990000	-2.79822300	-1.26617700
C	-5.16071500	-2.47142100	-1.10498400
C	-5.52583700	-1.18816000	-0.67649200
C	-4.57282600	-0.20352000	-0.40438600
C	-0.89843600	-0.67327900	-0.68691900
C	-1.41516500	-1.87850700	-1.07104400
H	-3.52184500	-3.78919000	-1.59414300
H	-5.92908100	-3.20960600	-1.30986200
H	-6.57550100	-0.94182600	-0.55325600
H	-4.91219800	0.76806500	-0.08342500
N	-2.00769100	0.20834000	-0.37382000
C	-1.67202500	1.45496600	0.11083400
O	-0.46498000	1.63581600	0.40265800
H	-0.83417900	-2.71580000	-1.43386000
C	-2.63100600	2.64094700	0.27850700
C	-3.51884700	2.40108000	1.52951700
H	-4.25029800	3.21067200	1.60836600
H	-4.06086200	1.45589300	1.52194000
H	-2.90270100	2.42077700	2.43359100
C	-3.43683700	2.88258800	-1.02162200
H	-3.99646100	2.01857900	-1.37591700
H	-4.14668200	3.69771000	-0.85404200
H	-2.76460200	3.19530700	-1.82703700
C	-1.79727000	3.91427100	0.54601300
H	-2.48140900	4.75928700	0.66483200
H	-1.19946700	3.82645700	1.45485700
H	-1.12235500	4.13723400	-0.28406200
C	2.75038800	0.49346700	-2.14272700
O	3.07364600	-0.61514800	-2.53663300
O	3.57612100	1.55756800	-2.14344600
C	1.40265500	0.87536700	-1.64787400
C	0.29620600	0.07569900	-2.08889700
H	1.25039100	1.94066400	-1.50841700
H	-0.57162100	0.59899500	-2.47875000
H	0.55589000	-0.83259600	-2.62236700
C	4.86652100	1.35816600	-2.75877500
H	4.74615200	0.99142400	-3.78014400
H	5.34357400	2.33705500	-2.75420300
H	5.46187300	0.64076700	-2.18998000

TS2(C7)

Sum of electronic and thermal Free Energies= -1439.241541

C	-2.20325100	-1.55622500	1.33425400
C	-1.69782400	-0.48282600	2.09911200
C	-2.22353500	0.77388400	1.54094100
C	-3.07916500	0.44764000	0.45456400
C	-2.98835100	-0.98668200	0.24513000
C	-3.82010200	-1.77430900	-0.72234200
H	-3.39251600	-2.76023200	-0.91395200
H	-4.82540200	-1.92980100	-0.31036500
H	-3.93767300	-1.25870800	-1.67860700
C	-2.00620700	-3.01839100	1.58684800
H	-1.16649100	-3.20322000	2.25929100
H	-2.90470000	-3.44385800	2.05034400
H	-1.81822900	-3.56812200	0.66172400
C	-0.83251000	-0.56074400	3.31795600
H	-0.05962000	0.21228100	3.30529500
H	-1.43655100	-0.40217300	4.21997100
H	-0.34383100	-1.53226200	3.41073300
C	-1.99648200	2.13443800	2.12376900
H	-2.17272200	2.91744300	1.38367200
H	-2.67438800	2.30816100	2.96887000
H	-0.97370500	2.24313200	2.49248400
C	-3.94600600	1.39979100	-0.31275300
H	-4.86930700	1.58881600	0.24855800
H	-3.45163100	2.35883300	-0.48206000
H	-4.23648200	0.99203400	-1.28350300
Rh	-0.96018400	-0.14053000	-0.04658900
C	1.66071500	-1.68724100	-0.53709900
C	2.42032400	-2.87903500	-0.62162800
C	1.83710800	-4.06085100	-1.09062000
C	0.50339800	-4.02793500	-1.48741400
C	-0.21941900	-2.83015700	-1.44916200
C	0.32725000	-1.61957400	-0.97967700
C	3.80423400	-1.26483800	0.13996800
C	3.76367500	-2.57267800	-0.19223400
H	2.42031400	-4.97331100	-1.16087600
H	0.02678800	-4.92624800	-1.86757700
H	-1.23013100	-2.82260400	-1.84647300
N	2.52215800	-0.67510600	-0.02681400
C	2.11527600	0.55385300	0.46091300
O	0.90594000	0.83354800	0.51418900
H	4.59819200	-3.25852700	-0.15234100
H	4.63293900	-0.68538700	0.49777800
C	3.13068600	1.61513700	0.94614700
C	4.15694400	1.92756600	-0.17235900
H	4.79784400	2.74860800	0.16189000

H	4.80737500	1.09073700	-0.43056500
H	3.64006700	2.24981600	-1.08041800
C	3.81027600	1.17331200	2.26895100
H	4.44426700	0.29052300	2.18060300
H	4.43898500	1.99387300	2.62621600
H	3.06216300	0.97060200	3.04240800
C	2.35660500	2.91872600	1.23887400
H	3.06998200	3.68040100	1.56570400
H	1.84642000	3.27760400	0.34401600
H	1.61818500	2.78287500	2.03272000
C	-0.21457000	2.25302500	-1.81396500
O	0.98749200	2.43717500	-1.88811100
O	-1.11720200	3.24618700	-1.66229000
C	-0.89123100	0.93395900	-1.90961800
C	-0.11553400	-0.20784100	-2.30801100
H	-1.92482300	0.98923600	-2.23741300
H	-0.58159600	-0.89847500	-2.99944400
H	0.93262300	-0.00573400	-2.50808000
C	-0.58440500	4.58658000	-1.65526400
H	-1.45088800	5.24602100	-1.68284300
H	-0.00127600	4.76247900	-0.74801700
H	0.05176100	4.74798600	-2.52754600

TS3'(C7)

Sum of electronic and thermal Free Energies= -1439.152630

C	-1.93809900	-2.05491900	-1.53527500
C	-2.39690700	-1.90953300	-0.13511800
C	-3.22911800	-0.74270400	-0.03867100
C	-3.07039700	-0.04569200	-1.28767300
C	-2.36943300	-0.93107400	-2.24244800
C	-2.16010400	-0.61790600	-3.69084900
H	-1.40554100	-1.26440100	-4.14320400
H	-3.09460900	-0.75497000	-4.25001400
H	-1.84981400	0.42046900	-3.84009300
C	-1.17447100	-3.23289200	-2.05888500
H	-0.67759800	-3.00613000	-3.00437300
H	-0.41134900	-3.56728800	-1.35057100
H	-1.84708100	-4.08268400	-2.23162300
C	-2.23149300	-2.96366400	0.91365000
H	-2.33745700	-2.55478300	1.92067900
H	-2.99622800	-3.74158100	0.78668900
H	-1.25714000	-3.45242100	0.84126900
C	-4.11448000	-0.34422100	1.09970000
H	-4.09670300	0.73561700	1.26828400
H	-5.15324200	-0.62724600	0.88356400
H	-3.82657400	-0.84414800	2.02769200
C	-3.76322700	1.22999000	-1.66185300
H	-4.78789600	1.01538600	-1.99241600
H	-3.81511000	1.91618400	-0.81413100
H	-3.25609200	1.73639200	-2.48726700
Rh	-1.08448700	-0.18760800	-0.40072600
C	2.77260400	1.02351900	-0.58072600
C	3.78577600	1.21959500	-1.55117600
C	3.82449300	2.39287300	-2.31261000
C	2.85495400	3.36307200	-2.08771400
C	1.89631000	3.18956900	-1.08112200
C	1.84392700	2.03655100	-0.27664800
C	4.19141800	-0.77089800	-0.56268500
C	4.65551100	0.06896700	-1.51388800
H	4.60218900	2.54028300	-3.05512100
H	2.85690400	4.28027800	-2.66774200
H	1.18935200	3.98830500	-0.87659500
N	3.00919300	-0.24323800	0.02504200
C	2.10328300	-1.02866000	0.73303500
O	0.88021700	-0.88339500	0.58615200
H	5.52561800	-0.10005000	-2.13244900
H	4.55127100	-1.74447000	-0.28294700
C	2.61027000	-2.08957200	1.73861400
C	3.91145700	-1.66417200	2.45446500
H	4.14208400	-2.40120900	3.22882500
H	4.77962600	-1.59971400	1.79815500
H	3.79169300	-0.69403800	2.94652300
C	2.78210100	-3.45070000	1.01365100
H	3.58372000	-3.44977700	0.27147800
H	3.02216500	-4.21840100	1.75494100
H	1.85610500	-3.74623500	0.51091300
C	1.51145000	-2.25985900	2.81480300
H	1.84160800	-3.00747300	3.54105300
H	1.33101000	-1.32410200	3.35255700
H	0.56718700	-2.59113500	2.38136600
C	-1.56959000	2.30360900	1.60867900
O	-2.68440700	2.65665000	1.27756300
O	-1.10902000	2.29070300	2.86598400
C	-0.53221000	1.83602500	0.63566800
C	0.89927100	2.04208400	0.86115000
H	-0.82478600	1.92932700	-0.43213500
H	1.23708900	2.22231200	1.87671700
H	0.13073200	0.85404000	0.96653800

C	-2.02815900	2.75986900	3.88106900
H	-1.47275900	2.71469200	4.81611000
H	-2.33875800	3.78299000	3.66221900
H	-2.90721300	2.11379900	3.92200600

TS3(C2)

Sum of electronic and thermal Free Energies=-1439.249175

C	3.54460900	-0.67792100	-0.08823500
C	3.74473200	-1.46202400	-1.24978200
C	4.98383800	-2.05890200	-1.51988900
C	6.01672300	-1.89481600	-0.60845400
C	5.80311000	-1.15877400	0.56663000
C	4.57786900	-0.55458100	0.84658500
C	1.56594600	-0.82282400	-1.24536500
C	2.49389500	-1.53898600	-1.93701800
H	5.11790800	-2.65035900	-2.42015600
H	6.98498500	-2.34847700	-0.79237800
H	6.60808400	-1.05456500	1.28710300
H	4.47005100	-0.01300000	1.77108500
N	2.18026000	-0.23894200	-0.09054000
C	1.48183900	0.56569600	0.81197000
O	0.25123500	0.43038000	0.92996900
H	2.30075200	-2.07787300	-2.85505600
C	2.12971200	1.66422800	1.69180400
C	3.30035700	2.39263100	0.99401500
H	3.62125900	3.21895400	1.63540100
H	4.17393100	1.77721400	0.79619500
H	2.95995700	2.81263700	0.04473800
C	2.49185900	1.05700800	3.07529700
H	3.14586400	0.18591600	3.03265300
H	2.98774800	1.82095400	3.68132400
H	1.58076500	0.75173600	3.59878200
C	1.04651300	2.74181100	1.95520600
H	1.48067200	3.51780700	2.59188300
H	0.72180700	3.20275100	1.02039700
H	0.17602700	2.32830700	2.46568700
C	-2.75164100	-1.03409500	1.70542200
C	-2.98487700	-2.00413100	0.69616300
C	-3.42434600	-1.29468800	-0.49687500
C	-3.61732500	0.10748000	-0.14417200
C	-3.14977300	0.28024800	1.18041600
C	-3.14251900	1.54839500	1.97574100
H	-2.23598700	1.63601300	2.57967100
H	-3.99784500	1.56965000	2.66273500
H	-3.20954900	2.42814200	1.33317900
C	-2.29659300	-1.27995300	3.11083800
H	-1.59072200	-0.51335900	3.44046400
H	-1.81456200	-2.25357400	3.21626500
H	-3.15314400	-1.25403200	3.79601300
C	-2.85181600	-3.49199600	0.82892900
H	-2.56348500	-3.96118300	-0.11393100
H	-3.81451700	-3.92374800	1.12949300
H	-2.11444000	-3.76893600	1.58474200
C	-3.88213400	-1.94112800	-1.76999000
H	-3.77777600	-1.27134100	-2.62685100
H	-4.94263700	-2.21260100	-1.69559400
H	-3.32404000	-2.85579800	-1.98303200
C	-4.21057600	1.16318800	-1.02667600
H	-5.27745300	1.28069500	-0.79974000
H	-4.12822000	0.90347000	-2.08364100
H	-3.72695900	2.13157400	-0.88425900
Rh	-1.41560300	-0.53615600	-0.05126100
C	-0.68179100	0.38968700	-1.86816400
C	0.15582700	-0.76593500	-1.67845000
H	-0.03767800	-1.56230700	-2.39411600
H	-0.38909300	-1.68921500	-0.49271800
C	-0.21052000	1.78944100	-1.75455500
O	0.87479000	2.15722400	-1.33978100
O	-1.15455200	2.63352200	-2.22013600
C	-0.78982200	4.02895400	-2.24753300
H	-1.62681600	4.53907600	-2.72209500
H	-0.63654200	4.40577800	-1.23342000
H	0.12603400	4.17158100	-2.82456100
H	-1.48445600	0.27064700	-2.58932900

TS3(C7)

Sum of electronic and thermal Free Energies=-1439.244686

C	-2.20654200	1.67409700	-1.55773800
C	-2.56159600	0.39215900	-2.05195900
C	-3.06674600	-0.37200600	-0.92066600
C	-3.20033000	0.53834200	0.21850900
C	-2.62419100	1.76848300	-0.14907500
C	-2.58472700	3.01073600	0.68582800
H	-1.70525600	3.62022000	0.47104600
H	-3.46767600	3.62932600	0.47776100
H	-2.58780100	2.77830700	1.75293600
C	-1.63319500	2.81037300	-2.34564700
H	-0.91952400	3.38862400	-1.75384900

H	-1.12692600	2.46455000	-3.24868500
H	-2.43454200	3.49498000	-2.65137100
C	-2.48066800	-0.07927400	-3.47417600
H	-2.31600400	-1.15659000	-3.53811500
H	-3.42144700	0.14247400	-3.99296000
H	-1.67622100	0.41622100	-4.02124700
C	-3.65532400	-1.74792900	-0.99516300
H	-3.47077700	-2.31113100	-0.07853700
H	-4.74066600	-1.68408500	-1.14418800
H	-3.24122900	-2.31566000	-1.83098400
C	-3.86260400	0.22764600	1.52571700
H	-4.71854100	0.89620000	1.67203000
H	-4.23743300	-0.79670500	1.54774300
H	-3.18818300	0.35636700	2.37781600
Rh	-0.99953500	0.12204900	-0.44948200
C	2.80073800	-1.07431100	-0.37596800
C	4.08489800	-1.58196600	-0.71323300
C	4.26337600	-2.86440100	-1.23972400
C	3.14604100	-3.66397000	-1.42313100
C	1.89014000	-3.19321200	-1.03653500
C	1.66967000	-1.92028000	-0.47386100
C	4.41614000	0.48669300	0.10533200
C	5.06745600	-0.57997300	-0.39442400
H	5.25866700	-3.21606100	-1.49149300
H	3.24088800	-4.66161900	-1.83855800
H	1.03571400	-3.85460100	-1.14491000
N	3.01274000	0.25806300	0.11491800
C	2.09052700	1.29132800	0.25031000
O	0.94484000	1.17632600	-0.19725300
H	6.13629400	-0.66473000	-0.52953300
H	4.81676700	1.42778200	0.42527800
C	2.46913800	2.60952300	0.98494200
C	3.30916900	3.54219300	0.07128300
H	3.40790100	4.51397500	0.56366800
H	4.31674200	3.18285700	-0.14079100
H	2.80434500	3.70408200	-0.88629000
C	3.16413800	2.33399500	2.34133700
H	4.13367900	1.84280700	2.26178800
H	3.32093200	3.28741300	2.85405600
H	2.53063800	1.71535500	2.98521900
C	1.15122100	3.35482100	1.29027400
H	1.38255600	4.26818400	1.84500700
H	0.63226400	3.63550100	0.37193700
H	0.47448100	2.74853400	1.89764300
C	-1.10509100	-1.54307100	2.16665500
O	-1.31690500	-1.01486700	3.24143000
O	-1.72697500	-2.67482200	1.75779500
C	-0.11417100	-1.01604000	1.19437000
C	0.27763900	-1.73325500	0.02299200
H	0.59515700	-0.36226800	1.68718000
H	-0.33580300	-2.60674300	-0.17422000
H	-0.19668300	-0.92579500	-1.33539700
C	-2.58083400	-3.29853200	2.74207400
H	-2.96724300	-4.19825100	2.26499300
H	-2.00316800	-3.55391700	3.63265000
H	-3.39530700	-2.63037300	3.02891900

TS-R1

Sum of electronic and thermal Free Energies=-634.189111

C	-1.08965600	-0.06034200	0.15423600
C	-2.13316500	0.85906100	-0.14731500
C	-3.44274500	0.37464100	-0.30996200
C	-3.68628400	-0.98286400	-0.14985200
C	-2.64344500	-1.87235200	0.17863200
C	-1.33625600	-1.42630000	0.33772200
C	-0.21053000	2.01745900	0.07273700
C	-1.54205300	2.16676000	-0.19446300
H	-4.25298400	1.05852400	-0.54722900
H	-4.69514600	-1.36710800	-0.26826600
H	-2.86435000	-2.92663500	0.31693800
H	-0.54421800	-2.11545500	0.61112100
N	0.09516700	0.66814000	0.24559900
C	1.38683000	0.19852500	0.73379800
O	1.66010400	0.33158100	1.90135400
H	-2.04515100	3.10137200	-0.39838100
H	0.57175600	2.75869700	0.14913700
C	2.36890500	-0.33749900	-0.31700300
C	2.79090500	0.87205300	-1.19161800
H	3.52780100	0.54041600	-1.93024900
H	1.93973200	1.29763300	-1.72972600
H	3.25375200	1.65936200	-0.58730800
C	1.72339300	-1.40802800	-1.22034300
H	0.82344400	-1.03787400	-1.71657000
H	2.44116000	-1.70203700	-1.99302700
H	1.46054000	-2.30765900	-0.65569400
C	3.59883600	-0.91656700	0.40061100
H	4.32449800	-1.27246600	-0.33756700
H	4.08169300	-0.16605800	1.03072100

H	3.32205500	-1.75760800	1.04299300

1a^{OAc}

Sum of electronic and thermal Free Energies=-1361.926908

C	-3.28276100	0.59045300	-0.69013400
C	-2.52556500	-0.02779900	-1.73202600
C	-2.26452100	-1.40521600	-1.35496200
C	-2.91765700	-1.64861100	-0.09071000
C	-3.50938200	-0.40715300	0.35058000
C	-4.32635800	-0.19491000	1.58519000
H	-4.15044100	0.79390200	2.01430800
H	-5.39329300	-0.27027600	1.34073800
H	-4.10634200	-0.94195400	2.34947400
C	-3.81004900	1.98966100	-0.66495300
H	-3.23266800	2.65561900	-1.30770300
H	-4.84832700	1.99822900	-1.01985000
H	-3.80487900	2.40271100	0.34637900
C	-2.06345100	0.60081100	-3.00716400
H	-1.00817700	0.38602400	-3.19521100
H	-2.64016200	0.19339100	-3.84625900
H	-2.19967900	1.68262400	-3.00224100
C	-1.55891400	-2.41953100	-2.19971400
H	-1.11004900	-3.20814200	-1.59240600
H	-2.26945600	-2.89468400	-2.88775600
H	-0.77046000	-1.96243200	-2.80140600
C	-2.94912800	-2.94941600	0.64311000
H	-3.82441000	-3.52785700	0.32155600
H	-2.05895800	-3.54749400	0.43985800
H	-3.01946900	-2.80384000	1.72223700
C	-0.27222100	0.04682000	2.46950400
O	-0.28551800	-1.03973200	1.79866100
O	-0.87743500	1.05485200	1.97216000
C	0.45841700	0.13308300	3.77707000
H	0.12445800	1.00122400	4.34653100
H	0.30581600	-0.78350200	4.35106100
H	1.53230000	0.22507200	3.58246200
Rh	-1.38239200	-0.12736800	0.18127100
C	3.07675700	-0.78019800	-0.30629900
C	4.46219300	-0.96269300	-0.09194900
C	5.01710200	-2.24551100	-0.11154300
C	4.17915900	-3.33225800	-0.34779300
C	2.80782400	-3.13864500	-0.56112100
C	2.23309800	-1.86526400	-0.54548900
C	4.06440900	1.26204500	0.03030400
C	5.04749800	0.34158700	0.11944100
H	6.08081600	-2.38624200	0.05299000
H	4.58950700	-4.33685600	-0.36729300
H	2.17094300	-3.99925600	-0.74211900
H	1.17540600	-1.73374100	-0.70409800
N	2.81657800	0.62721000	-0.23153600
C	1.58805100	1.22249200	-0.40185700
O	0.61044100	0.47727100	-0.62526400
H	6.08861100	0.55522000	0.31797800
H	4.13056500	2.32666900	0.14281200
C	1.43341600	2.76355300	-0.38040000
C	2.27757100	3.40950400	-1.51187200
H	2.09019200	4.48726900	-1.51616500
H	3.35265900	3.26271000	-1.41472700
H	1.97803000	3.01665100	-2.48893300
C	1.77562300	3.34190200	1.01719100
H	2.80487600	3.17201100	1.33450900
H	1.61071600	4.42344600	1.00053200
H	1.11071100	2.91354500	1.77240300
C	-0.04017000	3.11539900	-0.66708600
H	-0.13921700	4.20430600	-0.69494600
H	-0.36292700	2.72112400	-1.63373100
H	-0.70064800	2.73585200	0.11420100

1c^{OAc}

Sum of electronic and thermal Free Energies=-1361.922656

C	2.92523500	-0.52972100	-1.65179000
C	2.98186600	0.88655400	-1.33102800
C	3.49202300	1.02900600	-0.00386100
C	3.76474400	-0.30629600	0.51678100
C	3.45669000	-1.25820800	-0.52636700
C	3.63422700	-2.73881500	-0.43748500
H	2.94367900	-3.26926800	-1.09521700
H	4.65587500	-3.00113600	-0.73996200
H	3.48126800	-3.10190200	0.58041600
C	2.49996200	-1.10752500	-2.96522500
H	1.70946900	-0.51169600	-3.42644300
H	3.34906900	-1.12991800	-3.65976400
H	2.13452800	-2.13068400	-2.85593700
C	2.56510000	1.98374600	-2.25621200
H	2.43740500	2.93164900	-1.73242400
H	3.33228800	2.12527200	-3.02723400
H	1.62700300	1.74134100	-2.76119500
C	3.73998300	2.30425400	0.73622000

H	3.50151200	2.20241500	1.79752600
H	4.79999400	2.57665200	0.65900600
H	3.15250400	3.13032300	0.33278600
C	4.38620100	-0.61169600	1.84248500
H	5.47785000	-0.52946000	1.76758800
H	4.05030600	0.08598600	2.61227600
H	4.15082800	-1.62446000	2.17453600
C	0.26434700	-1.13236800	2.01463200
O	0.72776500	0.05427700	2.07917200
O	0.55677500	-1.82660600	0.98095900
C	-0.61497800	-1.69728400	3.09079600
H	-0.27802500	-2.70333400	3.35305000
H	-0.60774900	-1.05419300	3.97119400
H	-1.63810300	-1.78453300	2.71084300
Rh	1.65894700	-0.19501500	0.09641600
C	-3.85157100	-0.18033600	-0.31834900
C	-4.27763700	-1.46976500	-0.72786500
C	-5.62264500	-1.84091900	-0.65302700
C	-6.54975400	-0.92347100	-0.16859400
C	-6.12955500	0.34819000	0.23516900
C	-4.78865900	0.73643200	0.16803700
C	-2.04398200	-1.40319900	-1.05071700
C	-3.11850600	-2.20390500	-1.17803200
H	-5.93070100	-2.83214300	-0.97094400
H	-7.59912000	-1.19202100	-0.10341900
H	-6.85611000	1.06070100	0.61237700
H	-4.52980800	1.72965100	0.49506300
N	-2.42419000	-0.13300200	-0.52205400
C	-1.43418000	0.82207900	-0.35639800
O	-0.28328300	0.51073700	-0.73808800
H	-3.10909000	-3.21966000	-1.54815500
H	-1.00665900	-1.58445900	-1.26103400
C	-1.68690700	2.22224700	0.22486700
C	-2.20312800	2.10810100	1.68433200
H	-2.46246800	3.10524500	2.05299600
H	-3.07462600	1.46759100	1.80737600
H	-1.40594800	1.70973000	2.31806000
C	-2.61261300	3.02363800	-0.73183000
H	-3.51912000	2.50073400	-1.03045300
H	-2.90352600	3.96250100	-0.25083900
H	-2.06716100	3.27483600	-1.64670000
C	-0.34849600	2.98767000	0.28872600
H	-0.53987700	3.98964800	0.68443000
H	0.36453400	2.49034500	0.94961900
H	0.10002400	3.09322800	-0.70168000

2(C2)^{OAc}

Sum of electronic and thermal Free Energies=-1361.926132

C	2.07928200	0.40940400	-1.96412000
C	2.94835600	1.13698100	-1.02465400
C	3.50187100	0.20510800	-0.13520000
C	3.00769200	-1.13101100	-0.50903700
C	2.23033400	-1.00462300	-1.70369700
C	1.71011900	-2.11810000	-2.55829300
H	0.75487500	-1.86489700	-3.02111700
H	2.42881900	-2.32460600	-3.36097600
H	1.58059500	-3.04180800	-1.99049800
C	1.40472500	1.02461000	-3.15150300
H	0.99729400	2.00959600	-2.91129500
H	2.12438700	1.15566200	-3.96956700
H	0.59032800	0.39837800	-3.52109300
C	3.13037800	2.62281400	-1.03455400
H	3.65350600	2.97544200	-0.14447800
H	3.71397100	2.92615000	-1.91189900
H	2.16751600	3.13960000	-1.08640100
C	4.40229100	0.46456000	1.03211300
H	3.97175900	0.06268400	1.95446500
H	5.37457700	-0.01832700	0.88079900
H	4.57610400	1.53128800	1.18057300
C	3.45112700	-2.40539300	0.14139400
H	4.44008500	-2.69724100	-0.23403300
H	3.53394600	-2.29119000	1.22496400
H	2.76298000	-3.22780000	-0.06466100
C	0.58944200	-0.99830600	2.96674900
O	-0.33877500	-1.84873600	2.57355100
O	1.19288400	-0.23540200	2.20078100
C	0.85569700	-1.02930900	4.44332900
H	1.66449800	-0.34516000	4.69439100
H	-0.05408900	-0.74542000	4.98110400
H	1.10717000	-2.04828400	4.75115600
Rh	1.18268800	0.01322900	-0.03781100
C	-2.97506100	-0.56461000	-0.37774600
C	-2.62333400	-1.91323800	-0.63149300
C	-3.60672300	-2.87111100	-0.89701300
C	-4.94188600	-2.47951700	-0.91219100
C	-5.28596900	-1.14600300	-0.66343900
C	-4.31722300	-0.17558200	-0.39405600
C	-0.64740000	-0.80485800	-0.28166700

C	-1.18207900	-2.02480300	-0.56228400
H	-3.32600900	-3.90217200	-1.08896600
H	-5.71960200	-3.20795700	-1.11730300
H	-6.32930500	-0.84778000	-0.67795400
H	-4.64066500	0.83637300	-0.21036100
N	-1.74320500	0.13663500	-0.14718300
C	-1.37751100	1.42214000	0.16891100
O	-0.14351200	1.63999100	0.28676200
H	-0.62009400	-2.93386400	-0.73052700
H	-0.48675100	-1.76399100	1.60028000
C	-2.32581900	2.60538500	0.39027500
C	-3.25503000	2.31387500	1.59703800
H	-3.98121700	3.12634900	1.69371800
H	-3.80485300	1.37657000	1.52624800
H	-2.66795800	2.28430800	2.52022600
C	-3.08512000	2.91566000	-0.92643000
H	-3.60719600	2.06242500	-1.35681500
H	-3.81948200	3.70442400	-0.73832900
H	-2.38560200	3.28829200	-1.68109000
C	-1.49126100	3.85540600	0.74549800
H	-2.17392300	4.69437900	0.90848900
H	-0.90613100	3.70699000	1.65557100
H	-0.80420600	4.12613300	-0.05916600

2(C7)^{OAc}

Sum of electronic and thermal Free Energies=-1361.925842

C	3.00002600	-1.21748300	0.11300400
C	2.18311200	-1.96596800	-0.73744100
C	1.70240300	-1.06983900	-1.80481500
C	2.37849800	0.19547900	-1.66573700
C	3.06909500	0.16194400	-0.41161500
C	3.96079100	1.22687500	0.15081700
H	3.94874100	1.22174500	1.24350500
H	4.99782300	1.05841100	-0.16652000
H	3.67258800	2.22374500	-0.18948000
C	3.66785300	-1.65654900	1.37826800
H	3.45754800	-2.70246600	1.60681200
H	4.75470500	-1.53953700	1.29935700
H	3.32961500	-1.05229300	2.22635000
C	1.78672500	-3.40382000	-0.61209600
H	0.70105900	-3.52014700	-0.67817200
H	2.23055000	-3.99516700	-1.42170700
H	2.11189400	-3.83444900	0.33618100
C	0.89729000	-1.51525800	-2.98680300
H	0.39870000	-0.67598700	-3.47585300
H	1.54899500	-1.99542600	-3.72808900
H	0.13775200	-2.24574600	-2.69794400
C	2.39876600	1.29114000	-2.68534100
H	3.14628500	1.05190300	-3.45204200
H	1.43402700	1.40628200	-3.18328700
H	2.67238500	2.25385100	-2.25182500
C	0.47351100	1.07012700	2.99681600
O	0.87191300	0.18554600	2.23065500
O	-0.09105400	2.19374200	2.59285600
C	0.59515000	0.96076400	4.48907200
H	-0.39272700	1.06795500	4.94623000
H	1.03433300	0.00256200	4.76164800
H	1.21464200	1.78044800	4.86559800
Rh	0.92475200	-0.12466400	-0.01331500
C	-1.64259400	1.38776100	-0.54306000
C	-2.46449000	2.48819800	-0.89036100
C	-1.90343100	3.75536400	-1.07790500
C	-0.53092900	3.89627600	-0.90994900
C	0.27127900	2.78635000	-0.59040300
C	-0.25021900	1.49028000	-0.40876500
C	-3.82816200	0.69969600	-0.65627600
C	-3.82648000	2.01503000	-0.96233700
H	-2.52826900	4.60411900	-1.33652400
H	-0.06606000	4.86999900	-1.03178700
H	1.33961800	2.94432800	-0.47996400
H	-0.13016600	2.21406900	1.60990400
N	-2.50704900	0.26003700	-0.37820400
C	-2.10831600	-0.98216200	0.04946600
O	-0.90366600	-1.20727300	0.28098400
H	-4.69893900	2.60226200	-1.21286600
H	-4.65855300	0.02178000	-0.60817000
C	-3.10960700	-2.13976200	0.28044600
C	-3.82098000	-2.52937600	-1.04049300
H	-4.44695800	-3.40714500	-0.85603100
H	-4.46283700	-1.75040800	-1.45302700
H	-3.09057700	-2.80061200	-1.80952900
C	-4.11881200	-1.77289500	1.39934600
H	-4.76681400	-0.92935500	1.16059200
H	-4.76054400	-2.63795000	1.58992900
H	-3.59452000	-1.53873100	2.33123200
C	-2.31780900	-3.37400900	0.76254900
H	-3.02130700	-4.18879200	0.95407200
H	-1.60302300	-3.71518700	0.01015600

H	-1.76803500	-3.16956800	1.68358900

TS1(C2)^{OAc}

Sum of electronic and thermal Free Energies=-1361.904371

C	-1.39757800	-1.94167300	1.15443800
C	-1.80951400	-0.85895100	1.99495400
C	-2.94549800	-0.19911500	1.37905700
C	-3.26272000	-0.91929100	0.17275000
C	-2.29224100	-1.96880400	0.00338400
C	-2.30713300	-3.01380500	-1.06939000
H	-1.31860500	-3.45091900	-1.21920200
H	-2.98861900	-3.82617100	-0.78716900
H	-2.65070600	-2.61065600	-2.02437500
C	-0.34367400	-2.95897300	1.46832000
H	0.44227500	-2.54752400	2.10493500
H	-0.79202000	-3.80594100	2.00225700
H	0.12683300	-3.34792300	0.56405500
C	-1.19807700	-0.46077500	3.29996900
H	-1.16767600	0.62578900	3.41060900
H	-1.80168600	-0.85939500	4.12483800
H	-0.18469500	-0.84983700	3.41284900
C	-3.72815600	0.94344800	1.94755800
H	-4.17521300	1.54759100	1.15540200
H	-4.54025700	0.56983100	2.58415600
H	-3.10247000	1.59738300	2.55888900
C	-4.38872300	-0.58199000	-0.75075900
H	-5.34604500	-0.73834100	-0.24068800
H	-4.33321800	0.46605800	-1.05849700
H	-4.37865000	-1.20238800	-1.64793600
C	-1.30165900	1.85234000	-2.36170800
O	-0.13728700	1.48216900	-2.66795400
O	-1.96987200	1.39006300	-1.37134800
C	-1.98607900	2.89088200	-3.22396200
H	-2.86405400	3.29970900	-2.72411800
H	-1.27928900	3.68615900	-3.46968700
H	-2.29193400	2.42063500	-4.16423000
Rh	-1.22853000	-0.04522600	-0.00598800
C	2.89084600	-0.63552600	-0.27753000
C	2.57547400	-1.71909200	-1.14629800
C	3.52290900	-2.72100400	-1.41993300
C	4.76517800	-2.64956400	-0.80998200
C	5.06102200	-1.59150000	0.06775200
C	4.14191000	-0.58171900	0.34761600
C	0.69671700	-0.40316000	-1.03058400
C	1.23245000	-1.54139100	-1.59479300
H	3.27571100	-3.53411000	-2.09536000
H	5.51367100	-3.41040700	-1.00445500
H	6.03574200	-1.55223700	0.54370300
H	4.42225300	0.20906500	1.02596800
N	1.73946200	0.18265500	-0.20641200
C	1.37530000	1.32587800	0.48663900
O	0.14866000	1.49904400	0.66310500
H	0.72655900	-2.15794700	-2.32690800
H	0.21119500	0.42888400	-1.81504800
C	2.33593000	2.41262300	0.98751100
C	3.45900700	2.69039800	-0.03646200
H	4.09212200	3.49623400	0.34577800
H	4.10046500	1.83496900	-0.24191600
H	3.03353000	3.02508200	-0.98728400
C	2.87363000	2.00403800	2.38536800
H	3.37797100	1.03682900	2.40355500
H	3.58649300	2.76048800	2.72598900
H	2.05445400	1.96514000	3.10962300
C	1.52701200	3.71925700	1.16447300
H	2.20159300	4.50022000	1.52642200
H	1.09609200	4.05302600	0.21693200
H	0.71578300	3.60188100	1.88448700

TS1(C7)^{OAc}

Sum of electronic and thermal Free Energies=-1361.904553

C	2.95259400	-0.91430500	-0.81523200
C	1.95332500	-1.08785300	-1.81343700
C	1.39513300	0.22783700	-2.12875000
C	2.07582900	1.20145300	-1.33771700
C	2.98118600	0.49540700	-0.44993300
C	3.95776800	1.10895500	0.50532700
H	4.15508600	0.44207200	1.34754500
H	4.91282300	1.30053000	-0.00010600
H	3.59645700	2.06037200	0.90088700
C	3.78747600	-1.97243300	-0.16768200
H	3.63815900	-2.94703600	-0.63429300
H	4.84946300	-1.71670400	-0.24654200
H	3.53390800	-2.06135500	0.89385700
C	1.54761200	-2.36711900	-2.47484500
H	0.46184500	-2.42753600	-2.58714000
H	1.98767600	-2.43160700	-3.47753100
H	1.87441900	-3.23831900	-1.90525400
C	0.39855700	0.50640000	-3.21134400

H	-0.16590400	1.42062800	-3.01592100
H	0.91425500	0.63342500	-4.17158600
H	-0.30960100	-0.31703200	-3.33001700
C	1.92402800	2.68473300	-1.45558500
H	2.52929900	3.04097900	-2.29866100
H	0.88805400	2.97542700	-1.64215400
H	2.26367400	3.20189200	-0.55846900
C	0.54269100	-1.37519000	2.75961500
O	1.30337900	-1.42133700	1.73430800
O	-0.40847800	-0.55371600	2.89105900
C	0.83059700	-2.33999400	3.88705700
H	-0.10549800	-2.67058400	4.34055900
H	1.41016300	-3.19249700	3.53245200
H	1.40588500	-1.81586100	4.65773800
Rh	0.98773800	-0.22440900	0.00982200
C	-1.45775900	1.54543200	0.38740200
C	-2.03495300	2.82647500	0.24793200
C	-1.36248700	3.94013600	0.76853000
C	-0.15178300	3.74955100	1.43713200
C	0.38733800	2.46655400	1.57894100
C	-0.24050300	1.31001800	1.05868100
C	-3.49486200	1.33889000	-0.62488100
C	-3.31036800	2.66223400	-0.41026900
H	-1.79272100	4.93292800	0.67659400
H	0.36265200	4.60262600	1.86867500
H	1.30733500	2.34219800	2.14398800
H	-0.27503200	0.34676900	1.90039300
N	-2.37093900	0.60966800	-0.15839000
C	-2.14211800	-0.75539700	-0.24502300
O	-0.98660500	-1.19649300	-0.13438700
H	-4.00575700	3.44495800	-0.67908900
H	-4.31710400	0.83772000	-1.10115200
C	-3.29577600	-1.76037300	-0.45157800
C	-3.77162200	-1.73366600	-1.92818900
H	-4.51694300	-2.52167500	-2.06881200
H	-4.23249700	-0.79188300	-2.23194500
H	-2.94060300	-1.93922500	-2.61066100
C	-4.45842900	-1.48406000	0.53157800
H	-4.96573600	-0.53345000	0.36296700
H	-5.20313100	-2.27786800	0.42483600
H	-4.10471300	-1.49692200	1.56702400
C	-2.74781600	-3.17428800	-0.15834200
H	-3.55637700	-3.89842300	-0.28965400
H	-1.93276700	-3.44330300	-0.83294500
H	-2.37871000	-3.25454900	0.86701300

1a^{F}

Sum of electronic and thermal Free Energies=-3297.565056

C	-1.35156300	-2.46752300	2.42082700
C	-0.12333000	-1.80608900	2.77063200
C	-0.40383900	-0.40374000	2.98718300
C	-1.82721900	-0.19958100	2.78342000
C	-2.41326700	-1.47170700	2.44338600
C	-3.85824700	-1.74832900	2.19513300
H	-3.99402000	-2.56254700	1.48083300
H	-4.33247400	-2.04727700	3.13905900
H	-4.38098100	-0.87018000	1.81725100
C	-1.54363000	-3.93199300	2.19090500
H	-0.61487300	-4.42089300	1.89438900
H	-1.88845600	-4.40589000	3.11882700
H	-2.29436000	-4.12655100	1.42185300
C	1.21336400	-2.45660100	2.90813100
H	2.03179900	-1.75226100	2.75524400
H	1.30774900	-2.85791000	3.92573300
H	1.33313900	-3.28983200	2.21319400
C	0.54293600	0.63913900	3.47590500
H	0.43907100	1.56848500	2.91423500
H	0.31514800	0.84709500	4.53006400
H	1.58189400	0.32272800	3.41287700
C	-2.53588400	1.10089500	2.97638900
H	-2.70125200	1.26486200	4.04884400
H	-1.93986000	1.93325300	2.59693900
H	-3.50476000	1.11640600	2.47806300
Rh	-0.97432600	-0.91500700	0.92334000
C	3.13283600	-0.32774300	-1.28459600
C	4.14840100	0.14752300	-2.14694300
C	5.18014800	0.94241600	-1.63920700
C	5.19662500	1.23648700	-0.27930100
C	4.19055900	0.74138500	0.56293000
C	3.14089400	-0.04165700	0.07368900
C	2.77289000	-1.15223400	-3.38327500
C	3.87504100	-0.37458200	-3.46494800
H	5.96386200	1.31180300	-2.29237800
H	5.99295000	1.84129400	0.13860000
H	2.36215300	-0.39399000	0.72912200
N	2.27028600	-1.15905400	-2.05565500
C	1.16436000	-1.83238000	-1.57914700
O	0.70054700	-1.47461300	-0.47642300

H	4.43727900	-0.17670100	-4.36655300
H	2.25480900	-1.67060000	-4.16801900
C	0.60729000	-3.06253000	-2.33804400
C	1.75668000	-4.04129200	-2.69243300
H	1.32255500	-4.94489600	-3.12961100
H	2.47423100	-3.64150500	-3.40875900
H	2.31078800	-4.33942500	-1.79628200
C	-0.19312300	-2.64980000	-3.60132100
H	0.41260000	-2.17419800	-4.37373100
H	-0.62972600	-3.55153700	-4.04100300
H	-1.00615800	-1.96565000	-3.35198400
C	-0.35780000	-3.81360300	-1.39744000
H	-0.70965200	-4.71564600	-1.90565700
H	0.14599900	-4.12208100	-0.47682400
H	-1.22747400	-3.20747800	-1.14340900
N	-1.31715400	0.91563600	-0.32655400
S	-2.26762000	0.22082400	-1.46485200
O	-1.93950500	0.39361500	-2.87088200
O	-2.40224200	-1.16799200	-0.89704900
S	-0.10539100	2.05167700	-0.61792800
O	0.67017200	2.06064000	0.62059400
O	0.51984400	1.90398300	-1.92405600
C	-3.98074600	0.95588100	-1.22133100
C	-1.04706800	3.67394700	-0.63577500
F	-3.98519400	2.22605600	-1.59651800
F	-4.83289300	0.25083600	-1.95227000
F	-4.32278600	0.87086100	0.07282600
F	-0.16457000	4.66261000	-0.61334800
F	-1.83297100	3.74295600	0.44330800
F	-1.79103800	3.74561200	-1.73614900
C	4.19326000	1.08385900	2.02592400
F	5.39393700	1.49398200	2.46182700
F	3.83887500	-0.00101700	2.78760500
F	3.29786100	2.05081300	2.32906200

1c^{F}

Sum of electronic and thermal Free Energies=-3297.556705

C	2.47440600	2.05184300	-2.05879800
C	2.03655800	3.15822200	-1.21954600
C	2.82788700	3.15512800	-0.02961600
C	3.78675200	2.05621900	-0.12751400
C	3.59946300	1.41668500	-1.40509500
C	4.41074000	0.29874300	-1.96684000
H	3.79674600	-0.38316200	-2.55622100
H	5.18300500	0.71970900	-2.62391500
H	4.91002300	-0.27336000	-1.18447600
C	1.95265500	1.72606600	-3.42000900
H	0.90962000	2.02866200	-3.53008700
H	2.53867800	2.26509400	-4.17573100
H	2.02284900	0.65754400	-3.62624900
C	0.94921600	4.11787700	-1.57643200
H	0.59577500	4.67808900	-0.71022900
H	1.33177400	4.83910200	-2.30948400
H	0.09757700	3.60642200	-2.03047600
C	2.73380000	4.10314900	1.12111300
H	2.86799700	3.58699100	2.07470500
H	3.52570600	4.85832200	1.03844300
H	1.77544400	4.62289100	1.14570600
C	4.85184300	1.75061600	0.87506900
H	5.72666000	2.38481700	0.68299700
H	4.51201000	1.95100200	1.89308100
H	5.17269200	0.70999500	0.82152300
Rh	1.79844700	1.21750900	-0.17945700
C	-3.83403500	-0.11452800	-0.82823600
C	-4.07334500	-0.87630500	-2.00106200
C	-5.32904300	-1.43866200	-2.24698400
C	-6.34937800	-1.24803500	-1.32396900
C	-6.10632500	-0.50422200	-0.16277700
C	-4.85774500	0.06577800	0.10171300
C	-1.90892900	-0.24907700	-2.07351300
C	-2.84682100	-0.93284600	-2.75659400
H	-5.49682500	-2.02419900	-3.14506900
H	-7.32924000	-1.68172400	-1.48808500
H	-4.74229100	0.61181900	1.02190000
N	-2.45490500	0.29579100	-0.87491000
C	-1.62034800	1.03997400	-0.05242300
O	-0.41910600	1.08963300	-0.39632000
H	-2.69641500	-1.44275600	-3.69759900
H	-0.87086800	-0.08565600	-2.29847700
C	-2.12165000	1.81017400	1.17976700
C	-2.50048200	0.79757200	2.29745800
H	-2.97865700	1.33510500	3.12190600
H	-3.16983200	0.00133400	1.97762100
H	-1.59752200	0.31721900	2.68273500
C	-3.25909300	2.78726900	0.77515700
H	-4.06721100	2.34282100	0.19955700
H	-3.69143500	3.22698600	1.67879600
H	-2.84631300	3.60539500	0.17597100

C	-0.98371300	2.68738800	1.74214600
H	-1.37460900	3.25275700	2.59332700
H	-0.14061100	2.09180100	2.09148300
H	-0.63156100	3.40776400	0.99825100
N	1.80493500	-0.97421300	0.12840400
S	1.24308000	-2.07158900	-1.01138300
O	0.01390700	-2.74342500	-0.62123600
O	1.37304900	-1.36808100	-2.29073000
S	1.44280000	-0.97489800	1.73476900
O	1.54080100	0.50474500	2.00350300
O	0.28209100	-1.71532600	2.19918100
C	2.59597300	-3.36773800	-1.00270600
C	2.94646700	-1.68419500	2.63245100
F	2.69716200	-3.87973800	0.22430800
F	2.27707300	-4.31518200	-1.87122500
F	3.75925400	-2.80885800	-1.34743500
F	3.00248900	-1.10831000	3.82665900
F	4.05337700	-1.39748400	1.93976300
F	2.81567700	-2.99366600	2.75617900
C	-7.23373000	-0.24959900	0.80628400
F	-7.93836600	0.85051200	0.45927700
F	-6.77522000	-0.04301100	2.06235800
F	-8.09814300	-1.28106800	0.84740000

2(C2)^{F}

Sum of electronic and thermal Free Energies=-3297.544678

C	2.87685100	1.01688900	0.48894100
C	2.25669600	2.04701300	-0.27580300
C	3.04407500	3.02057800	-0.91925400
C	4.42195400	2.93586200	-0.82389900
C	5.01988400	1.88114700	-0.10361600
C	4.26825700	0.90925300	0.55129300
C	0.60672500	0.70420900	0.50952900
C	0.84342900	1.84655100	-0.22138800
H	2.57203600	3.82240100	-1.47769500
H	5.05279200	3.67753600	-1.30085500
H	4.77571900	0.12506800	1.09264500
N	1.85082100	0.20131400	1.00191700
C	1.84028800	-1.07588400	1.57627600
O	0.98583700	-1.86612700	1.13661700
H	0.06182800	2.49566500	-0.60125900
H	-0.30904300	0.48757000	1.04738800
C	2.72231100	-1.49296600	2.75733800
C	3.22048100	-0.28708700	3.57869300
H	3.76424000	-0.66034200	4.45058600
H	3.89595200	0.37152400	3.03269800
H	2.38258100	0.31354500	3.94461800
C	3.89588200	-2.35663000	2.22390600
H	4.55782900	-1.81749400	1.54167700
H	4.49972800	-2.69106100	3.07193800
H	3.51910300	-3.24342400	1.70636600
C	1.84701300	-2.38384500	3.67685500
H	2.45425600	-2.70958400	4.52548300
H	0.98797000	-1.83036100	4.06653800
H	1.47787700	-3.26626400	3.15258100
C	-0.37713200	-0.90906800	-2.83256200
C	0.94762100	-1.42826700	-2.51397500
C	0.78163800	-2.75829300	-1.99403700
C	-0.63873300	-3.04639800	-1.92843100
C	-1.34663100	-1.91272700	-2.49488100
C	-2.81186600	-1.84535600	-2.76581900
H	-3.19690700	-0.82625200	-2.71339600
H	-2.98478700	-2.22787500	-3.78151300
H	-3.38592000	-2.45689600	-2.07009400
C	-0.67433600	0.39251100	-3.49975400
H	-1.62830900	0.80972200	-3.16978300
H	0.11245700	1.12839400	-3.32800300
H	-0.73996500	0.22340400	-4.58330800
C	2.24537500	-0.75189200	-2.82325700
H	3.05172100	-1.10299800	-2.17641100
H	2.53460300	-0.96725700	-3.85956800
H	2.17328500	0.33198200	-2.71778200
C	1.86773400	-3.69955500	-1.58866900
H	1.59925000	-4.26236600	-0.69187700
H	2.03270300	-4.42448000	-2.39590400
H	2.81257000	-3.18446700	-1.40896200
C	-1.26256800	-4.32535900	-1.47498300
H	-1.40080600	-4.99403400	-2.33459700
H	-0.63799500	-4.84421600	-0.74521600
H	-2.24268700	-4.15128200	-1.02703400
Rh	-0.21102400	-1.33253100	-0.65773700
N	-2.55336800	1.02586800	0.48029300
S	-3.04728700	-0.46500700	0.74253600
O	-4.15964400	-1.02370600	-0.02269300
O	-1.79811800	-1.33468900	0.82930900
S	-3.10110400	2.03181700	-0.69356400
O	-2.09711900	3.09074700	-0.81770400
O	-3.55561600	1.33078900	-1.90190500

C	-3.54705100	-0.43319100	2.54808100
C	-4.61839800	2.82743600	0.06183300
F	-4.57881700	0.39031400	2.68879300
F	-3.88864700	-1.66413500	2.91494300
F	-2.52206400	-0.00869400	3.28752800
F	-5.16073700	3.64719500	-0.83140100
F	-4.26372800	3.50711700	1.14829300
F	-5.49035500	1.87394000	0.39454400
C	6.52898100	1.77711700	-0.09436000
F	6.96667200	0.96057000	0.88627600
F	7.10069300	2.98106800	0.07689800
F	6.97504000	1.27819300	-1.26670200

2(C7)^{F}

Sum of electronic and thermal Free Energies=-3297.545792

C	3.00253200	-0.70392200	-2.15705800
C	3.62799400	-0.24990000	-0.92515600
C	3.49804200	-1.30430900	0.04461100
C	2.73823000	-2.38574700	-0.55319600
C	2.48152700	-2.03410900	-1.93364400
C	1.77434400	-2.89761100	-2.92274400
H	1.53285300	-2.35714600	-3.83835500
H	2.41618100	-3.74780600	-3.18490300
H	0.84464000	-3.28893100	-2.50219700
C	2.94931600	0.05308400	-3.44179400
H	2.06035100	-0.19728400	-4.02366000
H	2.95618800	1.13099600	-3.27254700
H	3.83035300	-0.19562800	-4.04761000
C	4.38711100	1.02730600	-0.74618400
H	4.38893100	1.35480000	0.29503000
H	5.43056400	0.88528900	-1.05400900
H	3.97228600	1.83162100	-1.35663100
C	4.08165000	-1.30753400	1.41689400
H	3.50642300	-1.92722300	2.10431400
H	5.09774600	-1.72066500	1.35892800
H	4.15655300	-0.30179500	1.83445600
C	2.38992100	-3.69326400	0.08265500
H	3.18987600	-4.41993800	-0.10856600
H	2.26376900	-3.60394100	1.16174500
H	1.46424100	-4.09549700	-0.33348100
Rh	1.48384200	-0.61122200	-0.60670400
C	1.19338800	1.69970000	1.52753900
C	1.97901500	2.25613300	2.56628400
C	2.27351100	1.48561500	3.69777100
C	1.78088500	0.18543300	3.78050400
C	0.96718100	-0.33595800	2.76579800
C	0.63609300	0.41088400	1.61740300
C	1.67879500	3.86239000	1.01209000
C	2.27154100	3.62129400	2.20553100
H	2.86174700	1.90177900	4.50961900
H	1.99855800	-0.42016600	4.65386800
H	-0.22515800	0.11482600	1.00991800
N	1.02434600	2.69645900	0.54669900
C	0.55280100	2.46816500	-0.74445000
O	0.55179800	1.30469900	-1.18134800
H	2.84218300	4.33523600	2.78211000
H	1.68047000	4.76022800	0.42178800
C	0.09200200	3.61633200	-1.66094700
C	1.35216400	4.24689400	-2.31890000
H	1.02328700	5.01736900	-3.02172100
H	2.03381500	4.72055200	-1.60805100
H	1.91471300	3.50039400	-2.88966500
C	-0.74640600	4.67917700	-0.91363400
H	-0.17389400	5.28208400	-0.20635300
H	-1.16271500	5.36584900	-1.65576500
H	-1.57406700	4.21264700	-0.37585300
C	-0.77857900	3.01361000	-2.78788800
H	-1.05245600	3.81881000	-3.47508800
H	-0.24592000	2.24650500	-3.35231500
H	-1.69918400	2.57222100	-2.40165900
N	-2.05167100	-0.13894600	0.00113900
S	-1.73038600	-1.01218100	-1.27873500
O	-1.88961400	-0.44554900	-2.61368200
O	-0.37266300	-1.64461200	-0.98016000
S	-3.05665700	1.16846200	0.04806200
O	-2.31876100	2.22858600	0.74851000
O	-3.75414800	1.46297200	-1.20125200
C	-2.80250100	-2.54886800	-1.19916700
C	-4.33727900	0.54119200	1.25729000
F	-4.06404200	-2.19251900	-1.40819800
F	-2.40170400	-3.39676500	-2.14824300
F	-2.68263400	-3.12452900	-0.00622000
F	-5.24717500	1.49325100	1.43874100
F	-3.75571800	0.24503400	2.41914400
F	-4.91698200	-0.55031100	0.75601700
C	0.40813800	-1.72275700	2.97169300
F	1.42512900	-2.60168000	3.23398100
F	-0.42704900	-1.77794400	4.01734700

F	-0.23678900	-2.18580400	1.88741600

3(C2)^{F}

Sum of electronic and thermal Free Energies=-1469.897693

C	-3.59713200	-0.58907900	1.29749400
C	-4.19309300	0.51903600	0.54617900
C	-4.24748000	0.13859900	-0.80401700
C	-3.71093800	-1.23151700	-0.91802400
C	-3.38259400	-1.70119500	0.38848100
C	-2.98872100	-3.09407200	0.77571900
H	-2.30862000	-3.10153300	1.63006400
H	-3.87951800	-3.66994200	1.05428300
H	-2.50484400	-3.61980800	-0.05022900
C	-3.42575400	-0.62613700	2.77982800
H	-3.17464600	0.35722000	3.18313000
H	-4.36858800	-0.94213500	3.24699000
H	-2.65175000	-1.33424300	3.08080900
C	-4.62431600	1.82084600	1.14795600
H	-4.71534700	2.60479700	0.39434000
H	-5.60141000	1.70822400	1.63329300
H	-3.91883400	2.16576400	1.90824900
C	-4.75592400	0.94169600	-1.95903500
H	-4.11962000	0.82746600	-2.84077300
H	-5.76145200	0.60237700	-2.23854400
H	-4.81841700	2.00445700	-1.71981700
C	-3.66630100	-2.01847400	-2.18804900
H	-4.66207400	-2.42762200	-2.40388000
H	-3.37832400	-1.39594200	-3.03855800
H	-2.96820100	-2.85457100	-2.12307600
Rh	-2.05248800	-0.03925100	-0.11223700
C	2.10807500	-0.41965500	-0.00409400
C	1.83867200	-1.81262900	-0.01345200
C	2.88441100	-2.74326900	-0.00185900
C	4.19520000	-2.28431800	0.01762400
C	4.45218900	-0.90678900	0.02512700
C	3.42175900	0.03985800	0.01481100
C	-0.20254500	-0.77292000	-0.03072400
C	0.41155200	-1.99249000	-0.02432400
H	2.67024500	-3.80712500	-0.00602600
H	5.02316800	-2.98419400	0.03369400
H	3.69008100	1.08268100	0.02905300
N	0.83492100	0.23772900	-0.01586400
C	0.38886700	1.53301200	-0.04068600
O	-0.86769500	1.68499500	-0.06616500
H	-0.09411300	-2.94830500	-0.02644700
C	1.25121700	2.79674300	-0.03927700
C	2.11781500	2.83947900	-1.32572700
H	2.78456900	3.70511800	-1.27641200
H	2.72922400	1.95323000	-1.48888300
H	1.47710700	2.96331700	-2.20403900
C	2.07579400	2.86594900	1.27331400
H	2.68343000	1.98472100	1.47364500
H	2.74220200	3.73211000	1.22848200
H	1.40728500	3.00530600	2.12834200
C	0.32577200	4.03323200	-0.06676600
H	0.94896500	4.93191700	-0.06546600
H	-0.29970700	4.05196800	-0.96181700
H	-0.32813300	4.06945000	0.80721400
C	5.88529900	-0.43015000	-0.01013100
F	6.66930000	-1.17583100	0.79121100
F	5.99296400	0.85754900	0.38449600
F	6.39167400	-0.51249600	-1.25779500

3(C7)^{F}

Sum of electronic and thermal Free Energies=-1469.888411

C	-1.64811500	-2.69990400	-0.35042400
C	-0.59651800	-2.85685500	0.55924700
C	-0.73734700	-1.80705800	1.57219100
C	-2.00938200	-1.12145500	1.35184900
C	-2.53290100	-1.61564800	0.13033400
C	-3.86222100	-1.31351900	-0.48247100
H	-3.80756500	-1.28505200	-1.57273100
H	-4.56595800	-2.11099900	-0.20957100
H	-4.26931100	-0.36529600	-0.13872700
C	-1.90199600	-3.48264300	-1.59876800
H	-1.02900400	-4.06211500	-1.90278400
H	-2.73282900	-4.18187100	-1.44141000
H	-2.18594200	-2.82909900	-2.42860100
C	0.52402200	-3.84762600	0.51147300
H	1.48624100	-3.37377600	0.72321000
H	0.36992800	-4.62876200	1.26556700
H	0.59552200	-4.33456300	-0.46247400
C	0.12172800	-1.66506500	2.78672600
H	0.08534800	-0.65202200	3.19170000
H	-0.23396600	-2.34968700	3.56849000
H	1.16261700	-1.92154200	2.57758800
C	-2.65612900	-0.19568500	2.33427000
H	-3.12361400	-0.78874900	3.13037500

H	-1.92712500	0.46876500	2.80381000
H	-3.42320400	0.41971900	1.87136200
Rh	-0.48469600	-0.67969200	-0.21472300
C	1.06768900	1.80221600	0.28065800
C	1.34614500	3.12921400	0.68703200
C	0.33610600	4.08942900	0.64323500
C	-0.90227900	3.70864600	0.13874400
C	-1.16697000	2.37500600	-0.21611500
C	-0.20564400	1.34589400	-0.07811600
C	3.30172600	1.99991400	0.78808700
C	2.74581400	3.20397000	1.03847900
H	0.52450300	5.11494200	0.94265400
H	-1.67799100	4.45362600	0.00204300
N	2.31702000	1.10028000	0.29434300
C	2.52526800	-0.08765800	-0.35054300
O	1.54163600	-0.76916000	-0.72578900
H	3.26614600	4.06829500	1.42701900
H	4.31836900	1.68218500	0.92435200
C	3.93361300	-0.63393800	-0.67636100
C	4.69083300	-0.99868300	0.62669600
H	5.64717200	-1.45622400	0.35789800
H	4.90727800	-0.14743500	1.27364400
H	4.12870800	-1.73144900	1.21483500
C	4.72727700	0.37745600	-1.54230100
H	4.95033400	1.31719900	-1.03706600
H	5.67923000	-0.07936600	-1.82714000
H	4.18362500	0.61132900	-2.46282100
C	3.77193900	-1.92762600	-1.50396600
H	4.76590300	-2.31004500	-1.75119600
H	3.23788500	-2.70292400	-0.95057000
H	3.23327400	-1.74544600	-2.43654500
C	-2.51737500	2.11278600	-0.83334500
F	-3.47069200	1.79661600	0.08941100
F	-2.98147100	3.18600200	-1.49516300
F	-2.48541200	1.08525200	-1.72137300

4(C2)^{F}

Sum of electronic and thermal Free Energies=-1776.296587

C	3.28504200	-0.50618900	1.66021500
C	2.15450900	-1.43755500	1.84090500
C	2.25672600	-2.45788100	0.83856800
C	3.31506500	-2.06752000	-0.04915600
C	3.99682400	-0.89475600	0.51713300
C	5.26657700	-0.31342100	-0.02181700
H	5.61682700	0.51658200	0.59362700
H	6.05191900	-1.07820300	-0.02901400
H	5.14470400	0.06591100	-1.03969000
C	3.56695600	0.64156500	2.57730700
H	4.37326700	1.27353500	2.20260400
H	2.67771000	1.26616300	2.70571100
H	3.85567300	0.27337700	3.56891700
C	1.24518800	-1.45128300	3.03147000
H	0.31929600	-1.99210500	2.82494500
H	1.73905500	-1.94663300	3.87680300
H	0.98921700	-0.43817200	3.35066500
C	1.46623900	-3.72739800	0.77115700
H	1.41697600	-4.12066000	-0.24632300
H	1.94950600	-4.49049000	1.39394400
H	0.44617200	-3.59519200	1.13509900
C	3.85463500	-2.89112700	-1.17771900
H	4.53311400	-3.65485400	-0.77605900
H	3.06476900	-3.41018300	-1.72482300
H	4.43065900	-2.28890300	-1.88300200
Rh	1.69642600	-0.46296700	-0.07596700
C	-2.49587800	-0.40445100	-0.26308800
C	-2.33290400	-1.63388400	-0.94775200
C	-3.44894900	-2.34239100	-1.40429700
C	-4.71897100	-1.82612800	-1.17591500
C	-4.87057400	-0.61116900	-0.49531500
C	-3.76863600	0.11277200	-0.03098100
C	-0.22707700	-0.92332400	-0.43988900
C	-0.91849000	-1.91971200	-1.04243700
H	-3.32216500	-3.28087300	-1.93436700
H	-5.59737900	-2.35418800	-1.52974300
H	-3.95078700	1.04466600	0.47746500
N	-1.17494200	0.05724500	0.05521100
C	-0.63173900	1.14655100	0.68032500
O	0.62756700	1.16894900	0.76445100
H	-0.49106800	-2.79110900	-1.51881900
C	-1.39479300	2.34252400	1.25978900
C	-2.29506400	1.87620700	2.43316500
H	-2.89798700	2.72115900	2.77787400
H	-2.97154100	1.05921600	2.18663100
H	-1.67511500	1.54785900	3.27323400
C	-2.16861700	3.05747300	0.12031400
H	-2.83979600	2.41178100	-0.44363500
H	-2.76281300	3.86916600	0.54978600
H	-1.46271400	3.50248500	-0.58775900

C	-0.37833000	3.35701100	1.82794800
H	-0.92956800	4.21648600	2.21959900
H	0.20834900	2.92977400	2.64447600
H	0.31180200	3.70936000	1.05849400
C	2.77624000	1.92765200	-1.85722500
O	3.95702500	1.69968800	-2.04025700
O	2.27086400	3.14045300	-1.58421800
C	1.68703200	0.91067800	-1.95232100
C	1.95076600	-0.37185500	-2.38216000
H	0.67380800	1.29704400	-1.95408500
H	1.15864900	-1.00876800	-2.75433300
H	2.97411200	-0.64932500	-2.60837100
C	3.22772700	4.22244400	-1.54857300
H	2.64207600	5.12331800	-1.37361000
H	3.94695600	4.06628900	-0.74149200
H	3.76170500	4.28544400	-2.49872200
C	-6.25733800	-0.09491800	-0.20167400
F	-7.10980900	-0.36775000	-1.20774300
F	-6.25936800	1.24362700	-0.00786300
F	-6.76377900	-0.65802800	0.91653000

4(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.282888

C	1.49436200	-0.98464600	1.98982600
C	0.10108900	-0.83447900	2.30867600
C	-0.61476400	-2.00718400	1.80212400
C	0.31417300	-2.80783300	1.11116400
C	1.62513700	-2.15648500	1.17420800
C	2.90741300	-2.83064700	0.79356100
H	3.74273600	-2.13499500	0.74968100
H	3.14018300	-3.59411100	1.54769600
H	2.83839700	-3.33619200	-0.17142300
C	2.59790100	-0.13013300	2.53005300
H	2.27177200	0.90058700	2.68344500
H	2.90974100	-0.52724900	3.50460700
H	3.46872600	-0.11752100	1.87771600
C	-0.48262400	0.20270900	3.21640900
H	-1.55073600	0.33882400	3.03558000
H	-0.36464400	-0.10850100	4.26214300
H	0.01666600	1.16718300	3.10098100
C	-2.06478300	-2.29446300	2.03408200
H	-2.41193900	-3.12344400	1.41551800
H	-2.23892600	-2.56054700	3.08365800
H	-2.68129600	-1.42122100	1.80639700
C	0.06299500	-4.15479000	0.50764200
H	0.15094200	-4.92355200	1.28589400
H	-0.93266200	-4.22825100	0.06776400
H	0.79835600	-4.39579900	-0.26317000
Rh	0.22500200	-0.65743600	0.11863000
C	0.49779800	2.33355600	-0.12481000
C	1.10978000	3.61223800	-0.15767000
C	2.46693900	3.73888400	-0.45358000
C	3.16696300	2.58582100	-0.74981400
C	2.55343600	1.31361400	-0.70657200
C	1.19992000	1.13423700	-0.33588400
C	-1.07068200	3.97240200	0.27905200
C	0.10714400	4.60820000	0.11921200
H	2.94596800	4.71161600	-0.48058900
H	4.21136600	2.65183500	-1.03457300
N	-0.89952400	2.57204100	0.13553300
C	-1.90295100	1.63736600	0.10787300
O	-1.62706900	0.42681500	-0.01134800
H	0.26227900	5.67629000	0.17826200
H	-2.03648700	4.39025900	0.48452800
C	-3.40236700	2.02656800	0.19493700
C	-3.79121700	2.91787000	-1.01401900
H	-4.86430900	3.12355700	-0.96477600
H	-3.27243600	3.87611200	-1.05180800
H	-3.59695700	2.39097500	-1.95303100
C	-3.73926000	2.69209600	1.55480200
H	-3.27590100	3.66466200	1.72180600
H	-4.82208100	2.83569400	1.60847800
H	-3.45435400	2.04187100	2.38851100
C	-4.25045200	0.73968600	0.09961700
H	-5.30665100	1.02298200	0.11264400
H	-4.04592100	0.18693100	-0.81778800
H	-4.07480200	0.07763000	0.95165400
C	-1.93444200	-1.82774200	-1.99464100
O	-2.67004000	-0.94344100	-2.37978700
O	-2.35399900	-3.05422500	-1.62443100
C	-0.44194600	-1.73014800	-1.93479600
C	0.18532900	-0.57948700	-2.32629900
H	0.10002000	-2.66637800	-1.85996400
H	1.22987900	-0.57391200	-2.59203500
H	-0.41290700	0.28916900	-2.57735400
C	-3.77041600	-3.30016700	-1.76937200
H	-3.90953600	-4.35410300	-1.53329100
H	-4.33817500	-2.67210900	-1.07921300

H	-4.08740300	-3.08772800	-2.79201900
C	3.51450300	0.21828600	-1.11051000
F	4.19575000	0.55961600	-2.22253300
F	2.94101300	-0.98154800	-1.37435200
F	4.45631200	-0.01644700	-0.15090200

5(C2)^{F}

Sum of electronic and thermal Free Energies=-1776.296538

C	2.04717500	0.22003400	2.45317900
C	0.86710800	-0.64784900	2.46483800
C	1.16077600	-1.76509700	1.66505100
C	2.52958800	-1.61847000	1.13866900
C	3.10676500	-0.44015800	1.73360800
C	4.53872100	-0.01080000	1.66551000
H	4.65506300	1.04258600	1.92777100
H	5.13130200	-0.59674200	2.37914800
H	4.95790800	-0.15577300	0.66887000
C	2.15413100	1.50339700	3.21253100
H	2.99105800	2.11321700	2.86863300
H	1.23964000	2.09440700	3.12067400
H	2.30662200	1.29181600	4.27866900
C	-0.39421700	-0.37624200	3.22716600
H	-1.23337100	-0.96038000	2.84317500
H	-0.26759000	-0.63924500	4.28470300
H	-0.66924100	0.68136100	3.18960300
C	0.27349400	-2.93708700	1.39381300
H	0.50025100	-3.39835100	0.43051100
H	0.42905400	-3.70160400	2.16600400
H	-0.78434300	-2.66629700	1.40511700
C	3.26582200	-2.67916600	0.37973300
H	3.45905700	-3.54084700	1.03080000
H	2.69765200	-3.03124100	-0.48456400
H	4.22707700	-2.31154300	0.01967500
Rh	1.47625500	0.11342500	0.34137900
C	-2.01060200	-0.03661400	-1.02769500
C	-1.41898500	-1.24636200	-1.47478200
C	-2.16430100	-2.43509100	-1.47909100
C	-3.46820100	-2.41109500	-1.00495500
C	-4.02338100	-1.21296300	-0.52190500
C	-3.30879300	-0.01461900	-0.52158700
C	0.15452200	0.39277000	-1.67040400
C	-0.06702100	-0.95243200	-1.86832500
H	-1.72737200	-3.35613600	-1.85155600
H	-4.06919700	-3.31359600	-1.00677900
H	-3.78390800	0.88260800	-0.15384300
N	-1.03744100	0.98984900	-1.15866600
C	-0.83492000	2.07681100	-0.27164000
O	0.22743000	2.06593500	0.36304100
H	0.64379100	-1.60603700	-2.35636000
C	-1.79864400	3.26083700	-0.17523900
C	-2.55172700	3.18071300	1.17814400
H	-3.19914900	4.05643400	1.27601200
H	-3.18175500	2.29195500	1.26428300
H	-1.84671200	3.18409900	2.01415000
C	-2.77224500	3.32992100	-1.36715100
H	-3.44918900	2.47697000	-1.42904600
H	-3.38735200	4.22866800	-1.26969100
H	-2.23180200	3.39803600	-2.31565700
C	-0.92621900	4.54368700	-0.17140100
H	-1.58096700	5.41360100	-0.07245400
H	-0.21689900	4.54322900	0.65773400
H	-0.36753000	4.65011000	-1.10662200
C	3.40777000	-0.11111400	-1.95141100
O	3.00425900	-1.00661900	-2.67917600
O	4.72014000	0.04933500	-1.65578100
C	2.54404300	0.92239100	-1.31827300
C	1.31551400	1.23479400	-2.18086700
H	3.11094800	1.79190400	-0.98746600
H	1.06205600	2.29359600	-2.11394200
H	1.48064300	0.99672500	-3.23626400
C	5.62741800	-0.84590400	-2.33410100
H	6.62429900	-0.55311000	-2.00714100
H	5.42256800	-1.88547500	-2.06827100
H	5.52974400	-0.73347800	-3.41568200
C	-5.41521100	-1.24326700	0.06493700
F	-6.24629700	-1.99754000	-0.67620600
F	-5.94598200	-0.00627300	0.16085100
F	-5.39513000	-1.77062200	1.30909300

5(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.298517

C	-0.92441800	0.82343800	2.72692900
C	0.25067400	1.57476800	2.63921900
C	0.07516800	2.56700900	1.55947500
C	-1.29404300	2.48829300	1.09231200
C	-1.87203700	1.34191900	1.71986200
C	-3.28735600	0.87467400	1.58744200
H	-3.37110400	-0.20326500	1.74415700

H	-3.90726600	1.36628800	2.34843600
H	-3.70340100	1.10885500	0.60827900
C	-1.23056400	-0.31132600	3.65454600
H	-0.34340200	-0.64748200	4.19409400
H	-1.97633100	-0.00303300	4.39742200
H	-1.64702200	-1.16915700	3.11715800
C	1.50377900	1.43097800	3.44487100
H	2.39073300	1.42610200	2.80445300
H	1.60882200	2.27648300	4.13545900
H	1.50535500	0.51445600	4.03733900
C	1.05404900	3.64378200	1.21773100
H	0.93167000	3.96687200	0.18307900
H	0.89514100	4.51282600	1.86994500
H	2.08480400	3.31007000	1.35752400
C	-1.96992800	3.45302700	0.16856200
H	-2.28991000	4.33822000	0.73228200
H	-1.30014200	3.77887500	-0.62941900
H	-2.85916200	3.01542300	-0.28950800
Rh	-0.13992300	0.71501000	0.50177500
C	0.08160300	-2.21253700	-0.05402600
C	-0.35512000	-3.29206800	0.76504000
C	-1.71184000	-3.58904700	0.87049600
C	-2.61365100	-2.84254300	0.11950900
C	-2.17687400	-1.84457000	-0.76168900
C	-0.80296500	-1.50068400	-0.90135900
C	1.89714700	-3.33263100	0.77694600
C	0.81246900	-3.96543500	1.27432600
H	-2.05446600	-4.41391700	1.48661700
H	-3.67033400	-3.07352300	0.16759600
N	1.50637300	-2.22078700	-0.01592100
C	2.33601600	-1.09970600	-0.14339300
O	1.85363400	0.03241200	-0.01065100
H	0.82505500	-4.83882700	1.91069500
H	2.93926300	-3.53716500	0.94362400
C	3.84018200	-1.24999400	-0.44394800
C	4.11819200	-2.43217800	-1.39833600
H	5.18533300	-2.44607700	-1.63607300
H	3.86480500	-3.40823300	-0.98033000
H	3.57170400	-2.31478400	-2.33872700
C	4.63099100	-1.39427400	0.88535200
H	4.45353700	-2.33559800	1.41048500
H	5.69932100	-1.34613600	0.65681400
H	4.39949200	-0.57234000	1.56968100
C	4.31235500	0.05570600	-1.12660200
H	5.36861900	-0.05348100	-1.38740200
H	3.74238000	0.26826300	-2.03252900
H	4.21204700	0.91336600	-0.45814800
C	0.73643200	1.70613600	-2.23672800
O	1.71685700	1.25455000	-2.80009200
O	0.49670600	3.04177500	-2.15535400
C	-0.34270100	0.89903500	-1.59583100
C	-0.31282500	-0.57220500	-2.01578100
H	-1.30988400	1.36981700	-1.75315000
H	-0.92154000	-0.73746400	-2.90831200
H	0.70863200	-0.84154300	-2.29064100
C	1.45198600	3.88028000	-2.83852300
H	1.08794500	4.89994400	-2.71631300
H	2.44617600	3.76962600	-2.39935200
H	1.50079400	3.61613300	-3.89678500
C	-3.23063700	-1.21833000	-1.65464400
F	-3.04542200	-1.53511100	-2.95333300
F	-3.22837900	0.14185800	-1.58039500
F	-4.47173500	-1.61325100	-1.32056600

6(C2)^{F}

Sum of electronic and thermal Free Energies=-1776.29011

C	2.85818500	0.10184900	-0.74758500
C	3.04339800	0.54455400	-2.07694400
C	4.32071400	0.57845100	-2.64862900
C	5.40366100	0.13763100	-1.90040900
C	5.20173800	-0.36384400	-0.60575000
C	3.93432300	-0.40416100	-0.02241800
C	0.80604600	0.54308300	-1.67807000
C	1.74286400	0.80786400	-2.62281800
H	4.45562200	0.92336400	-3.66862900
H	6.40284900	0.14578900	-2.32024100
H	3.83095300	-0.83953100	0.95744500
N	1.45876100	0.14587200	-0.46258500
C	0.78359900	0.01628600	0.74891600
O	-0.41499400	-0.31949100	0.74424500
H	1.52881600	1.13188000	-3.63236300
C	1.40740700	0.28645000	2.14469100
C	2.48016100	1.39889500	2.14907100
H	2.69054900	1.66400200	3.18919800
H	3.42731400	1.12334600	1.69289500
H	2.10084800	2.29099500	1.64443900
C	1.90153700	-1.05091100	2.75761600
H	2.67064300	-1.55912500	2.17490500

H	2.31585300	-0.85413000	3.75058400
H	1.06493700	-1.74683800	2.87183000
C	0.25517700	0.79300800	3.05198600
H	0.66032600	0.98575200	4.04893600
H	-0.16532400	1.72265800	2.66254400
H	-0.54311200	0.05529600	3.14428900
C	-3.45251800	-1.91608300	0.96938600
C	-3.66460200	-2.30221300	-0.36034500
C	-4.21126000	-1.14089700	-1.08530800
C	-4.43993700	-0.07899100	-0.14723600
C	-3.85848800	-0.50182700	1.10360900
C	-3.89810000	0.26370700	2.38777900
H	-3.06583800	-0.00134600	3.04282800
H	-4.82820000	0.03916600	2.92662100
H	-3.86708800	1.34059400	2.20933000
C	-2.89196300	-2.73559300	2.08815700
H	-2.11388300	-2.18881000	2.62828500
H	-2.46204400	-3.67262200	1.73099300
H	-3.68088800	-2.98017000	2.80979800
C	-3.41085900	-3.64296000	-0.97812900
H	-2.97279700	-3.55440100	-1.97576800
H	-4.35451700	-4.19177200	-1.08769100
H	-2.74178800	-4.25272000	-0.36860500
C	-4.65594400	-1.17709800	-2.51485400
H	-4.76588300	-0.17606300	-2.93560600
H	-5.63122300	-1.67528800	-2.58617500
H	-3.95879800	-1.73980900	-3.14093600
C	-5.15758700	1.21306800	-0.39233000
H	-6.17411900	1.15266800	0.01514300
H	-5.24433800	1.43213300	-1.45838800
H	-4.64980600	2.05543300	0.08280100
Rh	-2.27922100	-0.40805600	-0.34416400
C	-1.67215200	1.39460100	-1.20922500
C	-0.66539200	0.54455100	-1.96605000
H	-0.77763000	0.71866500	-3.04094800
H	-0.98792800	-0.55555000	-1.89858800
C	-1.23538300	2.46422300	-0.28160200
O	-0.12771900	2.59610800	0.21160000
O	-2.25903900	3.31342600	-0.02807500
C	-1.95107900	4.42416100	0.83932800
H	-2.85050800	5.03820200	0.85720200
H	-1.70764000	4.07263100	1.84507100
H	-1.10540400	4.99154600	0.44606800
H	-2.49074200	1.74181500	-1.83786200
C	6.38069600	-0.82584000	0.21350000
F	6.03488400	-1.82373000	1.05941800
F	7.38646000	-1.27207200	-0.56193000
F	6.87120900	0.17930600	0.97205600

6(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.297677

C	1.01277600	-1.94670000	1.51928100
C	1.86977200	-2.60876500	0.63290500
C	3.17166500	-1.91829000	0.67505500
C	3.13416700	-0.89917500	1.67811700
C	1.76544800	-0.82799700	2.13232900
C	1.22705500	0.05670300	3.20906600
H	0.26500100	0.49626500	2.93414500
H	1.07918300	-0.53162400	4.12433100
H	1.91241900	0.87247400	3.44249100
C	-0.40954200	-2.27644400	1.83903400
H	-0.88661700	-2.84871300	1.04153700
H	-0.45603400	-2.87593000	2.75712800
H	-1.00059200	-1.37398900	2.01274300
C	1.56637900	-3.80468000	-0.21504300
H	2.01990100	-3.72246000	-1.20663200
H	1.96873700	-4.71303000	0.25056000
H	0.49159100	-3.94605500	-0.34312000
C	4.37185700	-2.32648000	-0.11474500
H	5.10209800	-1.51886500	-0.18494800
H	4.85990300	-3.18026700	0.37420100
H	4.10164800	-2.64423200	-1.12521900
C	4.29532400	-0.07967200	2.15323900
H	3.96514300	0.80005400	2.70859300
H	4.92722400	-0.67476100	2.82305900
H	4.91176700	0.26441500	1.31908000
Rh	1.75810900	-0.35239900	0.02742700
C	-1.96348400	0.25269400	-0.61433300
C	-1.12089400	-0.52406400	-1.44327000
C	-1.60033300	-1.72740400	-1.97935400
C	-2.88100700	-2.14795400	-1.64394000
C	-3.68131600	-1.38661700	-0.77066300
C	-3.23616200	-0.17815400	-0.23954500
C	0.01024800	1.35907800	-0.77681900
C	0.14871100	0.17080000	-1.52116800
H	-0.98318800	-2.31925800	-2.64814600
H	-3.27784100	-3.06911400	-2.05639100
H	-3.87122500	0.38839600	0.42941200

N	-1.25556600	1.41411500	-0.24073800
C	-1.66293100	2.38060600	0.78637100
O	-1.01043200	2.40950900	1.80353200
H	0.88837100	0.08205800	-2.31680100
C	-2.80629200	3.36103800	0.49002400
C	-3.87519700	3.20701100	1.59806200
H	-4.62855300	3.99137500	1.48376100
H	-4.39326300	2.24429300	1.54146500
H	-3.42569500	3.29994800	2.58946600
C	-3.42955000	3.20747800	-0.90715700
H	-3.95220400	2.25784800	-1.03908600
H	-4.16369500	4.00446800	-1.05443000
H	-2.68074800	3.29970600	-1.69945500
C	-2.16406000	4.77171700	0.60742200
H	-2.94045700	5.52822800	0.46412400
H	-1.71036300	4.91560900	1.59011800
H	-1.39859400	4.93040700	-0.15967000
C	3.29349100	1.48142400	-1.49688700
O	2.92002600	1.39428000	-2.65744100
O	4.59514700	1.40015100	-1.13187900
C	2.38700600	1.64390800	-0.32641100
C	1.08396700	2.40522400	-0.63464900
H	2.91417200	2.01120700	0.55196500
H	0.85068100	3.08716800	0.18357200
H	1.15524200	2.98803400	-1.56137700
C	5.53483200	1.24731000	-2.21744400
H	6.52088100	1.26695700	-1.75503200
H	5.37063000	0.30061100	-2.73842100
H	5.42935400	2.06662900	-2.93090100
C	-5.02688300	-1.93101100	-0.35695000
F	-4.88730800	-2.88862700	0.58739700
F	-5.67411500	-2.48896800	-1.39699700
F	-5.81846900	-0.96904200	0.16070800

7(C2)^{F}

Sum of electronic and thermal Free Energies=-1776.285228

C	2.73373700	-0.34495400	-0.64563400
C	2.82372400	-1.08919200	-1.84688400
C	4.04698800	-1.61529600	-2.28405900
C	5.17785300	-1.41880400	-1.50793000
C	5.07654100	-0.71569700	-0.29713200
C	3.86769200	-0.18273700	0.15143600
C	0.63703500	-0.54124200	-1.56520000
C	1.50571100	-1.19837200	-2.38485500
H	4.09810700	-2.18019700	-3.20912500
H	6.13612200	-1.82128100	-1.81576300
H	3.86212400	0.33094500	1.09618300
N	1.36172000	0.02570700	-0.46635700
C	0.73992700	0.70758600	0.58181800
O	-0.45453800	0.47509900	0.84400400
H	1.22730600	-1.70473100	-3.29917500
C	1.42803500	1.77619700	1.46400300
C	2.43418900	2.65055400	0.68135200
H	2.83716700	3.40608100	1.36220000
H	3.27812200	2.11591000	0.25390200
H	1.91825800	3.16594100	-0.13192700
C	2.02179200	1.08178300	2.72293300
H	2.70809200	0.26102900	2.51599000
H	2.55929400	1.82544600	3.31814000
H	1.21339000	0.67718900	3.33913800
C	0.32642000	2.73883300	1.97710600
H	0.80015000	3.49790300	2.60585800
H	-0.17115700	3.23996100	1.14483200
H	-0.42230400	2.21897000	2.57618700
C	-3.23972400	-1.29471300	1.77715200
C	-3.50575200	-2.21105500	0.70190200
C	-4.08585300	-1.44736500	-0.37395300
C	-4.35832100	-0.09238700	0.12527200
C	-3.82567800	0.00105800	1.42472500
C	-3.84159800	1.19062500	2.33331100
H	-2.85158700	1.37806400	2.75904500
H	-4.52963800	1.02052300	3.17024900
H	-4.16581300	2.09371800	1.81369300
C	-2.68311000	-1.63631300	3.12566800
H	-2.08868700	-0.81435400	3.53171900
H	-2.05152100	-2.52583700	3.08947700
H	-3.49945900	-1.83299900	3.83208000
C	-3.30023600	-3.69657500	0.72231800
H	-3.08160800	-4.09262800	-0.27098900
H	-4.21650900	-4.18294900	1.07948500
H	-2.48738100	-3.98636100	1.39003700
C	-4.60725300	-2.00985300	-1.66230800
H	-4.56321800	-1.28067500	-2.47509000
H	-5.65865200	-2.30225500	-1.54713000
H	-4.05017200	-2.89713000	-1.96970500
C	-5.12589100	0.95901200	-0.61551400
H	-6.19771400	0.85038900	-0.40651400
H	-4.99741600	0.87478300	-1.69661600

H	-4.82705400	1.96699000	-0.32357500
Rh	-2.05624800	-0.66449000	0.00480700
C	-1.70990800	0.57501800	-1.83713100
C	-0.79779600	-0.49192000	-1.86254600
H	-1.08059400	-1.31907900	-2.50650700
H	-1.07076500	-1.86996100	-0.05154900
C	-1.36114900	2.00014200	-1.59984800
O	-0.26238700	2.42759400	-1.29635800
O	-2.43178800	2.78290000	-1.83100100
C	-2.20133400	4.20598600	-1.74774200
H	-3.13630500	4.67036000	-2.05730900
H	-1.95093200	4.49271800	-0.72367500
H	-1.38591100	4.49743900	-2.41242000
H	-2.62293100	0.44329600	-2.40750200
C	6.32158100	-0.47468600	0.52179100
F	6.02752900	-0.25971900	1.82411000
F	6.99191800	0.61079100	0.08094500
F	7.16636500	-1.52148100	0.45729100

7(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.278755

C	0.08264700	-1.19259100	-2.59319100
C	-0.06421400	-2.51215500	-1.93818600
C	-1.41873900	-2.64574900	-1.50512900
C	-2.03828200	-1.35589300	-1.68392200
C	-1.12084600	-0.50151100	-2.45964900
C	-1.47499400	0.83874700	-3.02557200
H	-0.58753400	1.39295400	-3.33733300
H	-2.11562000	0.71635100	-3.90811000
H	-2.02468900	1.45413700	-2.31112400
C	1.31942100	-0.74639400	-3.31095500
H	1.35148300	0.33791100	-3.43290500
H	2.22704300	-1.05843200	-2.78683000
H	1.35937800	-1.19512900	-4.31157700
C	0.96567600	-3.59963400	-1.98653300
H	0.77121900	-4.37236300	-1.24036200
H	0.96458500	-4.07885000	-2.97384900
H	1.97209200	-3.20942600	-1.81453100
C	-2.09889700	-3.89192600	-1.01892200
H	-2.88816600	-3.66722100	-0.29915100
H	-2.56102900	-4.41037800	-1.86831800
H	-1.39745700	-4.58315200	-0.54843200
C	-3.48754700	-1.05552000	-1.44584200
H	-4.08556500	-1.44138300	-2.28139100
H	-3.85167000	-1.52318600	-0.52862500
H	-3.67422300	0.01807000	-1.38040100
Rh	-0.38171600	-1.15490800	-0.20596800
C	1.52812200	1.81734900	-0.08088800
C	2.09693200	2.89725500	-0.80287300
C	1.31166300	3.98462900	-1.19039800
C	-0.02098400	4.00406900	-0.81565800
C	-0.58756900	2.95841000	-0.06752000
C	0.16525500	1.81434500	0.30772200
C	3.78073800	1.48685200	-0.33280700
C	3.50425900	2.64935600	-0.96021400
H	1.74628100	4.81278800	-1.74007600
H	-0.63610300	4.85833900	-1.06700900
N	2.60185400	0.91645400	0.20869500
C	2.60090700	-0.38067100	0.73586700
O	1.62823700	-1.13450800	0.61483400
H	4.21551000	3.27764200	-1.47680700
H	4.71520100	0.96202900	-0.26080000
C	3.82129600	-0.91966200	1.52837800
C	4.48068700	0.16767700	2.40739800
H	5.25021000	-0.30528800	3.02371500
H	4.96123100	0.96901200	1.84521100
H	3.75093700	0.62210500	3.08468900
C	4.84311000	-1.57832600	0.56381600
H	5.34932600	-0.87408500	-0.10070600
H	5.61582900	-2.07220100	1.15961000
H	4.35963100	-2.34238200	-0.05265300
C	3.28956600	-2.03054400	2.46812900
H	4.12315400	-2.40744800	3.06636800
H	2.52473700	-1.64980200	3.15044800
H	2.86087800	-2.86354400	1.90930100
C	-1.99346000	-0.61382200	2.43929200
O	-1.25251300	-0.83410900	3.37365400
O	-3.28192000	-0.99177000	2.37657200
C	-1.61566500	0.14714200	1.20168600
C	-0.34794100	0.70499800	1.13617300
H	-2.43661100	0.48541200	0.58893200
H	0.30236000	0.40092400	1.95308800
H	-0.62425500	-2.14987600	0.94076500
C	-3.78003700	-1.69344800	3.53705600
H	-4.83181800	-1.88621900	3.33183900
H	-3.23359100	-2.62884300	3.67773100
H	-3.66704500	-1.07441000	4.42916600
C	-2.02438600	3.16579300	0.37079200

F	-2.21709100	2.88443700	1.67321100
F	-2.43107100	4.42901500	0.17303600
F	-2.89541700	2.37677300	-0.33746300

8(C2)^{F}

Sum of electronic and thermal Free Energies=-2004.145709

C	-2.14348700	-1.08686100	2.26182700
C	-1.37005300	0.15223400	2.37812500
C	-2.18788600	1.22307600	1.94218900
C	-3.46621000	0.66354800	1.49293400
C	-3.45660700	-0.74984500	1.78399300
C	-4.59960100	-1.69917100	1.63943900
H	-4.25131700	-2.68291500	1.32506700
H	-5.10549500	-1.79434700	2.60921500
H	-5.33399800	-1.34258600	0.91525200
C	-1.69714600	-2.45371200	2.66263000
H	-0.62390600	-2.48681500	2.85529500
H	-2.21493600	-2.75793200	3.58075500
H	-1.93997200	-3.16640600	1.87038900
C	0.01231100	0.27070100	2.93844200
H	0.52074000	1.16133000	2.56339900
H	-0.03489600	0.34779500	4.03195300
H	0.62259900	-0.60269400	2.69950700
C	-1.83753800	2.67523500	2.00720300
H	-2.57023400	3.29343000	1.48951900
H	-1.81837000	2.99019700	3.05786300
H	-0.85676400	2.88868300	1.57587600
C	-4.65112000	1.45656900	1.04056500
H	-5.37772700	0.82618200	0.52564100
H	-5.15109300	1.90419300	1.90899100
H	-4.36585100	2.26032000	0.35987800
Rh	-1.92718700	-0.25927100	0.24694500
C	2.79716000	0.52398100	-0.56143800
C	2.69227000	1.92685200	-0.74015900
C	3.79260500	2.75970100	-0.47619400
C	4.96298400	2.19194000	-0.00181200
C	5.03223800	0.80487900	0.23163400
C	3.95681100	-0.04159400	-0.02782400
C	0.65074300	1.04516500	-1.19467700
C	1.35035100	2.22171400	-1.13295300
H	3.71486700	3.83173300	-0.62493100
H	5.82401400	2.81219800	0.22011300
H	4.05021000	-1.09277700	0.19660500
N	1.54063200	-0.03859300	-0.88139500
C	1.06636200	-1.34673700	-0.69025200
O	-0.07820800	-1.50576900	-0.24699100
H	0.93829900	3.19047200	-1.36452500
C	1.84613400	-2.60551100	-1.13167500
C	2.38571000	-3.33733000	0.12302400
H	2.87202400	-4.26523200	-0.19025500
H	3.11973600	-2.75618300	0.68673300
H	1.56487100	-3.59676000	0.79738500
C	2.95223600	-2.32483800	-2.16791200
H	3.80029800	-1.76192900	-1.78187100
H	3.33715000	-3.28337800	-2.52689800
H	2.55419000	-1.78660900	-3.03360200
C	0.79783300	-3.53508200	-1.80471700
H	1.29541600	-4.46395000	-2.09621300
H	-0.02935700	-3.76903600	-1.13414600
H	0.39035700	-3.07780800	-2.71261100
C	-2.03251700	2.89524300	-1.38131000
O	-1.18927100	3.66546400	-0.95853400
O	-3.29881100	3.26501500	-1.66171400
C	-1.84830500	1.45818400	-1.70566800
C	-0.68128000	0.72962500	-1.67041900
H	-2.68935500	0.98701500	-2.20123600
H	-0.78125000	-0.24123100	-2.14649400
C	-3.58344800	4.67673400	-1.54327900
H	-4.61922800	4.79043100	-1.85829700
H	-3.45284200	5.01165800	-0.51173600
H	-2.91630500	5.24938300	-2.19064800
C	-2.92123800	-2.58645500	-1.29008500
O	-2.66636100	-3.28332000	-0.31015000
O	-2.75349100	-1.28159100	-1.35724100
C	-3.48374400	-3.17056100	-2.57716300
H	-4.46728800	-2.73814400	-2.78454100
H	-2.83675300	-2.91983600	-3.42280600
H	-3.57068400	-4.25317300	-2.48434500
C	6.32710000	0.21513200	0.73812200
F	7.21188400	0.05151400	-0.26618400
F	6.13469300	-0.99543800	1.30741600
F	6.90397300	1.01467600	1.65593000

8(C7)^{F}

Sum of electronic and thermal Free Energies=-2004.136007

C	-0.33790400	0.24761800	2.70101000
C	-1.78634800	0.34625100	2.50167000
C	-2.28001100	-0.96596600	2.19966000

C	-1.14398800	-1.84856900	2.08842700
C	0.04863400	-1.09671500	2.48696600
C	1.40301700	-1.68113800	2.72633900
H	2.18277100	-0.91823400	2.72739200
H	1.40973800	-2.16365200	3.71236700
H	1.67340400	-2.43956600	1.99189100
C	0.54095700	1.37115000	3.15374800
H	1.58491600	1.20782100	2.88230800
H	0.22279600	2.32614800	2.73044200
H	0.48800500	1.46569000	4.24550500
C	-2.62520000	1.56303800	2.72120700
H	-3.34188400	1.67332100	1.90442100
H	-3.17160900	1.47079000	3.66821800
H	-2.01523500	2.46667700	2.77718500
C	-3.71281500	-1.35059900	2.03227100
H	-3.81924500	-2.22738600	1.39104600
H	-4.13086200	-1.60245900	3.01574500
H	-4.29243200	-0.52992300	1.60857700
C	-1.21796800	-3.32640300	1.85371800
H	-1.67646000	-3.81893500	2.71974100
H	-1.81789900	-3.55839400	0.97076200
H	-0.22785300	-3.76302700	1.71110700
Rh	-0.92810300	-0.30337700	0.56595000
C	2.26403700	1.37762000	-0.12753200
C	3.46155800	1.88157200	0.44804400
C	4.54425800	1.03574700	0.69445700
C	4.44553200	-0.29186700	0.31570300
C	3.27933400	-0.79870700	-0.28176700
C	2.12969600	0.01267300	-0.48884200
C	2.10233900	3.64390600	0.15846600
C	3.31834200	3.29884200	0.63433400
H	5.45902300	1.42211900	1.13152600
H	5.29560300	-0.94946900	0.44182000
N	1.40592800	2.50402300	-0.30330000
C	0.06001600	2.56715000	-0.69939300
O	-0.70725100	1.62855000	-0.48439300
H	4.04875000	3.96930600	1.06366100
H	1.62591400	4.60697400	0.14508300
C	-0.49419300	3.80585800	-1.44566400
C	0.52959000	4.41357100	-2.43023000
H	0.02865700	5.19181500	-3.01251500
H	1.39525800	4.87340900	-1.95135900
H	0.89438000	3.66024000	-3.13536000
C	-0.99867900	4.85535400	-0.41799800
H	-0.20348800	5.32407500	0.16743800
H	-1.51152500	5.65310500	-0.96238000
H	-1.71911400	4.40690000	0.27232000
C	-1.72301500	3.32689900	-2.25717600
H	-2.13352000	4.18216800	-2.80076000
H	-1.44240400	2.56421700	-2.98978200
H	-2.49866300	2.91432300	-1.61106000
C	-0.62709600	-2.20808100	-2.05090100
O	-0.79085500	-1.66030200	-3.11801400
O	-1.18319800	-3.37611500	-1.68654100
C	0.30609900	-1.71811300	-0.98288100
C	0.90447200	-0.49575800	-1.14084800
H	0.67520100	-2.46360500	-0.29382800
H	0.50104200	0.10202000	-1.95421100
C	-2.05903600	-3.97237700	-2.66710000
H	-2.35078000	-4.93607700	-2.25221100
H	-2.93295800	-3.33624600	-2.82243000
H	-1.53335100	-4.10178500	-3.61507100
C	-3.39674900	0.19450200	-0.99875600
O	-2.35206100	-0.59612400	-0.89308400
O	-3.70901800	1.07981300	-0.20445900
C	-4.23429300	-0.12263800	-2.22971100
H	-4.87696500	-0.98348000	-2.01410500
H	-4.87086600	0.73021900	-2.46892400
H	-3.59654600	-0.38218400	-3.07708100
C	3.37537800	-2.23503800	-0.77218000
F	2.86134100	-2.39884400	-2.00496900
F	2.72094700	-3.11085900	0.05187500
F	4.64933700	-2.65678400	-0.81584300

p1[F]

Sum of electronic and thermal Free Energies=-1276.433466

C	-0.28799100	-1.69457700	-0.01154000
C	-0.17992200	-3.10714300	0.02041800
C	1.08563000	-3.70120400	-0.00470500
C	2.20179900	-2.87999800	-0.04844700
C	2.09255800	-1.47719800	-0.01145300
C	0.83227900	-0.83494000	0.03372800
C	-2.36694800	-2.58440800	0.12460100
C	-1.51292500	-3.64062900	0.10886300
H	1.19536100	-4.78083800	0.02005500
H	3.18998800	-3.32100900	-0.06897600
N	-1.65859000	-1.37237400	0.04132700
C	-2.24459000	-0.18111800	-0.52067500

O	-1.65220600	0.40596400	-1.39809200
H	-1.79096900	-4.68390300	0.15586900
H	-3.44397900	-2.58097600	0.14244400
C	-3.58945400	0.32849000	0.04526600
C	-3.79235400	-0.02528700	1.53206100
H	-4.70912000	0.45348300	1.89085000
H	-3.88947100	-1.09773200	1.71501500
H	-2.96431600	0.34585600	2.14369500
C	-4.74935600	-0.22359600	-0.82080500
H	-4.87713200	-1.30623000	-0.72794200
H	-5.68774500	0.24588400	-0.50838100
H	-4.58811300	0.00998500	-1.87732700
C	-3.56333500	1.86806400	-0.10218900
H	-4.50051100	2.28337500	0.28200100
H	-2.73128200	2.30932200	0.45439700
H	-3.45370000	2.15748900	-1.14879500
C	0.71663700	3.01715300	0.18490400
O	-0.21803900	3.24164100	0.93537700
O	1.44842500	3.99509300	-0.39622200
C	1.20653900	1.68199500	-0.22200400
C	0.59323500	0.59708200	0.27177800
H	2.02818900	1.64395300	-0.92345200
H	-0.23772200	0.80389200	0.94425400
C	1.04631700	5.33408600	-0.07504000
H	1.72713000	5.98620800	-0.62217700
H	0.01300900	5.51126300	-0.38481900
H	1.12491900	5.51327000	1.00049600
C	3.38527700	-0.69402900	0.02897000
F	3.44322700	0.16936400	1.06443800
F	3.57589600	0.03083400	-1.10531800
F	4.46307500	-1.50294400	0.14005900

p2^{F}

Sum of electronic and thermal Free Energies=-1276.439757

C	0.73003400	-0.30471900	-0.08576600
C	0.08812500	-1.55715300	0.10826400
C	0.86595000	-2.71631700	0.29278000
C	2.24479800	-2.61629800	0.25115200
C	2.86404500	-1.36992300	0.00807200
C	2.12286100	-0.20777400	-0.17461100
C	-1.52825500	0.00439100	-0.22792800
C	-1.31532100	-1.33452200	0.03022900
H	0.38437800	-3.67582200	0.45335700
H	2.86318300	-3.49623500	0.39267700
H	2.62751100	0.72379600	-0.39067400
N	-0.25879900	0.65922000	-0.25839600
C	-0.06314400	2.04704300	-0.58435200
O	-0.60475000	2.49777300	-1.57179900
H	-2.10943700	-2.05390400	0.14894400
C	0.70123900	2.97712600	0.39086900
C	1.92779200	3.56664200	-0.34159800
H	2.38158600	4.34877600	0.27510700
H	2.69862900	2.81526100	-0.53765200
H	1.62929800	4.00701900	-1.29640400
C	1.10266000	2.33358800	1.72893700
H	1.87679900	1.57211300	1.62730900
H	1.49477700	3.11208800	2.39112100
H	0.24190900	1.87694300	2.22678100
C	-0.29218400	4.13327000	0.68696700
H	0.19388700	4.87169300	1.33191400
H	-0.60846100	4.62095900	-0.23667600
H	-1.18343900	3.76802400	1.20867900
C	-4.70187500	-0.84214000	-0.01581100
O	-4.18065800	-1.92245300	0.20834500
O	-6.05059500	-0.67948300	-0.01936100
C	-4.05753700	0.44744400	-0.31152800
C	-2.74285900	0.77384000	-0.38872500
H	-4.76659400	1.24930800	-0.48917500
H	-2.57022900	1.81473900	-0.63945100
C	-6.81112600	-1.86333100	0.25514900
H	-7.85677600	-1.55846700	0.21156400
H	-6.60607100	-2.63683500	-0.48977700
H	-6.56832400	-2.25900700	1.24501600
C	4.36312600	-1.32878000	-0.10004000
F	4.80235000	-1.96858000	-1.20891200
F	4.95491000	-1.93728300	0.95398000
F	4.84129800	-0.06480500	-0.15548300

R3

Sum of electronic and thermal Free Energies=-971.238652

C	-0.10362700	0.67058600	-0.00365600
C	-0.43668100	2.04809600	0.00109600
C	-1.78274600	2.44197300	-0.00820400
C	-2.76708900	1.46582500	-0.02124500
C	-2.41796900	0.10161200	-0.02481600
C	-1.08936800	-0.31977700	-0.01556600
C	1.81262300	1.88620300	0.01281300
C	0.79784400	2.78770500	0.01197900

H	-2.04758400	3.49495300	-0.00810600
H	-3.81491200	1.74697800	-0.03536800
H	-0.83302800	-1.36727400	-0.02134300
N	1.30841800	0.57289100	0.00273300
C	2.01703500	-0.65110300	-0.00073900
O	1.38564200	-1.69281900	-0.00449100
H	0.90941400	3.86286500	0.01860000
H	2.87064100	2.07065000	0.02092400
C	3.56808200	-0.66597400	-0.00095300
C	4.13655200	-0.02126700	1.28701600
H	5.22447500	-0.14371800	1.29783600
H	3.92491900	1.04488700	1.38365200
H	3.73750100	-0.52044700	2.17577500
C	4.13732400	-0.00125600	-1.27826600
H	3.92701100	1.06653200	-1.35737100
H	5.22509600	-0.12494200	-1.29110900
H	3.73767400	-0.48524800	-2.17511300
C	3.99814600	-2.14788100	-0.01234600
H	5.09134400	-2.20553700	-0.01247100
H	3.62027400	-2.67901000	0.86391000
H	3.62098900	-2.66514200	-0.89722700
C	-3.52655500	-0.91426400	0.00092600
F	-4.47977000	-0.63422500	-0.92042600
F	-4.15444200	-0.93705800	1.20201600
F	-3.08793200	-2.16717400	-0.24092600

TSa(C7)^{F}

Sum of electronic and thermal Free Energies=-1698.922859

C	0.73488100	-1.57174500	2.95243900
C	1.87490500	-0.71656000	2.68411000
C	1.43396600	0.65195000	2.72572400
C	0.00987600	0.65002800	3.01177700
C	-0.41902700	-0.71099000	3.17178200
C	-1.78612400	-1.17034700	3.55218100
H	-2.02255100	-2.13504300	3.10199800
H	-1.83489600	-1.27855300	4.64364400
H	-2.55088300	-0.45423000	3.24966500
C	0.72780200	-3.05955300	3.06182000
H	-0.14623700	-3.48215500	2.56038500
H	1.62454900	-3.50584200	2.62996600
H	0.68397200	-3.34667100	4.12023000
C	3.28032900	-1.17008700	2.46298100
H	3.81828600	-0.49786100	1.79203600
H	3.81183200	-1.17754200	3.42336100
H	3.32245200	-2.18140400	2.05514500
C	2.32790200	1.84676700	2.69930000
H	1.80509300	2.75474200	2.40519800
H	2.72235400	2.00114700	3.71292100
H	3.17873800	1.70804800	2.03080600
C	-0.85851300	1.84753300	3.21029100
H	-1.01447800	1.99128600	4.28758200
H	-0.41631500	2.75319700	2.80136900
H	-1.83902600	1.71014700	2.74899500
Rh	0.32972000	-0.51645200	1.14281100
C	2.91097800	0.82803000	-1.04806800
C	4.11517900	1.56507300	-1.16300100
C	4.12814300	2.93654400	-0.88594900
C	2.94085800	3.54766500	-0.50765500
C	1.74723000	2.80987400	-0.43483000
C	1.69712100	1.43640700	-0.71109300
C	4.56833200	-0.55063000	-1.80991300
C	5.13743400	0.66354000	-1.63670800
H	5.04320300	3.51186600	-0.98108000
H	2.92373100	4.60772700	-0.27934400
H	0.73812200	0.94786900	-0.81676300
N	3.20121200	-0.50705200	-1.43817200
C	2.33482500	-1.57668500	-1.30903000
O	1.31225900	-1.44497600	-0.61645000
H	6.17083600	0.90922500	-1.83639700
H	5.01731500	-1.46731600	-2.14379800
C	2.58207000	-2.91889500	-2.02973500
C	3.70909700	-3.71107400	-1.31249100
H	3.79931400	-4.69095200	-1.78948700
H	4.69173300	-3.23746100	-1.35217000
H	3.45733700	-3.88166300	-0.26026900
C	2.90028200	-2.69645400	-3.52854500
H	3.83414300	-2.16385400	-3.71413200
H	2.97527500	-3.67239400	-4.01609700
H	2.09313500	-2.14416100	-4.01878200
C	1.28951300	-3.75782700	-1.93309600
H	1.45694200	-4.71124600	-2.44143700
H	1.01642200	-3.96459500	-0.89630300
H	0.44079500	-3.25936200	-2.40425100
N	-1.65860700	-0.06101900	-0.66951700
S	-1.97842700	-1.64296500	-0.63311200
O	-1.87050300	-2.42947600	-1.85354500
O	-1.14863400	-2.08093600	0.55946000
S	-2.17203500	0.89656000	-1.95095700

O	-1.08850200	1.82772300	-2.25182200
O	-2.83824100	0.13271800	-2.99900100
C	-3.72703000	-1.90651800	0.00759500
C	-3.52424000	1.89633500	-1.11804100
F	-4.60202600	-1.67301600	-0.95574500
F	-3.82965200	-3.16451100	0.43217300
F	-3.94792200	-1.07580000	1.03578200
F	-3.93277300	2.83248100	-1.96564400
F	-3.07770500	2.47097600	0.00306500
F	-4.54072300	1.08596600	-0.81154000
C	0.50026300	3.55863600	-0.04412800
F	-0.47935700	2.72102100	0.37573500
F	0.00972500	4.32096700	-1.02277500
F	0.75856700	4.38744900	1.01383800

TSc(C2)^{F}

Sum of electronic and thermal Free Energies= -3297.540896

C	-3.04392900	-1.06410300	0.02595400
C	-2.61514100	-1.87021900	-1.06307800
C	-3.56520600	-2.50030000	-1.88313800
C	-4.91273100	-2.29244300	-1.63254200
C	-5.31850300	-1.44959000	-0.58077100
C	-4.39809000	-0.81831600	0.25393300
C	-0.75856500	-1.03058600	-0.08115100
C	-1.17863400	-1.84213300	-1.09294100
H	-3.24542800	-3.13720400	-2.70149500
H	-5.66514700	-2.77501600	-2.24622400
H	-4.75598400	-0.18002500	1.04810700
N	-1.87992600	-0.55732800	0.65073500
C	-1.67761500	0.40344100	1.63859000
O	-0.75246800	1.21874200	1.45793700
H	-0.51457900	-2.39779600	-1.74107800
H	0.24173900	-0.96411000	0.33310300
C	-2.42878700	0.43514300	2.97740500
C	-3.03908800	-0.93014200	3.35093800
H	-3.46937800	-0.85525500	4.35320400
H	-3.83227900	-1.25921800	2.68042300
H	-2.27195900	-1.70968100	3.37830300
C	-3.49766900	1.55736400	2.93909100
H	-4.28461900	1.38265600	2.20123000
H	-3.97653400	1.62129300	3.92005100
H	-3.03610600	2.52585900	2.72574600
C	-1.37718000	0.80719100	4.05756400
H	-1.86837400	0.80892300	5.03411900
H	-0.56020000	0.08048000	4.08683100
H	-0.94822800	1.79439400	3.88078000
C	0.80734900	1.82069300	-2.48833300
C	-0.56022900	2.15432000	-2.10660400
C	-0.49972300	3.22130600	-1.14735200
C	0.90253100	3.50973600	-0.88209900
C	1.70527400	2.65669900	-1.74490200
C	3.19378900	2.68470400	-1.86179800
H	3.60370400	1.70617700	-2.11949700
H	3.47172100	3.39308300	-2.65351900
H	3.66524000	3.01394400	-0.93507000
C	1.18997200	0.81844300	-3.52330200
H	2.23417600	0.51832300	-3.43752600
H	0.57342400	-0.08057700	-3.46951700
H	1.03910700	1.26979600	-4.51371700
C	-1.79395300	1.58260200	-2.72879100
H	-2.64786700	1.61103600	-2.04918500
H	-2.05813500	2.16706500	-3.61934500
H	-1.64152800	0.54877900	-3.04134800
C	-1.65889000	3.92701200	-0.52630400
H	-1.46715500	4.17440800	0.52008700
H	-1.83551200	4.86823500	-1.06246000
H	-2.57363600	3.33547600	-0.58490800
C	1.43408300	4.55750300	0.03719700
H	1.67207300	5.46111500	-0.53918700
H	0.70905500	4.83059300	0.80562400
H	2.35018500	4.22291700	0.52832200
Rh	0.51299100	1.47581100	-0.31165400
N	2.40920900	-0.89853100	0.02962800
S	3.12281900	0.17966200	0.97552000
O	4.47067800	0.64909800	0.67632800
O	2.07131400	1.25207100	1.20911600
S	3.05576900	-1.58409500	-1.32266500
O	1.92894600	-2.23225500	-1.99744000
O	3.92609000	-0.67365200	-2.07358500
C	3.15321800	-0.66495300	2.64854400
C	4.15010700	-2.95815000	-0.67162300
F	3.94482800	-1.72859100	2.58706900
F	3.60457900	0.19487600	3.55329800
F	1.91088300	-1.04568100	2.96805800
F	4.69722400	-3.58934700	-1.70310700
F	3.41242200	-3.80509000	0.04281900
F	5.10090800	-2.43125200	0.10000900
C	-6.79161800	-1.17290900	-0.39462300

F	-7.05819700	-0.70056200	0.84219700
F	-7.52920600	-2.28100300	-0.58536200
F	-7.22076200	-0.24569700	-1.27872300

TS1(C2)^{F}

Sum of electronic and thermal Free Energies=-3297.530171

C	-1.31441800	-2.91873100	-2.03105600
C	-0.68650500	-3.66146800	-0.95481500
C	-1.70452100	-3.90472400	0.06862000
C	-2.89270500	-3.23752000	-0.32243600
C	-2.63963200	-2.58125100	-1.60828000
C	-3.66501200	-1.80933400	-2.37763800
H	-3.21882000	-1.24580600	-3.19881900
H	-4.40578000	-2.49570700	-2.80621400
H	-4.19713600	-1.10685900	-1.73171400
C	-0.70752000	-2.62592000	-3.36683000
H	0.37973800	-2.55839400	-3.31499700
H	-0.95864600	-3.44078300	-4.05756900
H	-1.09407500	-1.70090500	-3.79893000
C	0.67214400	-4.28963100	-0.99032000
H	1.08410800	-4.40876200	0.01418700
H	0.61362000	-5.28761900	-1.44293300
H	1.37561600	-3.69780100	-1.57955000
C	-1.48725100	-4.70277900	1.31425300
H	-2.23561100	-4.47969400	2.07584700
H	-1.54924500	-5.77328000	1.08276700
H	-0.49989800	-4.51555800	1.74312700
C	-4.19225000	-3.17317700	0.41296500
H	-4.94100400	-3.78844400	-0.10104800
H	-4.10162600	-3.53946600	1.43640800
H	-4.57105800	-2.14869700	0.45073200
Rh	-1.21800800	-1.72313000	-0.16522700
C	2.64029200	-0.13955500	-0.27670100
C	2.36927900	0.16027800	-1.64081000
C	3.40705700	0.51391600	-2.52187500
C	4.70574600	0.53565600	-2.04748900
C	4.96781800	0.20612700	-0.70339300
C	3.95653800	-0.13198700	0.19262000
C	0.34835200	-0.34813000	-0.66521600
C	0.96762600	0.01950800	-1.84676500
H	3.18706800	0.76113900	-3.55531500
H	5.52780200	0.80779300	-2.69981200
H	4.22332800	-0.36365600	1.21036000
N	1.40639300	-0.45250100	0.33208900
C	0.99628900	-0.84887900	1.59241100
O	-0.13021100	-1.39986300	1.64685300
H	0.44375700	0.24527000	-2.76656300
H	-0.48603400	0.61923300	-0.32535600
C	1.75381400	-0.63934300	2.90807200
C	2.36609500	0.77805200	2.99674100
H	2.89326500	0.86663900	3.95080200
H	3.07014300	1.02168300	2.20355900
H	1.58097000	1.53778800	2.97621700
C	2.80796700	-1.77105600	3.05692600
H	3.52270100	-1.82889500	2.23506600
H	3.37170800	-1.60629800	3.97939200
H	2.31292000	-2.74375700	3.13679900
C	0.74280800	-0.78435000	4.07021200
H	1.27598300	-0.62820400	5.01188700
H	-0.05534500	-0.04109300	4.00102600
H	0.28630500	-1.77538700	4.09398900
N	-1.21173000	1.68079100	0.16485600
S	-0.37330100	3.12645000	0.38861000
O	-0.99215400	3.97852800	1.39105000
O	1.04607400	2.78299900	0.40892000
S	-2.49685900	1.20973300	1.05453500
O	-2.70480900	-0.21043100	0.62229100
O	-2.45542500	1.51247100	2.47491900
C	-0.69085600	3.89629400	-1.28836300
C	-3.99953100	2.07158200	0.32036000
F	-1.99780300	4.08620900	-1.45509200
F	-0.04784300	5.05352400	-1.35271500
F	-0.23768900	3.07286800	-2.24265600
F	-5.08024400	1.57653400	0.91346200
F	-4.04638200	1.81342400	-0.98850800
F	-3.91229500	3.37607300	0.52401600
C	6.40740200	0.16958800	-0.23932800
F	7.01939700	-0.94728700	-0.68503700
F	6.50040600	0.17522000	1.10589400
F	7.09729200	1.22352200	-0.71053500

TS1(C7)^{F}

Sum of electronic and thermal Free Energies=-3297.529182

C	3.60928200	-0.79247800	-1.28629000
C	3.69887200	-0.47552200	0.13831400
C	3.17139100	-1.59751000	0.87850800
C	2.63448300	-2.53345200	-0.07120600
C	2.95091800	-2.04413800	-1.41301000

C	2.60579700	-2.76714700	-2.67385000
H	2.74803900	-2.14289300	-3.55665000
H	3.24402600	-3.65330400	-2.77668400
H	1.56620300	-3.10372600	-2.66017600
C	4.12086900	0.07862100	-2.38858400
H	3.73125600	-0.22456400	-3.36116600
H	3.84925900	1.12519600	-2.22771900
H	5.21545300	0.02285200	-2.43036900
C	4.42770200	0.69710000	0.71644400
H	4.05772100	0.95655700	1.71018000
H	5.49501800	0.45917400	0.81023600
H	4.34564300	1.57820100	0.07632600
C	3.25701700	-1.77481400	2.35983600
H	2.47652700	-2.43081200	2.74121500
H	4.22800600	-2.22618700	2.60194100
H	3.19587600	-0.82142900	2.88815800
C	2.05153900	-3.87965100	0.21987800
H	2.84091600	-4.63918600	0.14943600
H	1.61759500	-3.93289900	1.21693100
H	1.27610600	-4.14098000	-0.50317400
Rh	1.58955000	-0.61003900	-0.34148600
C	0.69600100	1.46369900	1.65720400
C	0.73898600	1.96914000	2.97803800
C	0.41833400	1.12504900	4.04525500
C	0.02450300	-0.18232000	3.77317100
C	-0.02275200	-0.65607300	2.45562400
C	0.32253900	0.14002700	1.33032500
C	1.21634800	3.69051400	1.60498400
C	1.08977000	3.36615000	2.91131500
H	0.44153500	1.49197900	5.06653500
H	-0.27042200	-0.83507900	4.58841100
H	-0.67493800	0.08492900	0.38483200
N	0.99771500	2.54938800	0.79533100
C	1.04032300	2.47808900	-0.58548300
O	1.15710400	1.36526100	-1.13274800
H	1.21682300	4.04203300	3.74495300
H	1.47554700	4.63459400	1.16307800
C	0.95286400	3.72829500	-1.48553800
C	2.31150900	4.48075100	-1.45971000
H	2.26482900	5.30025400	-2.18220400
H	2.56377300	4.91514800	-0.49004600
H	3.13352200	3.82321000	-1.76194700
C	-0.21736300	4.65416100	-1.07484600
H	-0.09201800	5.12014300	-0.09696000
H	-0.29412200	5.45706900	-1.81325900
H	-1.16529800	4.11189300	-1.06253300
C	0.70385800	3.25112600	-2.93429500
H	0.61937600	4.13034300	-3.57839400
H	1.52390200	2.63322300	-3.30630200
H	-0.21848800	2.67256900	-3.01972700
N	-1.71127800	0.13127100	-0.43158200
S	-1.41854500	-0.58994000	-1.87239300
O	-1.55269600	0.24734400	-3.05259800
O	-0.12812800	-1.30969300	-1.63069900
S	-2.88679000	1.31222100	-0.17289900
O	-2.23935000	2.36774700	0.60334200
O	-3.65909400	1.58824900	-1.37355000
C	-2.66766500	-1.99034700	-2.03118300
C	-3.99732500	0.39001100	1.02132200
F	-3.87132100	-1.47157400	-2.22504400
F	-2.30637800	-2.73240100	-3.07292400
F	-2.65542700	-2.72340800	-0.92326200
F	-4.99256200	1.19383000	1.37070200
F	-3.28905700	0.04557000	2.09817300
F	-4.47450700	-0.70286700	0.42981400
C	-0.56302200	-2.05889500	2.29221700
F	0.22348800	-2.96697100	2.94231300
F	-1.79184800	-2.17570700	2.82396600
F	-0.63488700	-2.45661100	1.00623300

TS2(C2)^{F}

Sum of electronic and thermal Free Energies=-1776.271789

C	3.08251900	0.36341700	1.93585600
C	1.86577200	-0.25191500	2.48942200
C	1.75444200	-1.56419000	1.96882300
C	2.84184500	-1.75286000	1.01922600
C	3.71615700	-0.59617100	1.10365600
C	5.07459500	-0.48958400	0.48779500
H	5.32733500	0.53949700	0.22512100
H	5.82099800	-0.84317200	1.21039600
H	5.15753700	-1.11142200	-0.40449600
C	3.61503300	1.70571600	2.33373700
H	4.35230300	2.07504000	1.61836300
H	2.81594900	2.44744800	2.41004100
H	4.10219400	1.64450800	3.31511200
C	0.97772600	0.40859300	3.49742600
H	0.01873900	-0.10332800	3.59599000
H	1.45983700	0.40671600	4.48272400

H	0.78537900	1.45142700	3.23133600
C	0.72772600	-2.59306100	2.32444900
H	0.37043000	-3.13139600	1.44363300
H	1.16376100	-3.33072000	3.00879400
H	-0.13823600	-2.15069500	2.82001600
C	3.15462000	-3.01630300	0.27829600
H	3.91797700	-3.59184700	0.81717500
H	2.27193600	-3.65228500	0.18224200
H	3.53389700	-2.79894400	-0.72285300
Rh	1.66616400	-0.03419900	0.25066400
C	-2.47399700	-0.35417600	-0.40656500
C	-2.18001800	-1.71329200	-0.69422100
C	-3.21122700	-2.65527300	-0.81607400
C	-4.52464200	-2.24354700	-0.64269700
C	-4.80523700	-0.90091800	-0.34752400
C	-3.79428100	0.05518200	-0.22456500
C	-0.16939000	-0.63493100	-0.58491800
C	-0.75710300	-1.84853800	-0.81343100
H	-2.98048000	-3.69211200	-1.03828300
H	-5.33888600	-2.95481800	-0.72450000
H	-4.07806100	1.06809400	0.00574900
N	-1.22072100	0.33049000	-0.33193200
C	-0.80892400	1.60780000	0.00080200
O	0.41544900	1.75667000	0.22348200
H	-0.23113300	-2.74835100	-1.10305300
C	-1.70861200	2.84789900	0.07935700
C	-2.55496900	2.77841400	1.38030800
H	-3.25441300	3.61919100	1.39435400
H	-3.13083800	1.86103800	1.49862400
H	-1.90363500	2.87317400	2.25445100
C	-2.55460200	2.99634000	-1.20908700
H	-3.17015200	2.13214400	-1.45219200
H	-3.21744700	3.85951900	-1.10107700
H	-1.90256900	3.18996400	-2.06681700
C	-0.81036900	4.10094900	0.18512400
H	-1.45270000	4.98374300	0.24812300
H	-0.17561300	4.07485300	1.07254100
H	-0.16586200	4.21102100	-0.69047300
C	3.49009100	0.05056200	-2.23858300
O	3.69146300	-1.13009900	-2.47349500
O	4.40649400	1.01856600	-2.42287100
C	2.20513200	0.62535400	-1.76151400
C	1.01533500	-0.11555300	-2.07528500
H	2.15741500	1.70965500	-1.75229200
H	0.18246100	0.44222800	-2.49303800
H	1.17845200	-1.09051300	-2.52180100
C	5.64380200	0.61251900	-3.04684000
H	5.44213800	0.12474300	-4.00259300
H	6.20817600	1.53195600	-3.19452500
H	6.19557100	-0.07575700	-2.40337400
C	-6.24452100	-0.46374800	-0.21535700
F	-6.80452100	-0.25893800	-1.42548300
F	-6.35218700	0.69201100	0.47733500
F	-6.98367400	-1.39510700	0.41677400

TS2(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.263905

C	1.75850200	-0.82510400	2.07926500
C	0.41568900	-1.06602800	2.44856100
C	-0.05366000	-2.25783400	1.72030400
C	1.02396700	-2.74263300	0.93082200
C	2.13236900	-1.82623700	1.09230500
C	3.52787800	-2.09586900	0.62205300
H	4.14216800	-1.19801000	0.60046500
H	3.99543300	-2.80597100	1.31724800
H	3.55055300	-2.54837200	-0.37040300
C	2.66971000	0.22487000	2.63599100
H	2.11159100	1.06719900	3.04975900
H	3.27497700	-0.20086600	3.44607100
H	3.35649200	0.60885700	1.88054700
C	-0.39006100	-0.32277100	3.46765400
H	-1.43614000	-0.23770800	3.16343700
H	-0.37162800	-0.85677800	4.42602200
H	0.00103700	0.68200700	3.64003600
C	-1.38604100	-2.91073800	1.90902000
H	-1.62279800	-3.57925200	1.07914300
H	-1.38775100	-3.50430000	2.83194800
H	-2.18503400	-2.17041500	1.98839500
C	1.04074300	-4.00636500	0.12620600
H	1.25037400	-4.86053600	0.78182400
H	0.08462700	-4.18081100	-0.37017100
H	1.81812500	-3.98427400	-0.64022800
Rh	0.35228900	-0.69129100	0.21517200
C	-0.13560100	2.32927100	-0.13055900
C	0.20744600	3.69281200	0.04234500
C	1.53459700	4.11122500	-0.08277100
C	2.48345900	3.16697300	-0.43136700
C	2.12899500	1.82417400	-0.66434200

C	0.80753700	1.34250700	-0.49720400
C	-2.02765200	3.56243100	0.27090600
C	-0.99966000	4.43574100	0.29419900
H	1.80562500	5.15224000	0.05687500
H	3.51636400	3.46815600	-0.57020900
N	-1.55263200	2.24614700	0.04390400
C	-2.29524200	1.08924300	0.20240300
O	-1.71991400	-0.00765700	0.26383600
H	-1.07736000	5.50184800	0.45341200
H	-3.07466700	3.75092800	0.40648500
C	-3.84126800	1.11053100	0.29314300
C	-4.44207800	1.81648500	-0.94925700
H	-5.53211900	1.74210800	-0.89868100
H	-4.18994900	2.87448700	-1.03273700
H	-4.11373800	1.31465700	-1.86392500
C	-4.31908900	1.74216800	1.62792300
H	-4.10370100	2.80542300	1.73690100
H	-5.40388900	1.62111700	1.69650200
H	-3.87657100	1.22287300	2.48448900
C	-4.34317300	-0.35012100	0.27736300
H	-5.43626400	-0.33934900	0.30429800
H	-4.01822500	-0.86928600	-0.62494100
H	-3.99181700	-0.90760300	1.14891500
C	-1.36799900	-1.70988700	-2.11147700
O	-2.33552400	-1.01269200	-2.36019100
O	-1.41546100	-3.05912000	-2.05801700
C	0.01093600	-1.20896600	-1.86828900
C	0.25889600	0.18440100	-2.07870500
H	0.80335100	-1.91264600	-2.10471900
H	1.14392600	0.45746900	-2.63288600
H	-0.62190400	0.77975500	-2.29740700
C	-2.68811700	-3.65445700	-2.38683100
H	-2.50812400	-4.72814100	-2.42199700
H	-3.43147000	-3.41588700	-1.62234000
H	-3.03981400	-3.29060400	-3.35403700
C	3.27806400	1.01473700	-1.22205000
F	3.74373800	1.57267700	-2.35905000
F	2.97868800	-0.26965800	-1.52649100
F	4.32379700	0.97910700	-0.35322200

TS3(C2)[F]

Sum of electronic and thermal Free Energies=-1776.280781

C	2.75354600	-0.29566000	-0.66996400
C	2.86618900	-0.88463500	-1.95183400
C	4.10231800	-1.33534700	-2.43603900
C	5.22035200	-1.22334000	-1.62633500
C	5.09554400	-0.67964100	-0.33688100
C	3.87548500	-0.22191800	0.15808200
C	0.66928700	-0.43004600	-1.61459400
C	1.55131500	-0.95918800	-2.50644000
H	4.17228200	-1.78090900	-3.42300100
H	6.18738700	-1.57340900	-1.96958200
H	3.84794600	0.16518600	1.16119500
N	1.37593600	0.02355900	-0.45613700
C	0.74028900	0.63020300	0.63436900
O	-0.45514400	0.37897300	0.85980200
H	1.28557100	-1.37001300	-3.47115000
C	1.42014400	1.63139300	1.60018700
C	2.44379300	2.55467500	0.90113800
H	2.80228700	3.28470700	1.63268200
H	3.31634400	2.05200300	0.49278600
H	1.95603000	3.09854900	0.08892400
C	1.99120300	0.85358800	2.81897300
H	2.68716500	0.05319600	2.56804700
H	2.51294200	1.55568600	3.47566000
H	1.17393400	0.40249400	3.38972400
C	0.30909000	2.56002700	2.15449500
H	0.76940400	3.27462400	2.84241600
H	-0.17094600	3.11595300	1.34686800
H	-0.45231500	2.00175600	2.70051000
C	-3.23246200	-1.40862700	1.73131900
C	-3.49446100	-2.27413500	0.63745800
C	-4.12763000	-1.47807700	-0.40430600
C	-4.40034000	-0.15319000	0.14134900
C	-3.80059400	-0.08819400	1.42207500
C	-3.81269600	1.07158300	2.36873000
H	-2.84281800	1.19884000	2.85641600
H	-4.55790800	0.90981900	3.15761500
H	-4.06268900	2.00484100	1.86109500
C	-2.59888700	-1.77073200	3.03866800
H	-1.95648100	-0.96706000	3.40666200
H	-1.99809500	-2.67875400	2.96110900
H	-3.37284500	-1.94485600	3.79673700
C	-3.21648200	-3.74600500	0.56832000
H	-2.99610600	-4.07211400	-0.45018100
H	-4.09661900	-4.30488400	0.90968800
H	-2.37641800	-4.03138600	1.20432500
C	-4.67168200	-2.01588000	-1.69403000

H	-4.72331200	-1.24630700	-2.46784900
H	-5.68989700	-2.39600100	-1.54361200
H	-4.06689100	-2.84183900	-2.07486800
C	-5.18819500	0.92827200	-0.53311900
H	-6.22923600	0.89660200	-0.18824500
H	-5.20124600	0.80591300	-1.61769300
H	-4.79180700	1.92147500	-0.31347800
Rh	-2.15630600	-0.57688200	-0.07541300
C	-1.70952900	0.67352500	-1.79047200
C	-0.78564400	-0.42701000	-1.87623600
H	-1.01206800	-1.12097100	-2.68282900
H	-1.11376300	-1.56172900	-0.79735800
C	-1.31794300	2.07345100	-1.50203600
O	-0.21421700	2.45979500	-1.15830900
O	-2.36416900	2.89757600	-1.71126000
C	-2.09777100	4.30603100	-1.54478400
H	-3.01521300	4.81246900	-1.84086900
H	-1.85604900	4.52900900	-0.50281500
H	-1.26476400	4.61328000	-2.18003800
H	-2.58205900	0.60261400	-2.43237500
C	6.33114800	-0.54857700	0.52035500
F	6.02132000	-0.37324200	1.82441600
F	7.07747600	0.50930000	0.13974100
F	7.11191200	-1.64273000	0.42667100

TS3(C7)^{F}

Sum of electronic and thermal Free Energies=-1776.271424

C	-2.69052200	0.86314600	-1.87603400
C	-2.61054100	-0.55113800	-1.95562500
C	-2.92002100	-1.06715000	-0.62906300
C	-3.39365700	0.04976800	0.19367900
C	-3.19775200	1.23261700	-0.54299300
C	-3.58138600	2.61483900	-0.11380700
H	-2.93998100	3.37498800	-0.56349700
H	-4.61124100	2.83227200	-0.42631600
H	-3.53508900	2.72547500	0.97192200
C	-2.43096200	1.84097700	-2.97867900
H	-1.92561300	2.73589900	-2.60681500
H	-1.81638300	1.40714700	-3.76931500
H	-3.37941400	2.16238700	-3.42715900
C	-2.29876200	-1.37691300	-3.16894300
H	-1.74915700	-2.28452600	-2.91236700
H	-3.23110800	-1.67972600	-3.66113300
H	-1.70578500	-0.81982200	-3.89681700
C	-3.03298900	-2.51806200	-0.27332900
H	-2.81559700	-2.68793900	0.78234000
H	-4.04992100	-2.87695600	-0.47689600
H	-2.34085600	-3.12617600	-0.85975100
C	-4.00401700	-0.05067900	1.55820000
H	-5.01246600	0.37758300	1.54260500
H	-4.09258700	-1.09014600	1.87753400
H	-3.42627200	0.48699100	2.31681300
Rh	-1.13548000	0.14592100	-0.40319800
C	2.81947200	0.16699900	-0.00794400
C	4.22392700	0.01740400	-0.16614900
C	4.79417200	-1.21563800	-0.47528500
C	3.95482500	-2.30594100	-0.63722800
C	2.58055900	-2.18972300	-0.39803300
C	1.97501800	-0.96539700	0.00100800
C	3.86572200	2.18544000	0.30730800
C	4.84516100	1.29597400	0.05911200
H	5.86752600	-1.31307900	-0.59811000
H	4.36065900	-3.26746200	-0.92383100
N	2.58769400	1.56310100	0.23685700
C	1.42481800	2.28594800	-0.04350400
O	0.46268000	1.72582900	-0.57740000
H	5.90462400	1.50721900	0.03456800
H	3.94877300	3.23696200	0.49836100
C	1.31698000	3.79348200	0.31569800
C	2.07267600	4.66576600	-0.72309800
H	1.85998400	5.71822800	-0.51428700
H	3.15622600	4.54362500	-0.71368500
H	1.72139300	4.44939800	-1.73680300
C	1.77385100	4.07799000	1.76871500
H	2.83025500	3.89033100	1.95972500
H	1.58507100	5.13177300	1.99296700
H	1.19666700	3.48254900	2.48353800
C	-0.17511000	4.17985700	0.22420200
H	-0.28248500	5.23621600	0.48493000
H	-0.56231000	4.03497700	-0.78607500
H	-0.78529900	3.59540300	0.91723000
C	-0.86078800	-0.62104000	2.58847600
O	-1.25609300	0.12438900	3.46513500
O	-1.11934000	-1.94749200	2.56385300
C	-0.02348400	-0.14885800	1.45508200
C	0.57173300	-1.04018900	0.51032600
H	0.45561100	0.78713800	1.71025700
H	0.21766300	-2.05421900	0.62603700

H	-0.04319500	-0.82404400	-1.01151300
C	-1.80321900	-2.46890900	3.72463900
H	-1.88852600	-3.54121300	3.55447600
H	-1.22016700	-2.26766300	4.62541600
H	-2.78913800	-2.01203900	3.83142500
C	1.75610100	-3.45061800	-0.57613000
F	0.66606200	-3.22826200	-1.36477700
F	1.28425800	-3.93665500	0.59819900
F	2.45768700	-4.43522100	-1.15522000

R1'

Sum of electronic and thermal Free Energies=-634.195699

C	1.01671800	-0.00281700	0.00011900
C	2.20037000	0.78995300	-0.00008500
C	3.46559500	0.18962100	-0.00028500
C	3.55974300	-1.19646300	-0.00021800
C	2.39565700	-1.97682800	0.00008300
C	1.12515200	-1.40020000	0.00028700
C	0.45046900	2.20512200	0.00038200
C	1.80233900	2.17245700	0.00005700
H	4.35764400	0.80955800	-0.00044500
H	4.53320900	-1.67746800	-0.00038500
H	2.47391800	-3.05993600	0.00017100
H	0.26748500	-2.05349700	0.00053100
N	-0.08494700	0.89906100	0.00029300
C	-1.51158100	0.79962300	-0.00015000
O	-2.14108600	1.84344100	-0.00048400
H	2.45816300	3.03182700	0.00004800
H	-0.23717600	3.03334800	0.00050400
C	-2.25194500	-0.55197900	-0.00000900
C	-1.94154600	-1.33480800	1.30046900
H	-2.40870100	-2.32434600	1.25352300
H	-0.87987100	-1.47084800	1.50119500
H	-2.36953700	-0.80664000	2.15845800
C	-1.94129000	-1.33520300	-1.30022900
H	-0.87956800	-1.47124000	-1.50071000
H	-2.40844800	-2.32471800	-1.25310600
H	-2.36910500	-0.80728000	-2.15847000
C	-3.76609700	-0.25246500	-0.00020800
H	-4.31700300	-1.19902600	-0.00016000
H	-4.05970200	0.32172000	0.88108800
H	-4.05949600	0.32153400	-0.88168600

TS-R1

Sum of electronic and thermal Free Energies=-634.189111

C	-1.08965600	-0.06034200	0.15423600
C	-2.13316500	0.85906100	-0.14731500
C	-3.44274500	0.37464100	-0.30996200
C	-3.68628400	-0.98286400	-0.14985200
C	-2.64344500	-1.87235200	0.17863200
C	-1.33625600	-1.42630000	0.33772200
C	-0.21053000	2.01745900	0.07273700
C	-1.54205300	2.16676000	-0.19446300
H	-4.25298400	1.05852400	-0.54722900
H	-4.69514600	-1.36710800	-0.26826600
H	-2.86435000	-2.92663500	0.31693800
H	-0.54421800	-2.11545500	0.61112100
N	0.09516700	0.66814000	0.24559900
C	1.38683000	0.19852500	0.73379800
O	1.66010400	0.33158100	1.90135400
H	-2.04515100	3.10137200	-0.39838100
H	0.57175600	2.75869700	0.14913700
C	2.36890500	-0.33749900	-0.31700300
C	2.79090500	0.87205300	-1.19161800
H	3.52780100	0.54041600	-1.93024900
H	1.93973200	1.29763300	-1.72972600
H	3.25375200	1.65936200	-0.58730800
C	1.72339300	-1.40802800	-1.22034300
H	0.82344400	-1.03787400	-1.71657000
H	2.44116000	-1.70203700	-1.99302700
H	1.46054000	-2.30765900	-0.65569400
C	3.59883600	-0.91656700	0.40061100
H	4.32449800	-1.27246600	-0.33756700
H	4.08169300	-0.16605800	1.03072100
H	3.32205500	-1.75760800	1.04299300

P2

Sum of electronic and thermal Free Energies=-939.403907

C	1.78397200	-1.10439600	-0.21705300
C	0.86790200	-2.15492800	0.05187200
C	1.35402900	-3.44998300	0.31524300
C	2.72346600	-3.66240600	0.31053500
C	3.61734400	-2.60290500	0.04487700
C	3.16779000	-1.31435900	-0.22051300
C	-0.33793800	-0.25899300	-0.30956500
C	-0.44555500	-1.60625400	-0.02498400
H	0.66190100	-4.26122500	0.52077700
H	3.11828200	-4.65435800	0.50874700

H	4.68542300	-2.79978700	0.03544100
H	3.85708800	-0.51224600	-0.45291100
N	1.04340200	0.06983500	-0.39377600
C	1.68962200	1.33848800	-0.53314800
O	2.61913200	1.42732100	-1.31087500
H	-1.38643200	-2.12516700	0.06447900
C	1.35426000	2.52659600	0.40995000
C	2.71574900	2.89372200	1.06099600
H	2.58539300	3.77010000	1.70351500
H	3.09119300	2.07343600	1.68198700
H	3.46360300	3.11860100	0.29901600
C	0.35360600	2.22420700	1.53859500
H	0.63804000	1.33004300	2.10125100
H	0.34753500	3.06767500	2.23679500
H	-0.66904900	2.09047800	1.18318100
C	0.88409600	3.72535800	-0.44315200
H	0.81453200	4.61946500	0.18474900
H	1.59344000	3.92294600	-1.25091700
H	-0.10391500	3.55789100	-0.88412800
C	-3.60799500	-0.23904100	-0.11411500
O	-3.35427300	-1.33136800	0.36647000
O	-4.87665900	0.24535200	-0.18232900
C	-2.67780300	0.74107600	-0.69135500
C	-1.32121700	0.70890200	-0.73458800
H	-3.16513800	1.61089100	-1.11906200
H	-0.88107100	1.58132000	-1.21282100
C	-5.88959600	-0.61975000	0.34684500
H	-6.83219800	-0.09000700	0.20786200
H	-5.90351800	-1.57323800	-0.18805200
H	-5.71491900	-0.81811200	1.40777300

TS-P2

Sum of electronic and thermal Free Energies=-939.401340

C	-1.66117800	1.07743000	-0.30620900
C	-0.73737700	2.11822600	-0.00086200
C	-1.23121600	3.40367400	0.30203900
C	-2.60040500	3.61409700	0.30238300
C	-3.49843000	2.56600100	-0.00379000
C	-3.04750900	1.28969400	-0.31299400
C	0.44473600	0.22772000	-0.44243300
C	0.56928100	1.56303200	-0.09038600
H	-0.54294200	4.21190500	0.53147400
H	-2.99562900	4.59842500	0.53462200
H	-4.56592200	2.76584400	-0.00734200
H	-3.74230000	0.49836300	-0.57600300
N	-0.93342400	-0.06410000	-0.57685100
C	-1.52484300	-1.38726700	-0.72309900
O	-1.81007800	-1.78883200	-1.82497300
H	1.51500400	2.05813300	0.05822400
C	-1.78119800	-2.22529900	0.54949500
C	-3.29514100	-2.54597000	0.57999800
H	-3.50858300	-3.22500100	1.41170700
H	-3.89304500	-1.64060300	0.72605600
H	-3.60950800	-3.02324400	-0.35128300
C	-1.36563300	-1.51419700	1.84663200
H	-1.91263900	-0.57849300	1.99003000
H	-1.58350600	-2.16414700	2.70022400
H	-0.29614700	-1.28776100	1.86458300
C	-0.99238000	-3.54754400	0.39033300
H	-1.22853600	-4.21645800	1.22396400
H	-1.25742200	-4.04760900	-0.54459700
H	0.08844500	-3.37352800	0.39881600
C	3.69167800	0.06589700	-0.06726300
O	3.46769200	1.19856700	0.32651100
O	4.93871600	-0.47661000	-0.04087200
C	2.74440600	-0.91026600	-0.62252000
C	1.39712400	-0.81058100	-0.75492300
H	3.20746100	-1.83286000	-0.95618100
H	0.93703500	-1.69041600	-1.20192200
C	5.96535300	0.37882800	0.47670600
H	6.88784100	-0.19940200	0.42010700
H	6.04793400	1.29099500	-0.12047600
H	5.75217700	0.65871100	1.51197500

3(C2)-b

Sum of electronic and thermal Free Energies=-1132.820682

C	-2.80285300	-1.01148400	0.07456800
C	-2.18409600	-2.19804300	-0.42259600
C	-2.92456300	-3.39223000	-0.53957900
C	-4.24439500	-3.39529200	-0.12475500
C	-4.82492800	-2.23149200	0.42294700
C	-4.12067900	-1.03602500	0.53904100
C	-0.61452400	-0.53465700	-0.29009400
C	-0.81967200	-1.87626400	-0.66463600
H	-2.45742300	-4.29060300	-0.93080600
H	-4.83546800	-4.30203200	-0.19716400
H	-5.85090100	-2.26889100	0.77558900
H	-4.58654000	-0.17173100	0.99259300

N	-1.83093200	0.00631100	0.09439800
C	-1.90463900	1.38521400	0.56300600
O	-1.14962400	1.71058400	1.45176200
H	-0.07367300	-2.55532500	-1.07614900
C	-2.73676300	2.40620400	-0.23400000
C	-4.17456000	1.97430700	-0.57759700
H	-4.62805900	2.75578600	-1.19432200
H	-4.21435800	1.04329500	-1.14608800
H	-4.79456500	1.87276500	0.31764200
C	-1.95741800	2.61204900	-1.56350800
H	-1.92130600	1.69569900	-2.15948100
H	-2.46439900	3.38127200	-2.15358500
H	-0.93388000	2.95102400	-1.37865900
C	-2.77505500	3.72509600	0.55904100
H	-3.32549600	4.47755200	-0.01268400
H	-3.27805900	3.59432600	1.52144300
H	-1.77187900	4.10724600	0.75727100
C	2.40737700	0.42388100	1.33240600
C	3.23934700	-0.71503700	0.95350300
C	3.64609100	-0.54535900	-0.39715200
C	3.07630300	0.68689800	-0.88924600
C	2.33850500	1.31560100	0.18887200
C	1.78641400	2.70443200	0.19018300
H	0.92425500	2.79540700	0.85197500
H	2.56132200	3.39804000	0.54308100
H	1.49461400	3.02305000	-0.81256900
C	1.87238000	0.71601800	2.69625800
H	1.76163900	-0.19391000	3.28916200
H	2.56823400	1.37762400	3.22954400
H	0.90148100	1.21124000	2.63799600
C	3.59443700	-1.85038100	1.86054700
H	3.86516200	-2.74958100	1.30394600
H	4.45575200	-1.57441500	2.48239000
H	2.77213400	-2.09895500	2.53563800
C	4.50417900	-1.47931800	-1.19581100
H	4.20209900	-1.51058100	-2.24566200
H	5.54986100	-1.14912900	-1.16776200
H	4.47233100	-2.49797300	-0.80415600
C	3.29373300	1.26935400	-2.24872100
H	4.19470100	1.89717200	-2.24283000
H	3.44013400	0.49468600	-3.00440600
H	2.45601500	1.89775600	-2.55766300
Rh	1.32182300	-0.53467700	-0.26278300

TS1(C2)-b

Sum of electronic and thermal Free Energies=-2960.470846

C	1.79754100	2.23556500	1.41405300
C	1.28502400	1.32526000	2.37504200
C	1.58935100	1.49173100	3.74125300
C	2.40782100	2.54581000	4.10895700
C	2.91807300	3.43862000	3.13782300
C	2.62525800	3.30482500	1.78723300
C	0.46686100	0.73582500	0.28110600
C	0.46923900	0.39942300	1.65887800
H	1.18341200	0.81151500	4.48388100
H	2.66183300	2.69674300	5.15307900
H	3.55771600	4.25515500	3.45811500
H	3.03267100	3.99120200	1.05591500
N	1.28503200	1.87916300	0.15889700
C	1.78384200	2.51512600	-1.04604900
O	2.98228100	2.70902100	-1.10788800
H	-0.16996400	-0.35140400	2.10681500
H	-0.90520800	0.38574400	-0.26098200
C	0.79871000	3.02310700	-2.10465200
C	-0.32038700	3.82799500	-1.40492400
H	-1.00471400	4.22179300	-2.16080700
H	-0.90681200	3.22356100	-0.71363200
H	0.09733400	4.67773600	-0.85467200
C	0.21727800	1.84896800	-2.92801400
H	-0.31846100	1.12297200	-2.31903300
H	-0.49470500	2.24593500	-3.65611900
H	1.01139100	1.33660400	-3.47999200
C	1.57248900	3.95337300	-3.05997700
H	0.88595400	4.33478900	-3.82108600
H	2.00266400	4.80597200	-2.52827100
H	2.38802600	3.42891800	-3.56335800
C	3.02723700	-1.26363700	-1.45604700
C	3.45180000	-1.15586800	-0.09074100
C	2.98514000	-2.35368700	0.60056100
C	2.30811200	-3.20057800	-0.35162800
C	2.28150800	-2.51213400	-1.60460900
C	1.68296200	-3.01229600	-2.87965400
H	1.30694200	-2.19435400	-3.49812200
H	2.44572300	-3.54370800	-3.46348500
H	0.86116300	-3.70680900	-2.69672900
C	3.41044700	-0.35748600	-2.57724100
H	3.60130300	0.66187400	-2.24120800
H	4.33778100	-0.74010100	-3.02581700

H	2.65485200	-0.34010600	-3.36464100
C	4.33699400	-0.09776500	0.48523500
H	4.15836800	0.03868800	1.55358400
H	5.38661700	-0.39354900	0.35898100
H	4.19315900	0.86489600	-0.00904800
C	3.25575100	-2.68707500	2.03048700
H	2.47721200	-3.32426200	2.45489600
H	4.20495200	-3.23527600	2.09972000
H	3.34873600	-1.79015300	2.64566200
C	1.68947100	-4.53004000	-0.05950200
H	0.83011100	-4.72439400	-0.70359900
H	2.42381200	-5.32705100	-0.23023200
H	1.35748300	-4.60205600	0.97814500
Rh	1.26422200	-1.20955100	-0.10918500
N	-2.02757000	-0.08180200	-0.43041700
S	-2.07209600	-1.71880100	-0.28823400
O	-2.56005200	-2.44105500	-1.44787100
O	-0.71566900	-2.06644300	0.25796500
S	-3.34626600	0.82973700	-1.02577300
O	-2.82037500	1.81336300	-1.95745100
O	-4.45498900	-0.05694400	-1.33376800
C	-3.15952500	-2.14198300	1.19783800
C	-3.77188300	1.76765300	0.54293900
F	-4.42693300	-1.89289500	0.93081600
F	-2.97768800	-3.43176200	1.45175400
F	-2.74973800	-1.41093700	2.23537900
F	-4.71882300	2.64809000	0.26098100
F	-2.67703800	2.39521300	0.98432300
F	-4.19556500	0.91168000	1.47030300

R1-Me

Sum of electronic and thermal Free Energies=-516.344689

C	0.36523900	-0.16388700	-0.00000800
C	1.17147100	1.00145400	-0.00000200
C	2.56761000	0.87701400	-0.00002800
C	3.12561300	-0.39709700	-0.00006100
C	2.30871700	-1.54123000	-0.00006700
C	0.91788400	-1.44706900	-0.00004100
C	-0.99044400	1.66396700	0.00004400
C	0.28153600	2.13855300	0.00003200
H	3.19873700	1.76117100	-0.00002400
H	4.20566200	-0.51191700	-0.00008200
H	2.76920700	-2.52485200	-0.00009200
H	0.28387700	-2.32228600	-0.00004400
N	-0.98168000	0.25715500	0.00002100
C	-2.10499400	-0.58038300	0.00003500
O	-1.99274900	-1.79303900	0.00000800
H	0.56623800	3.18157000	0.00004500
H	-1.92374300	2.20383200	0.00006800
C	-3.45803900	0.10723200	0.00005300
H	-3.58644700	0.73786300	0.88553100
H	-3.58645200	0.73790900	-0.88539100
H	-4.22088600	-0.67039100	0.00003600

$1a^{OAc}$-Me

Sum of electronic and thermal Free Energies=-1244.076495

C	2.64797600	-0.58555600	1.56972400
C	1.56317200	-1.50427100	1.41481600
C	1.62140800	-2.06132900	0.07526000
C	2.78878700	-1.51541700	-0.57716900
C	3.40317600	-0.56982200	0.32136900
C	4.65988800	0.20575300	0.08127500
H	4.61295200	1.19285300	0.54622200
H	5.51580300	-0.32862400	0.51189700
H	4.85339200	0.34071200	-0.98431300
C	2.99518400	0.20574700	2.79041000
H	2.14338600	0.30930500	3.46475400
H	3.79889400	-0.29686400	3.34270600
H	3.34944800	1.20584700	2.52928900
C	0.52930500	-1.85215500	2.43774200
H	-0.45847200	-1.96315800	1.98437100
H	0.78627900	-2.80853600	2.90930600
H	0.46552000	-1.10062700	3.22663000
C	0.69975600	-3.10518400	-0.47417000
H	0.68012800	-3.09032200	-1.56565800
H	1.02997900	-4.10332700	-0.16052500
H	-0.32256500	-2.96566600	-0.11552400
C	3.25377900	-1.83544800	-1.96023500
H	4.00125900	-2.63758000	-1.91890900
H	2.43247100	-2.17392700	-2.59397900
H	3.71474000	-0.96894600	-2.43773900
C	1.38779100	2.18786200	-1.56979100
O	1.20410200	1.02194000	-2.05297900
O	1.63718700	2.27522100	-0.31815500
C	1.28169300	3.41129200	-2.43050900
H	1.95364000	4.19021500	-2.06547200
H	1.50516800	3.16463100	-3.46949500
H	0.25661900	3.79496800	-2.38202300

Rh	1.39636200	0.10827700	-0.10540400
C	-3.55258000	-0.06989300	-0.08710800
C	-4.92700100	0.03702100	0.22379100
C	-5.84477700	-0.83451800	-0.37070100
C	-5.37271000	-1.79057500	-1.26729800
C	-4.00685000	-1.87374000	-1.57463700
C	-3.07101600	-1.01512700	-0.99218700
C	-3.85847200	1.65601100	1.39770800
C	-5.08033200	1.13036000	1.16164900
H	-6.90292900	-0.76167500	-0.13995200
H	-6.06977800	-2.47475300	-1.74051700
H	-3.66558000	-2.61801900	-2.28746900
H	-2.02280300	-1.07164100	-1.24738700
N	-2.87798400	0.94465300	0.65300900
C	-1.53280500	1.16878700	0.69957000
O	-0.77054100	0.39600400	0.07905100
H	-6.00656300	1.47415200	1.60065000
H	-3.57097800	2.46898900	2.04334300
C	-1.02611500	2.33201800	1.51387000
H	-1.61784600	3.23327100	1.33844000
H	-1.08253900	2.09781600	2.58302300
H	0.00845700	2.52967400	1.23681200

1c^{OAc}-Me

Sum of electronic and thermal Free Energies=-1244.074773

C	-2.17931600	-1.95981800	-0.31134900
C	-2.05413100	-1.66326400	1.11005700
C	-2.99845400	-0.63610800	1.43321700
C	-3.68652500	-0.25425100	0.21209400
C	-3.20779400	-1.11939000	-0.85088600
C	-3.68726700	-1.08702500	-2.26553600
H	-2.96759600	-1.53797800	-2.95021800
H	-4.62690100	-1.64767300	-2.34595000
H	-3.87889400	-0.06427000	-2.59761300
C	-1.39556500	-3.00309800	-1.04315600
H	-0.35236000	-3.01504400	-0.71855800
H	-1.81807400	-3.99655000	-0.84942200
H	-1.41139600	-2.83782600	-2.12169100
C	-1.14796900	-2.37990300	2.06145500
H	-0.92466200	-1.77830300	2.94466900
H	-1.62633600	-3.30606100	2.40327700
H	-0.20435200	-2.65530200	1.58524600
C	-3.23272400	-0.02024300	2.77449600
H	-3.35509000	1.06275600	2.69611600
H	-4.15164700	-0.42954200	3.21211500
H	-2.41365700	-0.22365600	3.46597400
C	-4.80575800	0.73421600	0.10882100
H	-5.76324600	0.24082300	0.31724800
H	-4.68658100	1.54817500	0.82682700
H	-4.86548000	1.16860600	-0.89100700
C	-1.22578000	2.58807000	-0.66463800
O	-1.25109800	2.20366600	0.55709200
O	-1.44422400	1.70856000	-1.56014300
C	-0.91767300	4.01044500	-1.02527700
H	-1.38826200	4.26962300	-1.97505000
H	-1.25034800	4.68363200	-0.23324800
H	0.16596500	4.12456800	-1.13979100
Rh	-1.58972200	0.14710300	-0.06483900
C	4.15546200	-0.01183700	0.14930400
C	4.99720100	-0.55800500	-0.84995900
C	6.38319200	-0.57449200	-0.67033000
C	6.91388100	-0.05392900	0.50722900
C	6.07116700	0.46798500	1.49673200
C	4.68299600	0.49421900	1.33838800
C	2.86991200	-0.78860400	-1.59500400
C	4.15486600	-1.03141800	-1.92839400
H	7.02966500	-0.99068700	-1.43659100
H	7.98754300	-0.05758400	0.66467300
H	6.49925800	0.86082400	2.41337500
H	4.07222400	0.89246100	2.13536000
N	2.81468400	-0.15031200	-0.32604300
C	1.62205900	0.22913600	0.22761000
O	0.57331700	-0.11499700	-0.36307400
H	4.49181000	-1.49350200	-2.84588500
H	1.95027500	-0.96954600	-2.12498200
C	1.60452500	1.03467400	1.49516700
H	1.88308800	0.40621500	2.34806000
H	2.31535500	1.86224100	1.44261300
H	0.60262300	1.43417900	1.64327100

TS1(C7)^{OAc}-Me

Sum of electronic and thermal Free Energies=-1244.043676

C	2.86615800	-0.63031200	0.35947500
C	2.15293400	-0.73880600	1.58724000
C	1.04723100	-1.67760100	1.38879900
C	1.10200500	-2.15063900	0.04508200
C	2.16938800	-1.43549400	-0.63309700
C	2.64181700	-1.66143900	-2.03611400

H	3.09626900	-0.75849600	-2.44972500
H	3.39847700	-2.45607700	-2.05703900
H	1.82555200	-1.96547400	-2.69447400
C	4.06540200	0.21536700	0.07370200
H	4.45439000	0.68367500	0.97876900
H	4.86224800	-0.39547500	-0.36356300
H	3.81137300	1.00891200	-0.63685800
C	2.47091700	-0.06227000	2.88298900
H	1.56533200	0.32162100	3.36032900
H	2.93532900	-0.77390000	3.57653300
H	3.15730900	0.77439500	2.74570400
C	0.12183500	-2.15824900	2.46354300
H	-0.82879500	-2.50503700	2.05300400
H	0.57659200	-2.99818500	3.00360100
H	-0.08390300	-1.37459800	3.19643500
C	0.26019600	-3.24015500	-0.53851700
H	0.71228800	-4.20930300	-0.29209900
H	-0.75506700	-3.23542600	-0.13709800
H	0.19537700	-3.16947500	-1.62418200
C	0.75602500	2.68482700	-1.44389300
O	1.50925200	1.84006600	-0.84373900
O	-0.47403000	2.50390700	-1.64801800
C	1.40884600	3.94692300	-1.96045500
H	0.71419100	4.78426600	-1.87595100
H	2.33367700	4.15650200	-1.42249100
H	1.64060500	3.81139100	-3.02234900
Rh	0.76463400	0.07026200	0.03914900
C	-2.28821500	-0.05710100	-0.29831000
C	-3.45197100	-0.78818500	-0.62024600
C	-3.47847300	-1.53675900	-1.80390200
C	-2.36364800	-1.51131500	-2.64505400
C	-1.23921500	-0.74579900	-2.31773100
C	-1.15218400	0.01618300	-1.12861300
C	-3.88483400	0.34035300	1.29287600
C	-4.43648500	-0.52200900	0.40775400
H	-4.36328800	-2.10398300	-2.07655800
H	-2.38464900	-2.06625400	-3.57784900
H	-0.41375000	-0.69517900	-3.02271500
H	-0.73356300	1.18840100	-1.32453100
N	-2.55316900	0.63531800	0.90373300
C	-1.65432300	1.38803100	1.62246100
O	-0.44052400	1.38935200	1.36435500
H	-5.43926900	-0.92220800	0.46010800
H	-4.30023600	0.77223000	2.18898500
C	-2.17556800	2.22021500	2.76577800
H	-3.00837100	2.85294500	2.44684100
H	-2.52750400	1.58090600	3.58270900
H	-1.36157300	2.84361500	3.13322100

TS1(C2)^{OAc}-Me

Sum of electronic and thermal Free Energies=-1244.045935

C	-1.02800500	-2.11787600	-0.63338300
C	-1.18786700	-2.09179400	0.78204800
C	-2.41868700	-1.35852100	1.08465600
C	-3.01370900	-0.96003500	-0.15163800
C	-2.11198600	-1.34292900	-1.22124000
C	-2.38541700	-1.16330500	-2.68259900
H	-1.46373800	-1.14723400	-3.26809600
H	-3.00271200	-1.98954100	-3.05765800
H	-2.92331300	-0.23178600	-2.87121600
C	0.01606800	-2.87142800	-1.39480100
H	0.95235200	-2.95372900	-0.84008500
H	-0.34776100	-3.88833900	-1.58893700
H	0.22809400	-2.40862100	-2.35969300
C	-0.32757100	-2.78129400	1.79476300
H	-0.27100500	-2.21221100	2.72572600
H	-0.74722100	-3.76547200	2.03752200
H	0.68742500	-2.93730900	1.42379500
C	-2.97300300	-1.14414400	2.45752200
H	-3.68553300	-0.31832100	2.47987500
H	-3.48956800	-2.04958300	2.79988800
H	-2.18035100	-0.92339600	3.17661000
C	-4.28072300	-0.18920400	-0.33783000
H	-4.86772700	-0.15261200	0.58102100
H	-4.05523700	0.83999400	-0.63892600
H	-4.89430500	-0.65077300	-1.11775900
C	-1.30920400	2.93301600	-0.66260300
O	-0.09540900	2.97855500	-0.96044300
O	-1.92352400	1.87265000	-0.25868400
C	-2.16422500	4.17942100	-0.76976800
H	-2.99952500	3.99598400	-1.45143900
H	-2.58671900	4.41531600	0.21108500
H	-1.56747300	5.01678900	-1.12966100
Rh	-1.00972600	0.00945200	0.06373700
C	3.18016800	0.22171300	0.18585100
C	3.17044600	-0.12026500	-1.19509000
C	4.34641000	-0.57367400	-1.81847000
C	5.49954600	-0.68985600	-1.05675200

C	5.49002000	-0.36122600	0.31204500
C	4.33994800	0.09422100	0.95515600
C	1.03912400	0.57005500	-0.66410000
C	1.84841000	0.11303100	-1.68744900
H	4.34584500	-0.82484500	-2.87446000
H	6.42022400	-1.03533300	-1.51495300
H	6.40535200	-0.45941400	0.88702000
H	4.37488500	0.34159100	2.00735200
N	1.87476300	0.63144200	0.51263200
C	1.29144600	0.96858200	1.70707300
O	0.04731900	0.93345500	1.79064100
H	1.54094400	0.03519600	-2.72275900
H	0.43545800	1.58769000	-0.85619200
C	2.11764000	1.38038100	2.88944200
H	2.56450900	0.49951300	3.36405100
H	2.92072100	2.06155800	2.59933500
H	1.46063500	1.86295500	3.61284000

2(C7)^{OAc}-Me

Sum of electronic and thermal Free Energies=-1244.065903

C	-3.03081100	-0.06302800	-0.13763200
C	-2.60574800	-1.39049800	-0.24479200
C	-1.74488400	-1.68300500	0.91593200
C	-1.78575000	-0.54815500	1.80289100
C	-2.46101600	0.50411400	1.10159600
C	-2.80088100	1.86204100	1.63624400
H	-2.83634400	2.60891600	0.83940200
H	-3.78938100	1.84419600	2.11280000
H	-2.08178200	2.19746200	2.38665500
C	-3.86188400	0.72311000	-1.10219100
H	-4.12821700	0.13533000	-1.98180200
H	-4.78964300	1.05836900	-0.62458900
H	-3.32374800	1.61318900	-1.44341500
C	-2.87911500	-2.36679100	-1.34623700
H	-1.94591100	-2.74474300	-1.77632000
H	-3.43984500	-3.22777600	-0.96471100
H	-3.46087800	-1.91724900	-2.15243400
C	-1.18360000	-3.03460800	1.23517300
H	-0.32665000	-2.96790700	1.90864400
H	-1.94654700	-3.65294300	1.72540100
H	-0.87036600	-3.55971400	0.32972600
C	-1.28007600	-0.51987800	3.21088400
H	-2.04471500	-0.94417300	3.87355900
H	-0.36968500	-1.11013700	3.32979100
H	-1.07390700	0.49414500	3.55591400
C	0.13991900	2.65131400	-1.67631300
O	-0.54932400	1.63259600	-1.55006100
O	1.09844200	2.99912800	-0.83752800
C	-0.04364500	3.61324400	-2.81375800
H	0.88794100	3.68517700	-3.38302700
H	-0.85278800	3.28013500	-3.46150200
H	-0.25805000	4.61108400	-2.41989200
Rh	-0.69111800	-0.06640100	-0.06648500
C	2.29637000	-0.19466200	0.38016700
C	3.55137300	0.04320600	0.99111800
C	3.64149000	0.92816600	2.07058300
C	2.47631100	1.55071400	2.50508000
C	1.23738600	1.27908700	1.89440200
C	1.09723800	0.38592900	0.81342200
C	3.91423500	-1.40828200	-0.70992800
C	4.54165400	-0.74076200	0.28432800
H	4.59567800	1.12830000	2.54708100
H	2.51520900	2.25424600	3.33131900
H	0.35926500	1.78781400	2.28156000
H	1.17435000	2.33061600	-0.11935100
N	2.53132700	-1.09784400	-0.69405900
C	1.60814500	-1.54633400	-1.59173300
O	0.41200200	-1.19882000	-1.54483000
H	5.59932700	-0.78662800	0.50345700
H	4.31384000	-2.08345800	-1.44886500
C	2.05583400	-2.48821700	-2.68126500
H	2.80969200	-2.01675500	-3.31926800
H	2.49081800	-3.40023300	-2.26110100
H	1.18912400	-2.74775600	-3.28727500

2(C2)^{OAc}-Me

Sum of electronic and thermal Free Energies=-1244.070455

C	-1.88914400	-1.98282400	-0.17472000
C	-2.88297800	-1.24477400	0.62271300
C	-3.27471400	-0.11433800	-0.11018900
C	-2.54521700	-0.12503000	-1.38946900
C	-1.78839500	-1.33988300	-1.46388000
C	-1.06934000	-1.87717700	-2.66116400
H	-0.17694000	-2.43995200	-2.38268300
H	-1.73676800	-2.55444000	-3.20839500
H	-0.77298200	-1.08346600	-3.34951400
C	-1.31535200	-3.31516300	0.19699200
H	-1.13711400	-3.38589700	1.27228500

H	-2.01420200	-4.11639000	-0.07502100
H	-0.37236500	-3.50566200	-0.31968100
C	-3.32216200	-1.65194600	1.99456700
H	-3.91904600	-0.87719500	2.47780800
H	-3.92935600	-2.56334800	1.94136000
H	-2.46354300	-1.86579300	2.63780400
C	-4.21643000	0.97290200	0.30315200
H	-3.72619300	1.95022600	0.25641300
H	-5.08464200	1.00279500	-0.36516300
H	-4.58022300	0.82878800	1.32143200
C	-2.76302000	0.86309200	-2.49394300
H	-3.67248900	0.60963900	-3.05329900
H	-2.89128900	1.87527200	-2.10311700
H	-1.93137800	0.87236500	-3.20143300
C	-0.24888300	3.08812000	0.18784400
O	0.82354400	2.93173300	-0.56294800
O	-0.97348600	2.15328000	0.55476200
C	-0.52292000	4.51285900	0.57026600
H	-1.43645400	4.57552700	1.15912500
H	0.32154100	4.90160600	1.14740700
H	-0.60678900	5.12653100	-0.33135900
Rh	-0.96668700	-0.05312300	0.13441100
C	3.21705200	-0.34104800	0.23996700
C	3.16335400	-0.18633000	-1.16502000
C	4.34546100	-0.19742200	-1.91177300
C	5.55774100	-0.36430000	-1.24512800
C	5.59460800	-0.51796200	0.14730300
C	4.42600000	-0.50887700	0.91372800
C	0.98461400	-0.10213100	-0.42651200
C	1.76757800	-0.04078200	-1.54297100
H	4.31690200	-0.07846300	-2.99048400
H	6.48509100	-0.37562500	-1.80867300
H	6.54894900	-0.64757300	0.64732300
H	4.48922800	-0.63130300	1.98650800
N	1.87098500	-0.28192900	0.69708300
C	1.31179100	-0.35298800	1.93272300
O	0.06105600	-0.26873000	2.02356700
H	1.40965400	0.08121400	-2.55696600
H	0.96130700	1.97342300	-0.76168700
C	2.13804800	-0.52780200	3.17055300
H	2.70230200	-1.46461100	3.12812300
H	2.85364800	0.29290600	3.27811000
H	1.47209300	-0.54397000	4.03241700