Supporting Information

Theoretical study on the palladium-catalyzed oxidative carbocyclization-alkoxycarbonylation of bisallenes to construct seven-membered carbocycles assisted by olefin

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Cartesian coordinates and SCF energies for all of the calculated structures

1a

Sum of electronic and thermal Free Energies= -1474.522452

C	0.71927000	-0.95893200	-0.31314500
C	0.56971600	-1.17398500	-1.65277600
C	1.19043800	-1.27762600	0.88238500
C	2.42825700	-2.16991000	0.93921400
H	2.39122300	-2.80698200	1.83037300
H	2.50865400	-2.80371500	0.05463700
C	3.66720600	-1.28170200	1.04588700
O	3.85387100	-0.48708000	1.94534700
O	4.50205400	-1.48436200	0.01753700
C	5.62598700	-0.56738400	-0.08079800
C	6.56890800	-1.11575400	-1.13488200
H	6.10382400	-0.49120900	0.89934500
H	5.21425100	0.40923700	-0.35150800
H	7.43962100	-0.45908000	-1.22760600
H	6.92310000	-2.11553400	-0.86433100
H	6.07974600	-1.17327100	-2.11151300
C	0.71632200	-0.68710400	2.19794000
H	1.36201600	0.15799000	2.45525200
H	0.90055800	-1.44416200	2.97495300
C	-0.73937500	-0.27775000	2.25169200
C	-1.10492700	0.97505200	2.54360900
H	-2.14946300	1.26832300	2.59723300
H	-0.36357600	1.75760200	2.66753100
C	-0.23038800	-2.38025200	-2.10369000
H	-0.97447200	-2.68656900	-1.36833100
H	-0.70855000	-2.21446200	-3.07404000
H	0.47933900	-3.20849300	-2.23685600
C	-1.77875100	-1.37385500	2.06414800
H	-1.30043000	-2.36177500	2.12540300
H	-2.48448900	-1.34273500	2.90503100
C	-2.62192700	-1.35713400	0.79752500
C	-2.39603800	-0.64771700	-0.28390600
C	-2.48637400	-0.08860400	-1.51609200
H	-2.15207400	-0.61856000	-2.40308200
H	-3.11626100	0.78143800	-1.66587800
C	-3.85241800	-2.26096700	0.86155100
C	-4.70376400	-2.38468600	-0.40474200
H	-4.47879200	-1.88806000	1.68505200
H	-3.51409000	-3.26004100	1.17626900
C	-5.90197600	-3.31894500	-0.20675100
H	-5.05758300	-1.39097600	-0.70227900
H	-4.08336500	-2.75369900	-1.23073100
H	-6.49990600	-3.39257800	-1.11988300
H	-5.57895700	-4.33120400	0.06201200
H	-6.55947700	-2.95846900	0.59220800
Pd	-0.63947200	0.75438600	-0.60965100
O	2.85141900	1.24961700	-0.81547000
C	2.18675600	1.94622700	-0.04192300
O	0.89343000	1.95842200	0.09992800
C	2.89976600	2.91565200	0.89983100
H	3.58356600	3.53921100	0.31733600
H	2.20229400	3.54490500	1.45402800
H	3.50088100	2.32287100	1.59678900
C	1.31988700	-0.45758000	-2.74752400
H	0.64818200	-0.17811100	-3.56675100
H	1.87060600	0.39988700	-2.36371800
H	2.04279100	-1.17781200	-3.15962700
C	-2.70920200	2.83927800	-0.10017000
O	-3.43775700	2.03279900	0.47479200
O	-1.58091400	2.57487000	-0.70762100
C	-3.05111400	4.32759600	-0.15611900
H	-2.45041400	4.85529600	0.59237200
H	-2.80887300	4.75288600	-1.13263200
H	-4.10853900	4.46845100	0.07319200

1b

Sum of electronic and thermal Free Energies= -1474.536007

C	-0.07623000	-1.81439100	0.40047200
C	-0.93033000	-2.75004100	-0.07224200
C	1.08116700	-1.32182700	0.80681500
C	2.23402200	-2.23773400	1.15683100
H	2.66188400	-1.98408600	2.13547000
H	1.90518500	-3.27912100	1.23036200
C	3.35291900	-2.17109300	0.12120600
O	3.30406200	-1.55579600	-0.92367100
O	4.40988000	-2.90038800	0.51945700
C	5.53924900	-2.93832400	-0.39097900

C	6.59763700	-3.82639100	0.23343800
H	5.89624500	-1.91563200	-0.54653700
H	5.19665400	-3.31928500	-1.35782600
H	7.46994400	-3.87954100	-0.42512500
H	6.92079200	-3.43117600	1.20066100
H	6.21864800	-4.84115000	0.38429100
C	1.30376400	0.16678700	0.93159500
H	2.34507800	0.40676800	0.68168900
H	1.16824800	0.47930300	1.97584700
C	0.40191800	1.00056600	0.03435400
C	0.11051300	0.60270900	-1.25810600
H	-0.39187700	1.28825900	-1.93298800
H	0.59340900	-0.26562100	-1.69392800
C	-0.86743800	-3.20800000	-1.51257900
H	-0.67797700	-4.28940000	-1.52263400
H	-1.83008700	-3.02229300	-1.99675700
H	-0.07372000	-2.70614300	-2.06819000
C	-1.86385000	-3.51372800	0.83339000
H	-2.81391600	-3.71609500	0.33561100
H	-1.38753300	-4.48128500	1.04633800
H	-2.05155000	-2.99579100	1.77260400
Pd	-1.60925200	-0.25677500	-0.12225800
O	-3.91099500	3.16031700	-0.12686600
O	-3.71790100	-1.73322800	-1.61019500
C	-3.32984100	2.17650000	0.30251400
O	-2.56896200	1.46377300	-0.52450000
C	-4.14343600	-1.49822900	-0.47928400
O	-3.41992200	-1.03785100	0.51237400
C	-3.42160300	1.75796600	1.76018900
H	-2.42549300	1.72105600	2.21495200
H	-4.03856200	2.47785700	2.29940400
H	-3.84839300	0.75535400	1.83231400
C	-5.60358800	-1.71793100	-0.10641500
H	-5.69693700	-2.13283900	0.90026200
H	-6.11599200	-0.74995000	-0.11451200
H	-6.07892200	-2.37391000	-0.83708500
C	0.14362500	2.42128500	0.49985600
H	-0.62277200	2.87849400	-0.13100100
H	-0.22197900	2.41497700	1.53032800
C	1.42864000	3.25728100	0.43910700
C	2.03962900	3.59677000	1.55000300
C	2.62141600	3.94500700	2.66880800
H	3.40096600	3.33675800	3.12389500
H	2.35321900	4.86263100	3.18907300
C	1.91276800	3.67393200	-0.93974700
C	3.19650100	4.50955200	-0.96754500
H	1.09892300	4.23107400	-1.42769600
H	2.05275400	2.77108700	-1.55217800
C	3.61170900	4.89687500	-2.39007200
H	3.05273600	5.41268900	-0.36259500
H	4.00473600	3.94694400	-0.48426300
H	4.53075100	5.49151400	-2.38607200
H	3.79256600	4.00987400	-3.00810600
H	2.83430200	5.49046000	-2.88417100

1c

Sum of electronic and thermal Free Energies= -1474.553114

C	-3.21486600	-1.71641500	-1.01541600
C	-3.71576700	-2.45878900	-1.97550700
C	-2.73028200	-0.95962100	-0.05799900
C	-2.75720700	0.55346300	-0.18362400
H	-1.74252100	0.96282500	-0.06890100
H	-3.10683600	0.85860200	-1.17495300
C	-3.63657200	1.24098500	0.85005400
O	-4.23974800	0.70391700	1.75423100
O	-3.66049800	2.57661400	0.63104500
C	-4.46056500	3.35282600	1.55480700
C	-4.38872400	4.80377500	1.11900700
H	-4.07064800	3.20698700	2.56721800
H	-5.48547100	2.96937200	1.53985400
H	-4.99138200	5.42228900	1.79152300
H	-3.35916300	5.17210000	1.14516600
H	-4.77291900	4.92674700	0.10230400
C	-2.13826200	-1.51958300	1.23644400
H	-2.92840300	-1.54489000	1.99319700
H	-1.40017800	-0.79061900	1.59929300
C	-1.47224700	-2.87441700	1.13760800
C	-1.87403000	-3.91107200	1.87972400
H	-1.37201100	-4.87423200	1.83878200
H	-2.72743800	-3.83361100	2.54740200
C	-5.16545100	-2.90112500	-1.96019400
H	-5.68780700	-2.54641600	-2.85814700
H	-5.23452100	-3.99658600	-1.96326200
H	-5.69277500	-2.52485000	-1.08136200
C	-2.88948300	-2.92304600	-3.15785200
H	-2.85259300	-4.01927400	-3.20044200
H	-3.34008200	-2.58444300	-4.09971500
H	-1.86539400	-2.54471700	-3.11455600
C	-0.30044300	-3.01083700	0.17632400

H	0.18059100	-3.98480700	0.32590000	C	-6.32080700	3.35045300	-0.99243800
H	-0.66903200	-2.98499500	-0.85351100	H	-5.52278300	1.32303300	-1.00020700
C	0.74172800	-1.90599500	0.36241500	H	-4.72896800	2.40790600	-2.14464800
C	0.92376400	-1.05611000	-0.62263300	H	-7.10333400	3.14411800	-1.72922300
C	0.85191900	-0.40144200	-1.82261100	H	-6.76229900	3.28403900	0.00604400
H	1.42365700	-0.75597600	-2.67895200	H	-5.96600700	4.37372700	-1.14478500
H	0.04903600	0.30366000	-2.02241000	C	-0.72978800	0.14175600	1.22349100
C	1.50532500	-1.86666300	1.67143500	H	-1.70466000	-0.20583600	1.58842900
C	2.74435900	-2.78558700	1.65861200	H	-0.01396800	-0.08698200	2.02195500
H	0.82784000	-2.17803900	2.47613600	C	-0.37486500	-0.76989500	0.07000700
H	1.81925300	-0.84064000	1.89027000	C	-0.03616000	-0.32042300	-1.18024400
C	3.47725600	-2.78857000	3.00372300	H	-0.00121500	-1.01094200	-2.01801400
H	2.44182300	-3.80916500	1.40302500	H	-0.09071900	0.73609400	-1.41453100
H	3.41832000	-2.45000400	0.86218300	C	2.18925000	3.31993500	-0.41631500
H	4.35731100	-3.43892300	2.97257000	H	2.33463700	4.39738600	-0.56560300
H	3.81600500	-1.78134400	3.27156900	H	3.17983800	2.85635800	-0.34496200
H	2.82775300	-3.14488200	3.81124600	H	1.67782900	2.91306400	-1.29149600
Pd	2.23601400	0.68035300	-0.57867800	C	2.05931400	3.59090000	2.13429900
O	4.01648800	-0.31876700	-0.93205700	H	3.01481900	3.08087100	2.29873000
O	1.67020000	3.23503500	-1.44611800	H	2.25658600	4.66656400	2.04556200
C	4.71209500	0.54419300	-0.26573900	H	1.42135800	3.42585100	3.00580400
O	4.10559200	1.48460300	0.32126200	Pd	2.12734800	-0.59428600	-0.56999600
C	0.80798600	3.00363200	-0.60210000	O	3.63218600	0.69918300	1.60769600
O	0.67387500	1.82772500	-0.01534500	O	2.59641300	-0.37203500	-2.59175600
C	6.20784300	0.42329800	-0.24066700	C	2.99350200	-0.23371800	2.08069400
H	6.60391100	0.87846000	0.66876900	O	2.11399100	-0.95980800	1.41624600
H	6.50751200	-0.62403400	-0.31305300	C	3.84666100	-0.55674500	-2.35302000
H	6.61954400	0.95892600	-1.10295700	O	4.19689000	-0.79202400	-1.15583300
C	-0.18293200	4.04397700	-0.11486800	C	3.15153600	-0.69242300	3.52395800
H	-1.19395700	3.63256400	-0.05595500	H	3.64932000	-1.66726500	3.54217100
H	0.10365700	4.36259500	0.89303700	H	3.75474600	0.03117600	4.07367300
H	-0.15964700	4.90680700	-0.78187300	H	2.17678100	-0.81444100	4.00431800
1d				C	4.85351300	-0.45912300	-3.46061900
Sum of electronic and thermal Free Energies= -1474.545112				H	5.23078700	0.56813800	-3.50827200
C	0.31431600	2.36538900	0.89516100	H	5.69627000	-1.12311200	-3.25864600
C	1.42774700	3.05765300	0.86467100	H	4.38925400	-0.70316700	-4.41797800
C	-0.78354200	1.64589600	0.97762300	C	-0.51708600	-2.25390300	0.36164100
C	-2.14315000	2.32390000	0.96218600	H	-0.11670000	-2.82562200	-0.48450900
H	-2.67369900	2.13131100	1.90732500	H	0.09331000	-2.48903500	1.23841100
H	-2.02881300	3.41007600	0.90396000	C	-1.96698500	-2.68025300	0.60618400
C	-3.08698000	1.89094200	-0.14874500	C	-2.32291400	-3.14463500	1.78098200
O	-2.91691100	0.97066400	-0.92319800	C	-2.65900600	-3.61880800	2.95297100
O	-4.18632700	2.67172000	-0.15722500	H	-3.03468900	-2.97487500	3.74594000
C	-5.18843100	2.35429900	-1.15281400	H	-2.57696000	-4.67920200	3.18428900

C	-2.92066400	-2.55686900	-0.57066400
C	-4.35304500	-3.03585300	-0.31559100
H	-2.49019200	-3.11880200	-1.41437200
H	-2.93813800	-1.50727300	-0.89413100
C	-5.25086700	-2.86948500	-1.54540600
H	-4.33859200	-4.08732900	-0.00368200
H	-4.77422300	-2.47674300	0.52905900
H	-6.27176600	-3.20845500	-1.34135200
H	-5.30201300	-1.82051900	-1.85897700
H	-4.87304400	-3.44847400	-2.39596500

1e

Sum of electronic and thermal Free Energies= -1474.552800

C	0.58909500	-1.06769400	-0.70700400
C	1.60592000	-1.66858600	-1.41542700
C	-0.63451400	-0.94179500	-0.22693500
C	-1.74726100	-1.76640900	-0.84849200
H	-2.50469800	-1.10864100	-1.29098200
H	-1.36679800	-2.39196400	-1.66397900
C	-2.43838500	-2.68852300	0.14678200
O	-1.98985000	-3.04211400	1.21484500
O	-3.63575800	-3.08750800	-0.33677200
C	-4.37155600	-4.02111900	0.49140500
C	-5.67019200	-4.34089800	-0.22367900
H	-4.54080900	-3.56415700	1.47122000
H	-3.75646900	-4.91307500	0.64675600
H	-6.25411300	-5.05165000	0.36927700
H	-6.27194700	-3.43868900	-0.36707300
H	-5.47842800	-4.78673000	-1.20387300
C	-1.00208600	-0.00354400	0.92222100
H	-0.42939900	-0.30351400	1.80390200
H	-2.05950000	-0.16209200	1.16115300
C	-0.77679900	1.47041100	0.64626300
C	0.06282700	2.19471500	1.39590000
H	0.21817600	3.25473600	1.21253700
H	0.63123500	1.75162900	2.20829700
C	2.20439600	-2.97125400	-0.92359600
H	3.29640800	-2.92023000	-0.92002100
H	1.85694100	-3.21233500	0.08044000
H	1.90018000	-3.77120900	-1.61193100
C	1.92872600	-1.28751200	-2.84532100
H	3.00528700	-1.34738800	-3.03132400
H	1.43963600	-2.01451400	-3.50872000
H	1.57913000	-0.28720300	-3.09695800
C	-1.57392400	2.08768400	-0.48984100
H	-1.21033600	3.10591000	-0.67035500
H	-1.40123400	1.51950100	-1.41008000
C	-3.07643500	2.13222000	-0.20000700
C	-3.91493100	1.37061000	-0.86223400
C	-4.75091600	0.60394000	-1.51719600
H	-5.23359200	0.93636800	-2.43459100
H	-4.99627700	-0.39911100	-1.17115400
C	-3.55984300	3.08642000	0.88223500
C	-3.57803800	4.56222300	0.43920800
H	-2.90390900	2.98256100	1.75711900
H	-4.56646100	2.79589700	1.20147800
C	-4.03969200	5.50284900	1.55688700
H	-2.57767700	4.86121500	0.10153100
H	-4.23852400	4.66301500	-0.43089200
H	-4.05271800	6.54461200	1.22049800
H	-5.05088100	5.24959800	1.89515800
H	-3.37587400	5.44173500	2.42673800
Pd	2.27306200	0.07910500	-0.14152400
O	2.29913000	1.52985000	-1.64495400
O	4.52138300	-1.40118500	0.89176600
C	3.05792300	2.31397600	-0.95696800
O	3.42979600	1.94506700	0.19392700
C	3.62752000	-1.46136300	1.73133700
O	2.40478000	-1.00352200	1.54882700
C	3.45263200	3.64681000	-1.52739700
H	4.34204200	4.02303600	-1.01984600
H	3.62960600	3.56010700	-2.60175500
H	2.63268100	4.35736700	-1.37672900
C	3.82635000	-2.07196700	3.10953200
H	3.85145300	-1.27324200	3.85793300
H	2.99491300	-2.73441800	3.36406500
H	4.77035200	-2.61781600	3.13512600

2

Sum of electronic and thermal Free Energies=-1474.545433

C	0.80929100	-1.23098400	0.56300600
C	0.77653200	-2.64163200	0.99751900
C	1.84311400	-0.38496600	0.71779700
C	3.15147200	-0.75945900	1.40166700
H	3.49290000	0.05694700	2.04640700
H	3.01897700	-1.65930200	2.00518800
C	4.22251500	-1.06151700	0.36326500
O	4.34577200	-2.12184900	-0.21588000
O	5.00596100	0.01136700	0.12517600
C	6.02738900	-0.16230400	-0.88920300

C	6.76791300	1.15424100	-1.02224600
H	5.54572600	-0.46318600	-1.82462700
H	6.68824400	-0.97876800	-0.58233400
H	7.55287200	1.06195200	-1.77918500
H	6.09017700	1.95678700	-1.32731800
H	7.23512700	1.43889500	-0.07519800
C	1.72676400	1.02399200	0.18818400
H	2.66937700	1.35458800	-0.27472000
H	1.55397300	1.72187200	1.01779300
C	0.60612100	1.16211800	-0.83400100
C	0.51275900	0.24632000	-1.88817800
H	-0.16555800	0.45173800	-2.71525500
H	1.27400900	-0.51887300	-2.01021900
C	1.18372600	-3.67370500	-0.02869900
H	2.24327900	-3.53343800	-0.27235200
H	1.03335900	-4.69372400	0.33698300
H	0.62010900	-3.54405400	-0.95939200
C	0.37181500	-2.98909100	2.24092200
H	-1.48176200	-2.56987300	1.29146700
Pd	-0.84284500	-0.49904500	-0.38570700
O	-2.14020500	0.97461900	-3.18795000
O	-3.92196000	-2.56845200	-0.55523700
C	-2.94412200	0.70800300	-2.28547100
O	-2.64878500	0.28886400	-1.09084400
C	-3.21747900	-2.86569400	0.36521700
O	-2.09850000	-2.10864400	0.67823700
C	-4.44595300	0.87264300	-2.50458500
H	-4.85755800	1.57249600	-1.77022000
H	-4.64495500	1.23618200	-3.51384100
H	-4.94110600	-0.08991300	-2.34555100
C	-3.43023400	-4.03452800	1.30448200
H	-2.54914900	-4.68467700	1.32321300
H	-3.59967300	-3.67202800	2.32364800
H	-4.29712800	-4.60370600	0.97126600
H	0.35945100	-4.02853300	2.55983600
H	0.13532200	-2.23656100	2.98924000
C	-0.06314600	2.52361700	-0.96296600
H	0.67083700	3.16760000	-1.46810800
H	-0.91633900	2.42665300	-1.64199800
C	-0.47883700	3.20703300	0.33567000
C	0.07157700	4.35236100	0.66795300
C	0.61641500	5.50256600	0.97189900
H	0.19476600	6.44397400	0.62407400
H	1.51172100	5.56860500	1.58766000
C	-1.55321700	2.53685500	1.17733600
C	-2.11343600	3.37672100	2.32936800
H	-1.13890000	1.59886200	1.58192500
H	-2.36136800	2.21437500	0.50868600
C	-3.16542200	2.61984600	3.14573500
H	-1.29393500	3.69681000	2.98456300
H	-2.55072700	4.29705800	1.92279100
H	-3.56110300	3.23980500	3.95693500
H	-4.00921900	2.31143200	2.51841000
H	-2.74246900	1.71419300	3.59667900

2’

Sum of electronic and thermal Free Energies=-1474.543368

C	-1.14838900	0.95079800	-0.34434000
C	-1.91594800	2.18788500	-0.60538400
C	0.17758600	0.77229800	-0.43951300
C	1.10436900	1.91378000	-0.85553300
H	2.01484500	1.51713200	-1.30923400
H	0.60998500	2.53798100	-1.60878600
C	1.51151200	2.87844700	0.24951800
O	0.81370600	3.24924700	1.17169900
O	2.75992800	3.34338500	0.03799000
C	3.23819700	4.32356000	0.98783500
C	4.63640600	4.72768600	0.56043500
H	3.22611600	3.87846800	1.98760600
H	2.54833700	5.17348300	0.99848000
H	5.03768800	5.47103400	1.25642100
H	5.30776300	3.86412900	0.55491800
H	4.62880200	5.16433400	-0.44250400
C	0.85246800	-0.57296300	-0.24380800
H	1.39619500	-0.81506600	-1.16910900
H	0.08771400	-1.35206000	-0.13443300
C	1.82265400	-0.71075000	0.91987300
C	1.80992600	0.08379600	1.99365700
H	2.49444400	-0.08625700	2.82084400
H	1.11487600	0.90949600	2.09389400
C	-2.44924600	2.93617600	0.59437500
H	-3.03200200	2.27170900	1.24139800
H	-1.60184300	3.29865100	1.18459100
H	-3.07680500	3.78056800	0.29571600
C	-2.16259800	2.59692300	-1.87186900
H	-3.44112500	0.88083700	-1.87164200
H	-2.73540000	3.49841500	-2.07271700
H	-1.73066700	2.08352300	-2.72793000
Pd	-2.41939400	-0.52088400	0.16638100

O	-1.61613100	-1.12946200	1.98695200
O	-5.60348900	0.27846800	-2.50352400
C	-2.52980500	-2.01103700	2.19723900
O	-3.44432300	-2.18805500	1.34230700
C	-4.84145500	-0.49008900	-1.97944200
O	-3.55230300	-0.07759200	-1.65862200
C	-2.49043700	-2.78866400	3.48719600
H	-3.05979700	-3.71394700	3.38678800
H	-1.45738400	-2.99939200	3.77170200
H	-2.94060000	-2.18377500	4.28172900
C	-5.08205600	-1.92754800	-1.62281400
H	-4.94439300	-2.08836100	-0.54903300
H	-6.09290000	-2.20051800	-1.92328200
H	-4.35354200	-2.56167100	-2.13779000
C	2.75207600	-1.90378700	0.84035400
H	2.16106600	-2.80233800	0.60131200
H	3.18674100	-2.09341600	1.83094400
C	3.90061300	-1.83748700	-0.16636100
C	4.26989600	-0.72827900	-0.76059600
C	4.65692100	0.36716300	-1.36367500
H	5.38804400	1.03893000	-0.91790800
H	4.26311800	0.65823600	-2.33614300
C	4.62094800	-3.15850700	-0.39720500
C	5.84809300	-3.10953800	-1.31185800
H	3.89117900	-3.87790600	-0.79992300
H	4.91145500	-3.56358600	0.58446200
C	6.49999400	-4.48387000	-1.49321400
H	5.55569600	-2.70470500	-2.28808700
H	6.57816600	-2.40276300	-0.89941300
H	7.37438600	-4.42498400	-2.14930800
H	6.83227900	-4.89769300	-0.53406000
H	5.80023900	-5.20172600	-1.93665400

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Sum of electronic and thermal Free Energies=-1245.530125

C	0.66625700	-1.07209900	0.44787300
C	0.86211000	-2.34925100	1.15267600
C	1.48529900	-0.00765200	0.39384500
C	2.85139300	0.04081000	1.03674800
H	2.96301100	0.90823300	1.70045300
H	3.01787400	-0.84334300	1.65980400
C	3.97188900	0.09244100	0.00518400
O	3.84966300	-0.11449000	-1.18494100
O	5.15026800	0.38393700	0.59399100
C	6.30461900	0.41766400	-0.27874100
C	7.50922400	0.77144900	0.57236800
H	6.12767000	1.15372400	-1.06926700
H	6.41220500	-0.55999800	-0.75919000
H	8.40726300	0.80709200	-0.05221700
H	7.38038500	1.74909100	1.04568500
H	7.66576400	0.02677200	1.35801100
C	1.03539400	1.23037100	-0.34905800
H	1.86996500	1.68144600	-0.90446200
H	0.69787600	1.99076700	0.36741800
C	-0.09148700	0.92502100	-1.32798700
C	0.06157500	-0.12918400	-2.22442300
H	-0.60678000	-0.22752400	-3.07673900
H	0.99815700	-0.67609400	-2.26970100
C	0.95704100	-3.59758300	0.30403600
H	1.75699100	-3.50667100	-0.44020000
H	1.14902300	-4.48055600	0.91976300
H	0.02019400	-3.75771900	-0.24119600
C	0.91453000	-2.39300300	2.49555400
Pd	-1.06035100	-0.94076200	-0.55810400
O	-2.37778000	-2.31361800	0.45982800
C	-3.35597500	-2.03668000	-0.32365400
O	-3.21230400	-1.18960100	-1.25488300
C	-4.67213300	-2.74525900	-0.11372400
H	-5.42697300	-2.36617200	-0.80356500
H	-4.53516900	-3.81959800	-0.27178100
H	-5.00359700	-2.60873500	0.91964500
H	1.05784900	-3.33134400	3.02481800
H	0.79866700	-1.49745000	3.09787300
C	-1.11576700	2.01866600	-1.60842500
H	-0.60782800	2.76447800	-2.23540900
H	-1.92538700	1.59465600	-2.21590800
C	-1.71113700	2.73422400	-0.40028300
C	-1.43321600	4.00161100	-0.19724200
C	-1.15844800	5.26835100	-0.02030700
H	-1.76556700	6.05242500	-0.46923100
H	-0.31504200	5.59273600	0.58643300
C	-2.64268800	1.93855800	0.49960000
C	-3.35417900	2.73905400	1.59470000
H	-2.06481700	1.12323800	0.96166600
H	-3.38178100	1.43223200	-0.13712200
C	-4.27118800	1.86287100	2.45383000
H	-2.60791400	3.23106400	2.23033000
H	-3.93638400	3.54588300	1.13247900
H	-4.77029000	2.45220000	3.22988500

H	-5.04881600	1.38685900	1.84566200
H	-3.70785700	1.06525300	2.95143500

4

Sum of electronic and thermal Free Energies=-1245.518026

C	-0.53861000	0.00154900	0.73917200
C	-0.93294000	0.34904500	2.12461000
C	-1.23895200	-0.75519600	-0.11857400
C	-2.59092800	-1.32866500	0.27521000
H	-2.64737600	-2.39903400	0.03077200
H	-2.75053100	-1.25919300	1.35389700
C	-3.77560800	-0.65395900	-0.40599500
O	-3.72578500	0.24480300	-1.21866900
O	-4.93360400	-1.19944000	0.02809100
C	-6.14482300	-0.63918600	-0.53059900
C	-7.31737000	-1.35278100	0.11477600
H	-6.12889000	-0.77362100	-1.61691700
H	-6.15944400	0.43732900	-0.33464300
H	-8.25739500	-0.95744300	-0.28276600
H	-7.28255500	-2.42688100	-0.08850600
H	-7.31415700	-1.20770400	1.19878100
C	-0.85238800	-1.09092400	-1.55287200
H	-1.66486800	-0.71575100	-2.18620700
H	-0.87245300	-2.18634000	-1.65713600
C	0.46419700	-0.56614700	-2.09815000
C	0.54258000	0.65301300	-2.65681900
H	1.47353600	1.02941900	-3.07146700
H	-0.32144200	1.30945600	-2.70840700
C	-1.47425000	1.74457000	2.34946800
H	-2.39977700	1.88458400	1.77752100
H	-1.68591100	1.92241400	3.40786400
H	-0.77496800	2.50313100	1.98552300
C	-0.82024700	-0.54070200	3.12807100
Pd	1.13247600	0.98461400	0.19189900
O	0.44529000	3.08427100	-0.04923600
C	1.64066600	3.45917300	-0.30038200
O	2.59607800	2.62156300	-0.30744500
C	1.90310400	4.91107300	-0.62687500
H	1.66867500	5.08703300	-1.68259500
H	1.25498400	5.55622700	-0.02955100
H	2.95269900	5.15784100	-0.45797300
H	-1.10859800	-0.28562100	4.14454200
H	-0.44861300	-1.54732500	2.95805600
C	1.65906000	-1.50083100	-2.08660600
H	1.34912400	-2.48028900	-2.47914100
H	2.42322900	-1.12830500	-2.78251400
C	2.32717700	-1.72143000	-0.73701900
C	2.20524100	-0.86107300	0.25636200
C	2.38576500	-0.26423100	1.47415600
H	1.79522200	-0.55099400	2.34048400
H	3.25696500	0.36104200	1.66304500
C	3.20541000	-2.95986500	-0.63880200
C	3.99344900	-3.14832700	0.66014500
H	3.90428600	-2.94233600	-1.48920100
H	2.56609700	-3.83961300	-0.80978700
C	4.84247000	-4.42374500	0.64793700
H	4.63905200	-2.27696500	0.82300300
H	3.29719100	-3.17728200	1.50702300
H	5.39494500	-4.54010300	1.58551700
H	4.21973700	-5.31597100	0.51646000
H	5.57350600	-4.40769600	-0.16825300

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Sum of electronic and thermal Free Energies=-1245.564384

C	0.55576100	-0.51580200	1.44476900
C	0.26460800	-1.91425100	1.91697000
C	1.82097300	-0.08858400	1.22212400
C	3.02110500	-1.00677000	1.35497000
H	3.80366600	-0.52793000	1.95150500
H	2.73812000	-1.94639200	1.83066200
C	3.57581200	-1.33406100	-0.02762900
O	3.04457000	-2.08390500	-0.81996500
O	4.71737700	-0.66282600	-0.27893200
C	5.28013300	-0.84867500	-1.60198900
C	6.57598900	-0.06332700	-1.66061700
H	4.55068300	-0.49796600	-2.33861100
H	5.43602700	-1.91820200	-1.77073500
H	7.03310800	-0.17645500	-2.64853200
H	6.39743700	1.00157800	-1.48536500
H	7.28636700	-0.42176900	-0.91008600
C	2.14365100	1.33077700	0.77466900
H	3.21323400	1.52424500	0.89094400
H	1.62271000	2.03507300	1.43707300
C	1.72214800	1.63128600	-0.65189300
C	2.51574800	2.26198500	-1.52250400
H	2.17944600	2.50427300	-2.52680900
H	3.52740700	2.55818900	-1.25907300
C	-0.05683900	-2.93193400	0.84821500
H	0.77155100	-2.99987400	0.13320500
H	-0.23898700	-3.91864800	1.28320500

H	-0.94843500	-2.63569800	0.28131700
C	0.31057300	-2.22048200	3.21983800
Pd	-2.26745400	-0.20716400	0.00100600
O	-2.95650700	-0.60991300	-2.05315300
C	-3.88013400	-1.35396000	-1.58893500
O	-4.00514200	-1.51359800	-0.33099900
C	-4.84190400	-2.04489000	-2.52588600
H	-5.84214500	-1.61996800	-2.39376300
H	-4.52822800	-1.91978300	-3.56288600
H	-4.90264800	-3.10725900	-2.27448700
H	0.10054900	-3.22769300	3.57022800
H	0.55984700	-1.47918900	3.97387000
C	0.33376700	1.13111800	-1.01220900
H	-0.02667000	1.62737600	-1.91765700
H	0.42490600	0.06504000	-1.25269500
C	-0.70209100	1.28486500	0.09849500
C	-0.59967500	0.41777900	1.25006900
C	-1.78655600	0.27385400	2.02405800
H	-2.43852900	1.12010000	2.21406400
H	-1.83521200	-0.52576400	2.75507900
C	-1.43163100	2.62567700	0.13172200
C	-0.55827900	3.82004300	0.58109800
H	-2.31128800	2.58417800	0.78020500
H	-1.81134400	2.82647400	-0.87775900
C	-1.32972000	5.14269500	0.53017900
H	-0.20620500	3.63910400	1.60501900
H	0.33373400	3.88929200	-0.05075900
H	-0.70464100	5.97813800	0.86136000
H	-1.66884800	5.36374000	-0.48805800
H	-2.21572500	5.11323000	1.17454900

6

Sum of electronic and thermal Free Energies=-1358.888770

C	-0.78582000	-0.67513300	-1.44056700
C	-0.48089000	-2.12203200	-1.71429900
C	-2.05239300	-0.23795300	-1.24777300
C	-3.24227600	-1.17857500	-1.24598800
H	-4.03475200	-0.78864700	-1.89208100
H	-2.95365300	-2.16936900	-1.59898300
C	-3.78298700	-1.32961900	0.17228500
O	-3.23565900	-1.96354500	1.05035200
O	-4.93209100	-0.64718900	0.34341800
C	-5.48440500	-0.66772500	1.68414400
C	-6.79340000	0.09692900	1.64980800
H	-4.75660000	-0.21202800	2.36273300
H	-5.62048800	-1.70854700	1.99183700
H	-7.24209700	0.10699500	2.64789100
H	-6.63501200	1.13239300	1.33461400
H	-7.50205400	-0.36905000	0.95910900
C	-2.38473600	1.22141400	-0.96899300
H	-3.45893300	1.38874200	-1.08284900
H	-1.88595900	1.84653800	-1.72196200
C	-1.93313000	1.68943400	0.40304400
C	-2.71468800	2.41013200	1.21243600
H	-2.35950000	2.77038700	2.17390000
H	-3.73529100	2.66421100	0.93949300
C	-0.15778000	-2.97122000	-0.50724300
H	-1.00661800	-2.97448400	0.18693600
H	0.07585100	-4.00008100	-0.79518300
H	0.69916100	-2.56297200	0.04325800
C	-0.52247500	-2.61418400	-2.95896300
Pd	2.16663800	-0.18104300	-0.19325000
O	2.33185200	0.08652100	1.89087600
C	3.31977500	-0.51062700	2.47959700
O	4.17359300	-1.22353600	1.93089000
C	3.37418600	-0.27534000	3.98570000
H	3.42533700	0.79821800	4.19015300
H	2.45584400	-0.65055000	4.44760300
H	4.23832400	-0.77858900	4.42004000
H	-0.30147100	-3.65919100	-3.15989400
H	-0.78240000	-1.99310900	-3.81151300
C	-0.53287600	1.24178700	0.78352600
H	-0.14964500	1.83506400	1.61715200
H	-0.60584800	0.21002600	1.14645900
C	0.46793700	1.27501800	-0.36581200
C	0.35477200	0.29774100	-1.40602500
C	1.50340700	0.07672600	-2.22926600
H	2.11844600	0.90999300	-2.55461700
H	1.49961200	-0.77867200	-2.89491900
C	1.23182100	2.58613300	-0.53089500
C	0.36281200	3.75375600	-1.05549500
H	2.08959600	2.47419100	-1.20002400
H	1.64373200	2.86274500	0.44684600
C	1.15609600	5.06155300	-1.14068000
H	-0.02464700	3.49253700	-2.04881500
H	-0.50746200	3.88975800	-0.40467500
H	0.53384200	5.87707100	-1.52272400
H	1.53133400	5.36152400	-0.15593800
H	2.02009300	4.96066200	-1.80731000

C	3.75976600	-1.35642700	-0.39934000
O	4.61100800	-2.03206500	-0.75581600

7

Sum of electronic and thermal Free Energies=-1474.577497

C	-1.14763500	-0.88177400	-1.18059400
C	-0.72588000	-2.32373800	-1.13098200
C	-2.45305200	-0.52447400	-1.14214700
C	-3.57085100	-1.53741200	-0.97919500
H	-4.35020400	-1.37199700	-1.72963900
H	-3.18756300	-2.55308900	-1.08647700
C	-4.18464200	-1.41590900	0.41045100
O	-3.64124300	-1.76648000	1.43761800
O	-5.40397800	-0.83966700	0.36920400
C	-6.03872600	-0.61392800	1.65121100
C	-7.40460500	-0.01137700	1.38366100
H	-5.40129300	0.05318300	2.24000300
H	-6.10464300	-1.56680500	2.18488600
H	-7.91955200	0.17602900	2.33107300
H	-7.31607200	0.93799800	0.84751700
H	-8.02111000	-0.68836200	0.78526400
C	-2.90431800	0.92830900	-1.20225100
H	-3.97702800	0.98319700	-1.40759300
H	-2.39279700	1.41885600	-2.04195300
C	-2.57729000	1.71232800	0.05554400
C	-3.44200800	2.54676900	0.63975600
H	-3.16795000	3.13054800	1.51432800
H	-4.45236000	2.67594300	0.26129100
C	-0.36661900	-2.86354200	0.23309900
H	-1.22233900	-2.76782300	0.91238200
H	-0.06455000	-3.91314300	0.17779500
H	0.46191700	-2.29184200	0.67029000
C	-0.70018900	-3.07566200	-2.23807300
Pd	1.90203100	-0.12257100	-0.17723500
H	-0.38867700	-4.11629200	-2.20636400
H	-0.98004000	-2.67439000	-3.20791700
C	-1.18165100	1.44457000	0.59302400
H	-0.89757400	2.22347200	1.30669700
H	-1.22716200	0.50022500	1.14996700
C	-0.11741600	1.31758600	-0.48920200
C	-0.08292000	0.17086000	-1.29531900
C	1.10671200	-0.11022200	-2.08974300
H	1.58546500	0.70482600	-2.62769900
H	1.14364200	-1.05861800	-2.61493400
C	0.66098900	2.58945600	-0.78955300
C	-0.15062700	3.62253300	-1.60727100
H	1.59232300	2.37945800	-1.32300300
H	0.95531700	3.05234700	0.16170200
C	0.62809200	4.92154200	-1.83637900
H	-0.41817900	3.17603600	-2.57358400
H	-1.09413600	3.84139700	-1.09395800
H	0.04358300	5.63568000	-2.42546000
H	0.88265800	5.40415000	-0.88584900
H	1.56507300	4.73442200	-2.37317800
C	5.98334700	-1.26751500	-0.34943500
H	5.95577500	-2.29946700	0.00964300
H	6.17779500	-1.27282200	-1.42378000
H	6.75480900	-0.70063600	0.17381400
C	3.56910300	-1.17143200	-0.67177800
O	3.72067700	-2.14561900	-1.36517200
O	2.17795800	0.22294900	2.02393400
C	3.16262000	0.40767800	2.74537900
O	4.41156100	0.31269300	2.34852400
O	4.73568100	-0.59369300	-0.07579300
H	4.47781100	0.01025000	1.38724500
C	3.01918700	0.76789200	4.20168300
H	3.46627800	-0.01882200	4.81696100
H	3.56555100	1.69244600	4.40903900
H	1.96684400	0.88521700	4.45649300

r-p1

Sum of electronic and thermal Free Energies=-1474.587257

C	-0.93203900	-0.19862100	-0.71228800
C	-0.09962500	-1.42687600	-0.42092900
C	-2.19300700	-0.28518600	-1.19373300
C	-2.86056100	-1.58716700	-1.59828800
H	-3.09846700	-1.56822700	-2.66733300
H	-2.20479200	-2.43893900	-1.40733400
C	-4.18656800	-1.79383300	-0.88005500
O	-5.28014200	-1.69105500	-1.39392100
O	-4.00177400	-2.08609700	0.42712400
C	-5.20654700	-2.21960600	1.21822900
C	-4.79232800	-2.61193200	2.62339700
H	-5.85271100	-2.97044200	0.75366300
H	-5.73912600	-1.26347000	1.19796400
H	-5.68001700	-2.71906700	3.25478500
H	-4.25478300	-3.56467800	2.62246200
H	-4.14473700	-1.85101300	3.06846200
C	-3.07036900	0.95520500	-1.30235500
H	-3.95400400	0.75356000	-1.91444700

H	-2.50224500	1.74971000	-1.80388500
C	-3.49489700	1.48173200	0.06073900
C	-4.74181200	1.88726300	0.32041800
H	-5.01519900	2.30521900	1.28593700
H	-5.53058300	1.81460300	-0.42300300
C	-0.41577900	-2.04753400	0.93819000
H	-1.46929000	-2.35261500	0.98199300
H	0.21099100	-2.92257200	1.13479800
H	-0.25439600	-1.32434500	1.74443900
C	0.50302900	-2.19630200	-1.42933000
Pd	2.04327700	-1.11373800	-0.37384200
H	0.71688600	-3.25129000	-1.26677800
H	0.44659000	-1.88222700	-2.46824400
C	-2.38927400	1.49647500	1.10856600
H	-2.68583500	2.13091400	1.94949500
H	-2.29978800	0.47391100	1.49792700
C	-1.03840400	1.93249200	0.55347200
C	-0.38108600	1.13960500	-0.32277000
C	0.83328200	1.60744700	-1.10251200
H	0.86633300	2.70399500	-1.12502300
H	0.73524500	1.29289400	-2.14555500
C	-0.54924600	3.29344100	1.00005700
C	-1.29781100	4.47010200	0.33853400
H	0.52651800	3.39789800	0.82926600
H	-0.68271400	3.36484100	2.08890400
C	-0.84808900	5.83289600	0.87400600
H	-1.13993200	4.42742800	-0.74720000
H	-2.37733800	4.34922200	0.49048100
H	-1.38379400	6.65134500	0.38220100
H	-1.03129400	5.91478200	1.95152100
H	0.22417900	5.99005600	0.70987200
C	4.49370200	1.39353400	-1.40913500
H	4.87886200	0.38060000	-1.26954500
H	4.95253400	1.84437000	-2.28978200
H	4.70391000	1.99857300	-0.52345200
O	3.08747100	1.36086100	-1.68396300
C	2.22359200	1.18769100	-0.64586900
O	2.60162300	1.17678100	0.55084500
H	3.89586700	0.48049200	1.26520100
O	4.28374000	-1.58175100	0.19077300
C	4.91721700	-1.13433500	1.14870200
O	4.66787500	0.02996500	1.72259900
C	6.06691400	-1.87669000	1.78031200
H	5.81126200	-2.12808800	2.81451300
H	6.27588300	-2.78713600	1.22012000
H	6.95316000	-1.23676800	1.81253000

ts1

Sum of electronic and thermal Free Energies=-1474.518479

C	-0.81070200	-1.64548900	0.55309000
C	-1.88375200	-2.57479400	0.52144000
C	0.47368000	-1.73511900	0.91650800
C	1.07804900	-3.00791300	1.49911400
H	1.79646700	-2.76227200	2.28744500
H	0.29525600	-3.64196700	1.92096400
C	1.77699100	-3.81407700	0.41241400
O	1.21523200	-4.57822900	-0.34651200
O	3.09599200	-3.54777200	0.36544900
C	3.84819100	-4.23265800	-0.67000600
C	5.29518700	-3.79810500	-0.54485500
H	3.41965900	-3.97337200	-1.64287100
H	3.72651600	-5.31112600	-0.53200900
H	5.89826100	-4.29733800	-1.30932700
H	5.39319900	-2.71731700	-0.68279000
H	5.69957300	-4.05922700	0.43710300
C	1.39129100	-0.54207500	0.78549200
H	2.37262900	-0.85071600	0.39957700
H	1.58849500	-0.12548700	1.78311600
C	0.83474600	0.55242600	-0.11774300
C	0.35033000	0.24255300	-1.38119600
H	0.14427100	1.03761000	-2.09114500
H	0.41340800	-0.76848400	-1.77073400
C	-2.01989600	-3.47446700	-0.67145400
H	-1.85651400	-2.92470500	-1.60292100
H	-1.21634700	-4.22272200	-0.61155300
H	-2.99126700	-3.97123000	-0.70561300
C	-2.92800100	-2.48745200	1.48259500
H	-3.42215500	-1.46290000	1.01806200
H	-3.68212100	-3.27149900	1.46571600
H	-2.63980600	-2.14002400	2.47689000
Pd	-1.44762600	0.24082800	-0.13331200
O	-2.50078200	4.24160400	-0.53008300
O	-5.43764000	-0.91895500	-0.25912000
C	-2.24875200	3.14912600	-0.04319900
O	-1.78324400	2.16012100	-0.78994000
C	-4.57659800	-0.06424700	-0.36611300
O	-3.46327100	-0.13077500	0.39672600
C	-2.44725500	2.87863600	1.44576200
H	-1.50979700	2.54601500	1.90646700

H	-2.78766900	3.78990700	1.93948700
H	-3.17927100	2.07933200	1.59281700
C	-4.70260200	1.12444300	-1.29323500
H	-5.56780600	0.97430500	-1.93945800
H	-4.84881600	2.03684200	-0.70612800
H	-3.79692400	1.28287500	-1.88130500
C	1.18139400	1.98055800	0.23686900
H	0.98649300	2.15589800	1.30364400
H	0.53223800	2.66361900	-0.32041400
C	2.64007400	2.35637200	-0.04008100
C	3.45310900	1.59144600	-0.72779500
C	4.26962600	0.82989000	-1.41149100
H	4.34760400	0.90116200	-2.49483200
H	4.91679100	0.10218600	-0.92358000
C	3.05343400	3.71391200	0.50940200
C	4.47271300	4.17174600	0.16164200
H	2.93106500	3.69109400	1.60310200
H	2.32704900	4.45872300	0.15194300
C	4.80499400	5.54553600	0.75245600
H	5.19293300	3.42743200	0.52235700
H	4.58568000	4.19935100	-0.92869700
H	5.82198400	5.85317800	0.48933300
H	4.11879000	6.31525500	0.38171700
H	4.73311200	5.53809300	1.84613300

ts1'

Sum of electronic and thermal Free Energies=-1474.526557

C	-1.15916300	0.99799800	-0.35484800
C	-2.00908200	2.11027400	-0.66822300
C	0.15624200	0.79348600	-0.47113100
C	1.07509400	1.89924800	-0.99187700
H	1.99479800	1.46880200	-1.39156000
H	0.57791700	2.43454900	-1.81126800
C	1.44859100	2.97225000	0.02219300
O	0.67911800	3.51241300	0.79296900
O	2.74867200	3.30177000	-0.07630100
C	3.20930200	4.34673100	0.81386100
C	4.68684400	4.55542500	0.54299100
H	3.01919400	4.03532700	1.84549700
H	2.62289900	5.25241300	0.62926300
H	5.07785900	5.33774100	1.20094500
H	5.25029800	3.63647100	0.72810400
H	4.85615200	4.86148700	-0.49340800
C	0.81971000	-0.53733300	-0.18241100
H	1.34099000	-0.86423200	-1.09372900
H	0.04736900	-1.29186000	0.01209400
C	1.81383500	-0.57643700	0.96847900
C	1.83143900	0.32102600	1.95804000
H	2.53276900	0.22959900	2.78313200
H	1.13869800	1.15461800	1.99424600
C	-2.47969300	3.01179700	0.43538200
H	-2.60677800	2.47029700	1.37484700
H	-1.67721500	3.74230000	0.60166900
H	-3.40194900	3.53548100	0.17159800
C	-2.54017600	2.22700800	-1.97277000
H	-3.26739500	1.16897000	-1.87581500
H	-3.15859800	3.09551200	-2.19193300
H	-1.91450600	1.87819300	-2.79621200
Pd	-2.51732200	-0.41515500	0.27877500
O	-1.70385400	-0.84795600	2.14846900
O	-4.78814300	-0.52651900	-3.27085100
C	-2.59857600	-1.73555900	2.40277100
O	-3.48206800	-1.98792600	1.52939300
C	-4.27823000	-0.92294600	-2.24385200
O	-3.57208200	-0.07959500	-1.46135500
C	-2.59238800	-2.42590200	3.73895300
H	-3.05943700	-3.40883200	3.65621600
H	-1.57179700	-2.51228600	4.11673600
H	-3.17055800	-1.82748700	4.45145600
C	-4.35581000	-2.34897800	-1.74336700
H	-4.67778200	-2.38764900	-0.69955700
H	-5.04490700	-2.90872400	-2.37630100
H	-3.36420100	-2.81190300	-1.79127500
C	2.73398400	-1.77874300	0.98349000
H	2.12967200	-2.69216100	0.86466500
H	3.20449100	-1.86464800	1.97202200
C	3.84318400	-1.83060700	-0.06717300
C	4.18477000	-0.79983300	-0.80247900
C	4.54587800	0.21361400	-1.54841700
H	5.29171600	0.93292100	-1.21559700
H	4.11610700	0.38323700	-2.53449100
C	4.56003200	-3.16991800	-0.16915700
C	5.73924800	-3.23355800	-1.14386500
H	3.81574100	-3.93334800	-0.44347300
H	4.90182600	-3.45098600	0.83897500
C	6.39368600	-4.61808600	-1.18326400
H	5.39443200	-2.95685800	-2.14732800
H	6.48295900	-2.47861200	-0.86186900
H	7.23212400	-4.64047900	-1.88676500

H	6.77952500	-4.90545000	-0.19834700
H	5.67892300	-5.38852500	-1.49474300

ts2

Sum of electronic and thermal Free Energies=-1474.543306

C	-0.78062300	-1.22719100	-0.59439500
C	-0.71941200	-2.62823800	-1.05468200
C	-1.83377100	-0.39989500	-0.71790900
C	-3.13687100	-0.78263200	-1.40736100
H	-3.49362300	0.04165900	-2.03361400
H	-2.98835900	-1.66583200	-2.03155000
C	-4.20223800	-1.12734200	-0.37664900
O	-4.30667400	-2.20245600	0.17844100
O	-5.00534200	-0.07452500	-0.11507200
C	-6.02386200	-0.28981300	0.89416500
C	-6.79181300	1.00810500	1.05239500
H	-5.53694200	-0.59922500	1.82408800
H	-6.66728300	-1.11357300	0.57022700
H	-7.57570700	0.88442300	1.80596700
H	-6.13134800	1.81835200	1.37454300
H	-7.26366400	1.30184700	0.11042600
C	-1.74597000	0.99645500	-0.14786700
H	-2.69277400	1.28960900	0.33135000
H	-1.59724100	1.72229300	-0.95775400
C	-0.61806800	1.13035500	0.86841800
C	-0.50079800	0.18814800	1.89579500
H	0.18799900	0.35212600	2.72401900
H	-1.24544300	-0.59640200	1.99627600
C	-1.11862400	-3.68425900	-0.04943000
H	-2.18248900	-3.56657600	0.18730300
H	-0.94702900	-4.69540200	-0.43017800
H	-0.56600300	-3.56009700	0.88866500
C	-0.29267000	-2.94882000	-2.29810000
H	1.53733100	-2.51294900	-1.32830400
Pd	0.85948500	-0.47334900	0.35843900
O	2.20293300	0.39985800	3.30241900
O	4.06761200	-2.33384200	0.39486000
C	2.95396000	0.52516200	2.32907600
O	2.61252600	0.42044200	1.07612800
C	3.32057100	-2.71122700	-0.46060300
O	2.15312300	-2.01792200	-0.73967100
C	4.43664700	0.83387000	2.51821700
H	4.72094500	1.71133700	1.92928000
H	4.65758900	1.00366600	3.57307100
H	5.02327900	-0.01135500	2.14535000
C	3.52386700	-3.92389100	-1.34439000
H	2.67943000	-4.61531600	-1.25418400
H	3.59653200	-3.61950800	-2.39362900
H	4.44211500	-4.42853200	-1.04678800
H	-0.25725800	-3.98274900	-2.63270300
H	-0.06208300	-2.18050200	-3.03208700
C	0.02962700	2.49993200	1.02766300
H	-0.69395300	3.11201900	1.58404100
H	0.91366300	2.39345700	1.66336800
C	0.39230200	3.23913200	-0.25563100
C	-0.20476600	4.37479000	-0.53670400
C	-0.79610300	5.51422800	-0.78981100
H	-0.39814800	6.45836500	-0.42206700
H	-1.70817900	5.56827900	-1.38162300
C	1.47100800	2.63365400	-1.13992000
C	1.96574700	3.52485300	-2.28292600
H	1.08502300	1.68974600	-1.55855500
H	2.30714800	2.32891200	-0.49760500
C	3.02692300	2.83395000	-3.14497200
H	1.11705500	3.82617400	-2.90936300
H	2.37479000	4.45257200	-1.86388300
H	3.37446200	3.48982000	-3.94999800
H	3.89937200	2.54673700	-2.54750600
H	2.63066300	1.92231400	-3.60789000

ts3

Sum of electronic and thermal Free Energies=-1245.514911

C	0.68257900	-0.31590100	0.80406200
C	1.03411000	-1.11267700	1.99744800
C	1.44039300	0.60411700	0.18848600
C	2.83170000	0.96902400	0.65740400
H	2.94156700	2.05520100	0.78314400
H	3.04102400	0.53026100	1.63748300
C	3.92419300	0.50760300	-0.29925400
O	3.76518700	-0.18257400	-1.28474800
O	5.12877700	0.96677500	0.10250700
C	6.26051700	0.57310500	-0.70875700
C	7.50279800	1.17614600	-0.08103600
H	6.10200100	0.92845800	-1.73196500
H	6.30620900	-0.51987300	-0.74489900
H	8.38555700	0.90153800	-0.66687200
H	7.43595600	2.26753700	-0.05071800
H	7.64100200	0.81154100	0.94087200
C	0.93836900	1.34319700	-1.03331800
H	1.74462300	1.41182700	-1.77464400

H	0.69340100	2.37657900	-0.74976500
C	-0.27569300	0.69353500	-1.69124500
C	-0.17799100	-0.55395800	-2.24207000
H	-0.99500300	-0.98506100	-2.81184600
H	0.76672400	-1.08913000	-2.22895700
C	1.42748100	-2.55562700	1.76685200
H	2.29014800	-2.60833200	1.09136700
H	1.68964600	-3.04699200	2.70837400
H	0.61316500	-3.10923800	1.29055400
C	1.00842300	-0.56491200	3.22646300
Pd	-1.07417200	-0.86647500	-0.00973800
O	-1.31046500	-3.20884900	0.04091100
C	-2.43141100	-3.05062100	-0.52262500
O	-2.87038200	-1.88504800	-0.81485700
C	-3.27616400	-4.25303000	-0.88987000
H	-4.31732600	-4.08163800	-0.60395600
H	-3.25330400	-4.39199200	-1.97608900
H	-2.89415600	-5.15390000	-0.40747100
H	1.27513600	-1.14282600	4.10753100
H	0.72758800	0.47260700	3.38357500
C	-1.49835500	1.57872800	-1.86138100
H	-1.19242600	2.52084800	-2.33939100
H	-2.22086900	1.10494900	-2.53830500
C	-2.19561400	1.88654300	-0.53827200
C	-2.10940900	1.02090900	0.45583700
C	-2.29719200	0.29003600	1.58345600
H	-1.67773300	0.42946200	2.46466900
H	-3.17739500	-0.33993800	1.68935000
C	-3.02652900	3.15565900	-0.47564400
C	-3.81621700	3.38651500	0.81593700
H	-3.71958400	3.14428900	-1.33089400
H	-2.35831700	4.01162900	-0.65730200
C	-4.61944300	4.69063200	0.78590400
H	-4.49190600	2.53915900	0.98267300
H	-3.12383900	3.39739900	1.66658200
H	-5.17449400	4.83457400	1.71819200
H	-3.96495500	5.55954200	0.65159100
H	-5.34472300	4.69279200	-0.03568600

ts4

Sum of electronic and thermal Free Energies=-1245.496043

C	-0.19170700	-0.86945500	-0.53233300
C	-0.22733200	-1.36132200	-1.93973900
C	0.44251000	-1.50617900	0.47803600
C	1.23797500	-2.78268700	0.23642600
H	0.90661300	-3.57713900	0.91272600
H	1.11840700	-3.12535600	-0.79308600
C	2.71954100	-2.56229200	0.52732200
O	3.32048200	-3.04393200	1.46379700
O	3.26625000	-1.72569000	-0.37743600
C	4.62597200	-1.28554300	-0.13518500
C	4.80177200	0.05475700	-0.82483200
H	5.30826100	-2.04808100	-0.52740300
H	4.78198800	-1.21990300	0.94421600
H	5.81349200	0.43258700	-0.64357600
H	4.66188300	-0.03743600	-1.90636300
H	4.07699600	0.77767500	-0.43884700
C	0.53187900	-0.97527600	1.89949900
H	1.36712100	-0.26702200	1.97119300
H	0.78802600	-1.82017800	2.55521800
C	-0.72910100	-0.33065000	2.43098000
C	-0.70081000	0.75046600	3.21574000
H	-1.60822000	1.17041900	3.64185500
H	0.23066000	1.25746400	3.44810000
C	0.84126700	-0.83501800	-2.87187800
H	1.83514000	-1.05279200	-2.46692600
H	0.75282900	-1.27786600	-3.86826500
H	0.77523800	0.25554500	-2.96724100
C	-1.15702900	-2.24076500	-2.34243200
H	-1.17457000	-2.61638600	-3.36214200
H	-1.92092500	-2.61100200	-1.66596200
C	-2.03075700	-1.01622900	2.05528300
H	-1.84858600	-2.09203300	1.89683500
H	-2.74791500	-0.94480800	2.88123300
C	-2.69800200	-0.46504100	0.81106200
C	-2.00674200	0.04509700	-0.21406500
C	-2.07728700	0.97652900	-1.26314300
H	-1.91887600	0.66517900	-2.29296500
H	-2.66027200	1.88403000	-1.12466600
C	-4.21136500	-0.60774800	0.78292500
C	-4.93747200	-0.35437500	-0.54216200
H	-4.62459300	0.05509000	1.55977600
H	-4.44692700	-1.62670600	1.12757600
C	-6.43902600	-0.64330000	-0.44049600
H	-4.78828900	0.68415900	-0.85638200
H	-4.49066700	-0.97890600	-1.32527200
H	-6.94274500	-0.45639600	-1.39395700
H	-6.62599800	-1.68742400	-0.16457600
H	-6.91640500	-0.01097000	0.31671400

Pd	-0.20157800	1.22566000	-0.37302000
O	0.40168500	3.32950800	-0.40772200
C	1.51821800	3.05411500	0.14453200
O	1.81506800	1.85204700	0.43649300
C	2.50229300	4.16691800	0.41952400
H	1.97444200	5.10085200	0.62175500
H	3.15243600	3.90325800	1.25581400
H	3.12739300	4.31631200	-0.46787700

ts5

Sum of electronic and thermal Free Energies=-1358.870244

C	0.62362500	-0.21275000	1.52671700
C	0.34092200	-1.51213600	2.23312600
C	1.89105600	0.19743800	1.28046800
C	3.09621700	-0.66154400	1.61335800
H	3.83726200	-0.07686300	2.16734900
H	2.80307800	-1.52193700	2.21579000
C	3.73433400	-1.18784800	0.33203200
O	3.27145800	-2.07617700	-0.35186400
O	4.86922500	-0.52344000	0.03198200
C	5.51586900	-0.90843200	-1.20697800
C	6.79536800	-0.10271000	-1.32260900
H	4.82624300	-0.70989500	-2.03331900
H	5.70557700	-1.98555000	-1.18426800
H	7.31513200	-0.36363500	-2.24971300
H	6.58329400	0.97034600	-1.33885100
H	7.46556100	-0.30879800	-0.48310500
C	2.21577600	1.53770400	0.63420800
H	3.27989900	1.75810800	0.75245200
H	1.67027800	2.32448500	1.17338100
C	1.83714500	1.62835900	-0.83154300
C	2.66105000	2.11990700	-1.76147000
H	2.35698800	2.21282500	-2.80036200
H	3.66815100	2.44379400	-1.51377800
C	0.11024300	-2.72827300	1.36754100
H	0.95570600	-2.86956600	0.68386900
H	-0.00505000	-3.62633000	1.98150000
H	-0.79222400	-2.61980200	0.75393900
C	0.31775600	-1.56041200	3.57164300
Pd	-2.11099900	-0.20115200	-0.09144100
O	-1.96655000	-1.12829300	-2.05746100
C	-2.54116300	-2.21965800	-1.71063200
O	-2.93433200	-2.41112000	-0.52436500
C	-2.77798800	-3.27408900	-2.77107500
H	-3.74704200	-3.08856600	-3.24796600
H	-2.00564700	-3.22427100	-3.54132500
H	-2.80561900	-4.26717700	-2.31850000
H	0.11701500	-2.48970900	4.09837300
H	0.49942200	-0.67884400	4.18016400
C	0.45598500	1.08741300	-1.15967800
H	0.11810900	1.46896100	-2.12710500
H	0.54141600	-0.00013000	-1.26762100
C	-0.60302500	1.37812100	-0.10083100
C	-0.53744300	0.64816100	1.14785300
C	-1.76648800	0.60091200	1.87361000
H	-2.40522800	1.47480700	1.94049400
H	-1.85341600	-0.10147900	2.69605900
C	-1.33980500	2.70373700	-0.25689200
C	-0.47734300	3.95269800	0.04042600
H	-2.22712300	2.74388100	0.37989100
H	-1.70358200	2.76622800	-1.28992700
C	-1.25263400	5.25128100	-0.20431300
H	-0.14386000	3.91583900	1.08552400
H	0.42566200	3.93993400	-0.57920300
H	-0.63560000	6.12725600	0.01945600
H	-1.57497600	5.32887500	-1.24865100
H	-2.14894600	5.30569100	0.42399300
C	-4.37827300	0.19384800	-0.06915700
O	-5.30750800	0.24079900	0.59207200

ts6

Sum of electronic and thermal Free Energies=-1474.572415

C	-1.15075200	-0.91696400	-1.29073000
C	-0.80118200	-2.37963500	-1.29422600
C	-2.43174700	-0.49270900	-1.18027600
C	-3.59227400	-1.45247500	-0.99899600
H	-4.39321600	-1.21898400	-1.70728100
H	-3.26952700	-2.48219700	-1.15785100
C	-4.13760200	-1.35035700	0.42137400
O	-3.57484100	-1.78183400	1.40602300
O	-5.31535800	-0.69512100	0.45818000
C	-5.88046100	-0.48652300	1.77645500
C	-7.21403100	0.21245700	1.59531900
H	-5.17670900	0.11204000	2.36312300
H	-5.98540500	-1.45639800	2.27160400
H	-7.67399200	0.39142300	2.57213300
H	-7.08656500	1.17656600	1.09446100
H	-7.89897700	-0.39755100	0.99938900
C	-2.80875400	0.98237500	-1.17686400
H	-3.88581700	1.09625900	-1.32597900

H	-2.31708100	1.47276000	-2.02816700
C	-2.38165400	1.70794000	0.08630200
C	-3.18403100	2.54774700	0.74662500
H	-2.84247000	3.08903100	1.62460900
H	-4.20870500	2.72240300	0.43021900
C	-0.43743400	-2.97832200	0.04391800
H	-1.27158700	-2.86309700	0.74636900
H	-0.18846100	-4.03910400	-0.04965900
H	0.42473500	-2.45954900	0.48155600
C	-0.83810400	-3.09617000	-2.42470600
Pd	1.82578600	-0.18942200	-0.22643500
H	-0.58319800	-4.15266800	-2.43131700
H	-1.12293600	-2.65239000	-3.37448400
C	-0.97117200	1.37539500	0.54042000
H	-0.61252100	2.12467600	1.25110600
H	-1.01525200	0.42408000	1.08416300
C	0.02992700	1.22807600	-0.59774600
C	-0.04031200	0.08155600	-1.43238800
C	1.12406200	-0.24841000	-2.21680300
H	1.68154500	0.53612800	-2.72017100
H	1.13696800	-1.20635500	-2.72494000
C	0.78775900	2.49631300	-0.97094800
C	-0.07683500	3.53131500	-1.72948000
H	1.67236800	2.27894900	-1.57605200
H	1.15990600	2.95761700	-0.04791600
C	0.69795000	4.81848700	-2.02857200
H	-0.42432400	3.08259000	-2.66903900
H	-0.97327100	3.76651300	-1.14472900
H	0.07640200	5.53660500	-2.57302600
H	1.03401800	5.30212400	-1.10453900
H	1.58618500	4.61668600	-2.63794800
C	6.07189800	-0.98167000	0.27023000
H	6.03571000	-1.94186700	-0.25511100
H	6.84016900	-0.35045800	-0.18758500
H	6.32130200	-1.15573600	1.32280600
C	3.48953300	-1.32402700	-0.47424300
O	3.88833800	-2.33341400	-0.91640500
O	1.89915900	0.26489600	1.89955400
C	2.88515000	0.47656100	2.65806400
O	4.11487200	0.43695100	2.33038000
C	2.59637400	0.80579400	4.11151800
H	1.52667300	0.93209600	4.27871900
H	2.97153800	-0.00579000	4.74304700
H	3.13575600	1.71319200	4.39666300
O	4.79992500	-0.34584400	0.15883400
H	4.42600100	0.05824600	1.17383300

ts7

Sum of electronic and thermal Free Energies=-1474.546173

C	-0.97726100	-0.24299800	-0.81088400
C	-0.21928100	-1.53077800	-0.59316900
C	-2.25068300	-0.21731300	-1.26335800
C	-3.03416400	-1.45546800	-1.65291200
H	-3.36250000	-1.38566800	-2.69510100
H	-2.42216800	-2.35344000	-1.54233300
C	-4.30138000	-1.61188400	-0.82263500
O	-5.43104600	-1.48365600	-1.24256900
O	-4.01175300	-1.90163400	0.46686600
C	-5.14841600	-2.00155300	1.35786400
C	-4.62745500	-2.40039600	2.72515200
H	-5.85050700	-2.73690100	0.95356600
H	-5.65687800	-1.03239300	1.37754200
H	-5.46093200	-2.48010500	3.43012300
H	-4.11915200	-3.36828200	2.68454500
H	-3.92360400	-1.65658700	3.10983300
C	-3.01704700	1.09508200	-1.34086900
H	-3.92203400	0.97908500	-1.94438900
H	-2.38314000	1.83960300	-1.84092800
C	-3.37609500	1.64804800	0.03010600
C	-4.56827600	2.18773900	0.30099100
H	-4.78770100	2.62301600	1.27246900
H	-5.36407600	2.21371100	-0.43805300
C	-0.29069400	-2.06111400	0.82824100
H	-1.32286300	-2.36224800	1.04912500
H	0.36754000	-2.92292200	0.96910500
H	-0.01762900	-1.28696200	1.55212600
C	0.28769700	-2.29476400	-1.61174700
Pd	1.97003400	-0.75189000	-0.79336500
H	0.67626400	-3.29131200	-1.42225000
H	0.18099900	-1.99345900	-2.64916600
C	-2.27186000	1.52311200	1.06964000
H	-2.50555300	2.15614500	1.93108700
H	-2.28810900	0.48341800	1.42513400
C	-0.87681700	1.83657800	0.54227100
C	-0.29051200	1.01817600	-0.36942000
C	1.02494300	1.31556300	-1.02945700
H	1.26652900	2.37520400	-0.96350500
H	1.02112600	1.08337700	-2.10026000
C	-0.24175900	3.10557900	1.06821000

C	-0.81136100	4.38840100	0.42423900
H	0.84535600	3.08157600	0.94875200
H	-0.41586000	3.15538700	2.15242800
C	-0.22678800	5.66635100	1.03361400
H	-0.60902600	4.36475000	-0.65451600
H	-1.90367000	4.39457600	0.52621700
H	-0.63868700	6.56117400	0.55557700
H	-0.44634300	5.73012400	2.10552900
H	0.86279300	5.69856700	0.91899700
C	4.72041000	2.28014700	-0.57741200
H	5.34808400	1.61311300	0.01990200
H	5.28335700	2.66287700	-1.42895200
H	4.37902500	3.10279400	0.05705100
O	3.60248500	1.57052600	-1.13974000
C	2.72517300	1.03410500	-0.23936400
O	2.88938200	1.18986600	0.98062200
H	3.57817800	-0.27315700	1.58646300
O	3.60562300	-2.15932600	0.06383500
C	4.18581500	-2.06375500	1.14531700
O	4.12321600	-1.02103100	1.95717700
C	5.06672200	-3.16413400	1.68265100
H	4.71238000	-3.47201000	2.67076100
H	5.06102400	-4.01233800	0.99942400
H	6.08747500	-2.79007600	1.80653300

8

Sum of electronic and thermal Free Energies=-1361.263510

C	-0.77120800	-0.58687700	-1.49996000
C	-0.42702900	-2.00951900	-1.84535200
C	-2.04798700	-0.19862800	-1.27411000
C	-3.20845200	-1.17543000	-1.30261000
H	-4.02276500	-0.77978200	-1.91731500
H	-2.89455300	-2.13773700	-1.70916500
C	-3.72267500	-1.41513600	0.11311500
O	-3.14190000	-2.07279000	0.95155000
O	-4.89209800	-0.78302300	0.33356800
C	-5.42272500	-0.88988300	1.67872700
C	-6.76459000	-0.18394200	1.69733500
H	-4.70565900	-0.43352500	2.36824000
H	-5.50816900	-1.94870800	1.93978100
H	-7.19785800	-0.23939200	2.70079200
H	-6.65719900	0.87081400	1.42803700
H	-7.46246700	-0.64959800	0.99550700
C	-2.42159500	1.23559600	-0.92626300
H	-3.50191300	1.37358000	-1.02115500
H	-1.95301600	1.90828000	-1.65683700
C	-1.97009900	1.65926300	0.46001600
C	-2.77016400	2.31259100	1.30804900
H	-2.41792200	2.64409100	2.28091100
H	-3.80287100	2.53871300	1.05661900
C	-0.07513000	-2.90720800	-0.68246900
H	-0.92081700	-2.97011800	0.01255000
H	0.18816800	-3.91361400	-1.02056200
H	0.76881600	-2.49584800	-0.11435600
C	-0.45649600	-2.44073400	-3.11280000
Pd	2.09407800	-0.01509800	-0.19108200
O	2.27397000	0.14776800	1.94016300
C	3.13335700	-0.49637200	2.63693800
O	4.02785100	-1.25862900	2.19129000
C	3.04835300	-0.27802100	4.14080200
H	3.38871000	0.73607700	4.37589600
H	2.01117400	-0.36048800	4.47585500
H	3.67664700	-0.99675100	4.66820700
H	-0.20762700	-3.46833700	-3.36512500
H	-0.73482100	-1.78592800	-3.93365600
C	-0.54983100	1.25205600	0.80974200
H	-0.18145600	1.82607300	1.66353600
H	-0.57799300	0.20508900	1.13319200
C	0.44223900	1.36711000	-0.34386000
C	0.34416600	0.41056300	-1.42439300
C	1.50440200	0.26615300	-2.23587600
H	2.10167000	1.12761100	-2.51678900
H	1.55847000	-0.57868800	-2.91385200
C	1.09906200	2.73638700	-0.50678100
C	0.15314500	3.84663100	-1.01976400
H	1.96148900	2.68741000	-1.17761800
H	1.49502500	3.03338000	0.47194300
C	0.85289900	5.20792700	-1.08654900
H	-0.21156000	3.57286000	-2.01845200
H	-0.72676200	3.91631500	-0.37120400
H	0.17637200	5.98281500	-1.46117400
H	1.20280900	5.52144200	-0.09664000
H	1.72428800	5.17667900	-1.75048300
H	4.06710100	-1.28533300	0.71482900
C	3.95619600	-2.48115500	-0.92228700
H	3.68733400	-2.36870600	-1.97574300
H	4.96628800	-2.90489500	-0.86236700
H	3.25242100	-3.17946700	-0.45076500
O	3.92918000	-1.19808000	-0.30816700

9

Sum of electronic and thermal Free Energies=-1361.220925

C	-0.69876500	-0.58079700	-1.42953300
C	-0.20157600	-1.95599900	-1.77797000
C	-2.01723300	-0.31799300	-1.27855600
C	-3.07778000	-1.39825400	-1.37852800
H	-3.89409500	-1.07224100	-2.03041200
H	-2.65329400	-2.32013600	-1.77831700
C	-3.63746800	-1.70804100	0.00543900
O	-3.03997800	-2.31890600	0.86741700
O	-4.87314800	-1.19531700	0.17168100
C	-5.45755100	-1.37339800	1.48577900
C	-6.85010100	-0.77402300	1.45005800
H	-4.81367600	-0.87906500	2.21975100
H	-5.47261600	-2.44144700	1.72244600
H	-7.32728700	-0.88657300	2.42855300
H	-6.81148100	0.29194400	1.20770300
H	-7.47365000	-1.27482000	0.70380000
C	-2.54007800	1.07275100	-0.94437600
H	-3.62036700	1.11642600	-1.10790100
H	-2.08786800	1.79229600	-1.63936300
C	-2.21630600	1.51855500	0.46972400
C	-3.12595800	2.08425100	1.26920900
H	-2.86895100	2.43315500	2.26570200
H	-4.15688300	2.21903700	0.95291000
C	0.20046200	-2.83189600	-0.61560000
H	-0.65929500	-2.99837400	0.04429100
H	0.58453800	-3.79761400	-0.95753500
H	0.97168200	-2.33663300	-0.01274100
C	-0.14209600	-2.36713400	-3.05108000
Pd	2.01262800	0.24841900	0.05146700
O	2.60718400	0.33925700	2.00109000
H	0.21954100	-3.35964800	-3.30786600
H	-0.45468300	-1.72928200	-3.87287400
C	-0.79093800	1.23687700	0.91041200
H	-0.54683700	1.83165100	1.79419600
H	-0.74926300	0.18617400	1.21976700
C	0.27165200	1.46196800	-0.16413900
C	0.31474600	0.51479800	-1.27578400
C	1.48650600	0.52250900	-2.06267700
H	2.02787600	1.44031400	-2.26516400
H	1.65697500	-0.29088500	-2.75933000
C	0.75555300	2.90573500	-0.30749800
C	-0.27267700	3.89804200	-0.89572100
H	1.66159500	2.95549700	-0.91855100
H	1.05095200	3.25578400	0.68975900
C	0.27761800	5.32729100	-0.94680800
H	-0.54339600	3.57521200	-1.90962500
H	-1.19375200	3.88125600	-0.30322600
H	-0.45363100	6.01973600	-1.37647600
H	0.52981000	5.68965300	0.05621000
H	1.18725800	5.38278200	-1.55584000
O	3.91327000	-1.01878300	-0.28290500
C	2.02151600	1.13405800	2.97767800
H	2.66192600	1.15585300	3.87780800
H	1.88684000	2.19116800	2.67440700
H	1.02995600	0.76942700	3.31113700
C	4.47367200	-1.76656400	0.51436300
O	5.75360500	-2.11648400	0.31604700
H	6.04770100	-1.65499800	-0.48867100
C	3.85348900	-2.36715700	1.73395600
H	3.33559500	-1.54788200	2.25305400
H	3.10164000	-3.09866000	1.41862300
H	4.59866400	-2.85798600	2.35954900

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Sum of electronic and thermal Free Energies=-1245.504062

C	-0.38503300	-0.77764500	-1.14883700
C	-0.08035800	-2.24581300	-1.25917100
C	-1.65144400	-0.30553300	-1.21472600
C	-2.85703900	-1.22006500	-1.30435100
H	-3.52969100	-0.89654800	-2.10434600
H	-2.54844700	-2.24841200	-1.49951300
C	-3.61123800	-1.20487900	0.02151900
O	-3.18013700	-1.66147200	1.06032600
O	-4.80851900	-0.59721700	-0.09022300
C	-5.57318500	-0.48008400	1.13595400
C	-6.89484800	0.17713200	0.78840200
H	-4.99140100	0.11210200	1.84925100
H	-5.70671400	-1.47802600	1.56380400
H	-7.50233900	0.28697500	1.69205500
H	-6.73800600	1.17019700	0.35746900
H	-7.45551000	-0.42625600	0.06872600
C	-1.97612000	1.18072000	-1.14262200
H	-3.00815400	1.35541600	-1.45934500
H	-1.33500700	1.71474600	-1.85662600
C	-1.75136600	1.78642600	0.23137400
C	-2.61005000	2.63971600	0.79687600
H	-2.40771600	3.09466100	1.76262400

H	-3.54355600	2.91338400	0.31281700
C	0.06598100	-3.00227000	0.04005000
H	-0.84895900	-2.90462700	0.63639500
H	0.26860800	-4.06180900	-0.13861800
H	0.88868500	-2.59293200	0.63939900
C	0.03040700	-2.83388500	-2.45718900
Pd	2.38155500	-0.27870800	0.47839300
H	0.25172500	-3.89419500	-2.54681400
H	-0.09532300	-2.27714100	-3.38149600
C	-0.47689100	1.31713200	0.91066300
H	-0.24316400	1.96597600	1.76021700
H	-0.67990600	0.31786900	1.31321800
C	0.72817500	1.23187100	-0.02298100
C	0.76108600	0.17958700	-0.99585000
C	2.00729400	-0.09832400	-1.63214800
H	2.68830100	0.70522100	-1.89508900
H	2.09517000	-0.99580200	-2.23309000
C	1.52722500	2.52347200	-0.18782800
C	0.86915300	3.55720700	-1.13093300
H	2.53976800	2.32376400	-0.55071200
H	1.65122700	2.97856900	0.80238600
C	1.68988300	4.84675600	-1.23325100
H	0.76023200	3.10918800	-2.12688100
H	-0.14144500	3.78944400	-0.77699100
H	1.21631400	5.56463300	-1.91052100
H	1.79237500	5.32992300	-0.25508200
H	2.69905700	4.64710000	-1.61096500
C	4.57805500	-1.95774900	-0.66934200
H	4.88806700	-1.18838400	-1.40144100
H	5.48136600	-2.54440200	-0.42907400
H	3.88627700	-2.64400200	-1.19322900
O	4.05995000	-1.43648900	0.51783000
C	2.46202800	-0.20316800	2.46040600
O	2.55449900	-0.18853200	3.59823200

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Sum of electronic and thermal Free Energies=-1245.504075

C	-0.70217500	-0.64114600	-1.59458200
C	-0.62617800	-2.07852100	-2.02588100
C	-1.87343200	-0.04789500	-1.26929200
C	-3.18538900	-0.80876600	-1.24209600
H	-3.96611000	-0.24467900	-1.76118000
H	-3.07695500	-1.78479100	-1.71630400
C	-3.61190100	-1.04182100	0.20381600
O	-3.09278000	-1.84612100	0.94989400
O	-4.61729200	-0.22175800	0.56647600
C	-5.03288100	-0.30801300	1.95291200
C	-6.18041200	0.66417300	2.14595500
H	-4.17410400	-0.06435000	2.58577600
H	-5.32391500	-1.34029500	2.16883700
H	-6.52437300	0.62897900	3.18431200
H	-5.86742100	1.68826500	1.92298300
H	-7.02296600	0.41129800	1.49582500
C	-1.96166200	1.41273400	-0.84644300
H	-3.00295100	1.74530400	-0.86741500
H	-1.42513600	2.02221900	-1.58508200
C	-1.36332900	1.69120400	0.52298300
C	-1.96371300	2.48233500	1.41760300
H	-1.50382000	2.70368200	2.37656600
H	-2.93145400	2.93607000	1.21941300
C	-0.26790900	-3.07390900	-0.94865600
H	-1.03943000	-3.07114700	-0.16943100
H	-0.16677300	-4.08508100	-1.35282900
H	0.67425400	-2.79738700	-0.45479200
C	-0.87740800	-2.43577900	-3.29201300
Pd	2.30708700	-0.59934000	-0.21161900
H	-0.81734000	-3.47396900	-3.60858400
H	-1.15609000	-1.70596900	-4.04679700
C	-0.05731400	0.97334500	0.80373900
H	0.44203100	1.37698000	1.68735100
H	-0.30918200	-0.06549700	1.04248400
C	0.92715800	0.97236700	-0.36488900
C	0.58785300	0.12667200	-1.53948100
C	1.57267400	-0.12254500	-2.47668800
H	2.43434800	0.52543100	-2.59532200
H	1.41585700	-0.87552300	-3.24024500
C	1.73188800	2.26283000	-0.54253500
C	0.95158600	3.46827100	-1.11450200
H	2.59933100	2.09175700	-1.18783900
H	2.13682400	2.52868100	0.44030500
C	1.83873700	4.71239900	-1.23127100
H	0.55809000	3.20718600	-2.10557400
H	0.08968600	3.69197700	-0.47757700
H	1.28069100	5.56010500	-1.64193500
H	2.22847800	5.01259500	-0.25223200
H	2.69784400	4.52963000	-1.88704300
C	4.38394000	-1.54266400	3.23905100
H	4.89388700	-0.61072500	3.49829800
H	3.60950600	-1.73824400	3.98568900

H	5.09547900	-2.36829800	3.20279100
O	3.80669900	-1.45772700	1.92038700
C	2.86127100	-0.47076400	1.73889000
O	2.54303300	0.27165500	2.64502700

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Sum of electronic and thermal Free Energies=-1245.490714

C	0.46785200	-0.55005600	1.39217000
C	0.13221000	-1.96243000	1.78249000
C	1.74722300	-0.13218400	1.25519400
C	2.92791600	-1.07293700	1.40172600
H	3.69006100	-0.63380000	2.05246800
H	2.61149700	-2.02852400	1.82170000
C	3.53654100	-1.34655000	0.02994000
O	3.01685400	-2.03367100	-0.82509800
O	4.71019600	-0.70570300	-0.13344800
C	5.32645700	-0.84144900	-1.43899100
C	6.63438700	-0.07486400	-1.40808900
H	4.63393100	-0.44761700	-2.18921300
H	5.47461000	-1.90495000	-1.64839300
H	7.13168600	-0.15286600	-2.37982400
H	6.46300500	0.98418500	-1.19458200
H	7.30698200	-0.47625000	-0.64461400
C	2.10693800	1.30078400	0.88589700
H	3.17124900	1.47633200	1.06336300
H	1.56152900	1.98253100	1.55172300
C	1.76166700	1.66453400	-0.54788200
C	2.59352800	2.35390200	-1.33452300
H	2.31406000	2.64194500	-2.34416700
H	3.58067000	2.65535600	-0.99454500
C	-0.15128000	-2.91887900	0.64873500
H	0.72152400	-2.98544800	-0.01166200
H	-0.39819700	-3.91697400	1.02139100
H	-0.98688400	-2.56030000	0.03382900
C	0.11131000	-2.33519500	3.06858600
Pd	-2.32510300	-0.13498600	-0.18685700
H	-0.13228600	-3.35456000	3.35657100
H	0.33928800	-1.63826800	3.87001900
C	0.41047600	1.15591300	-1.01735400
H	0.11468200	1.66503200	-1.93901900
H	0.53295100	0.09576500	-1.26615600
C	-0.70690500	1.28618500	0.01641400
C	-0.66470200	0.41275000	1.17837200
C	-1.84274500	0.28952300	1.94047700
H	-2.52944400	1.12023100	2.06341200
H	-1.91465800	-0.50097600	2.67802700
C	-1.39638300	2.65189300	0.06516600
C	-0.58013100	3.76654600	0.75837300
H	-2.37008100	2.58825700	0.56114700
H	-1.60949600	2.95727600	-0.96602600
C	-1.31489800	5.11078100	0.73760600
H	-0.38307500	3.47116300	1.79701800
H	0.39396500	3.87203000	0.26840500
H	-0.73043200	5.88962300	1.23775900
H	-1.50251400	5.44336500	-0.28948500
H	-2.28394200	5.04319900	1.24518700
C	-4.34509800	-2.61184100	-0.72576400
H	-4.08518000	-3.03327300	-1.70931100
H	-3.75538500	-3.13193900	0.04206300
H	-5.40639000	-2.82650500	-0.54240100
O	-4.15416800	-1.20930100	-0.70481700
C	-3.01958200	-0.61323600	-2.00627300
O	-3.24884000	-0.96180000	-3.09199600

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Sum of electronic and thermal Free Energies=-1358.832696

C	-0.48475000	-0.17752400	0.79414700
C	-0.73887900	-0.23591800	2.24910700
C	-1.27873700	-0.66696500	-0.16888900
C	-2.58731000	-1.36374900	0.16209300
H	-2.61857400	-2.36976600	-0.27928400
H	-2.69324100	-1.50891500	1.24089500
C	-3.83136800	-0.62972200	-0.32076000
O	-3.87189700	0.46977500	-0.82985800
O	-4.93237100	-1.38257400	-0.09051400
C	-6.19401300	-0.79040400	-0.47495100
C	-7.28766000	-1.78402400	-0.13102100
H	-6.16741300	-0.56214900	-1.54533300
H	-6.31757600	0.15785500	0.05794600
H	-8.26391100	-1.37293700	-0.40657000
H	-7.14573500	-2.72475500	-0.67092300
H	-7.29589100	-2.00109900	0.94103000
C	-1.02873300	-0.50259200	-1.66545300
H	-1.57666900	0.38847100	-1.99044500
H	-1.50620700	-1.34923700	-2.18287900
C	0.40042300	-0.41954600	-2.16147600
C	0.86570900	0.68755000	-2.75977400
H	1.86370100	0.72926800	-3.18886900
H	0.26292300	1.58700800	-2.83556300
C	-1.19015500	1.04849900	2.91102000

H	-2.16192500	1.35804100	2.50901300
H	-1.27791700	0.92912300	3.99482400
H	-0.49874500	1.86712300	2.69130200
C	-0.57019700	-1.37163000	2.95272800
Pd	1.20197300	0.89055400	0.32862300
O	-0.07599500	2.55261900	0.17092100
C	0.43770300	3.68117600	-0.19063400
O	1.63430200	3.89829500	-0.45782400
C	-0.57037700	4.82053700	-0.27209800
H	-1.40653500	4.52704200	-0.91243400
H	-0.97788500	5.01231800	0.72523400
H	-0.09695400	5.72419700	-0.65638400
H	-0.75290100	-1.40652900	4.02379100
H	-0.26012000	-2.29588700	2.47345800
C	1.25089700	-1.67789200	-2.11003900
H	0.61032400	-2.55576200	-2.27911100
H	1.95965500	-1.66859000	-2.94967700
C	2.05740500	-1.94296500	-0.84864700
C	2.17472400	-1.10288200	0.15815600
C	2.51174400	-0.58283700	1.36675100
H	1.94882600	-0.84299000	2.26075800
H	3.46411000	-0.07909600	1.51663100
C	2.77238900	-3.28965400	-0.83311100
C	3.67315900	-3.59023800	0.36762200
H	3.36289300	-3.36248200	-1.75880500
H	2.00363600	-4.07279300	-0.91770400
C	4.33509900	-4.96847000	0.26661600
H	4.44576000	-2.81575200	0.44637200
H	3.08379500	-3.53202300	1.29050700
H	4.97472200	-5.16367600	1.13292500
H	3.58650700	-5.76747800	0.21948400
H	4.95882800	-5.04611700	-0.63107700
C	2.87796800	2.09723400	-0.12926200
O	3.94989900	2.43991000	-0.34378800

r-p3

Sum of electronic and thermal Free Energies=-1245.545675

C	0.50271600	0.25098300	1.38594400
C	0.40102900	-0.93517500	2.32191500
C	1.73904000	0.70056900	1.06720800
C	3.00733900	0.01954400	1.56486600
H	3.67908200	0.76866900	1.99706500
H	2.78133800	-0.72399000	2.32808700
C	3.73766800	-0.69322100	0.43345600
O	3.43091600	-1.77701100	-0.01810400
O	4.78092100	0.03326200	-0.02690200
C	5.51914800	-0.55008800	-1.12762400
C	6.70627100	0.35101100	-1.40994000
H	4.85017700	-0.63442100	-1.99010000
H	5.82634600	-1.56212100	-0.84802800
H	7.29172800	-0.05596600	-2.24029700
H	6.38045500	1.35933900	-1.68204200
H	7.35725800	0.42552000	-0.53408600
C	2.00793200	1.92222500	0.20940400
H	3.08454200	2.10086000	0.16057400
H	1.55698700	2.80494100	0.68311000
C	1.45351000	1.79721200	-1.18979600
C	2.25521200	1.76293900	-2.27068600
H	1.84971600	1.69713800	-3.27648600
H	3.33589900	1.80054600	-2.17598200
C	0.42721600	-2.31382200	1.70244800
H	1.34559000	-2.45417800	1.12040100
H	0.36591200	-3.09131000	2.46992300
H	-0.41625300	-2.44379700	1.01210500
C	0.37207100	-0.75710400	3.64962100
Pd	-2.29613000	-0.79025000	0.57454300
O	-1.68663600	-1.44190700	-2.41905600
C	-2.44776700	-2.42401000	-1.95038600
O	-2.85381600	-2.46451600	-0.78885000
C	-2.75797400	-3.48233300	-2.97017700
H	-3.42738800	-4.22568400	-2.54005400
H	-3.21442300	-3.02527600	-3.85263900
H	-1.82793400	-3.95954100	-3.29376100
H	0.31969200	-1.60240700	4.33122800
H	0.40094900	0.23256500	4.09673400
C	0.00398800	1.85630500	-1.30701500
H	-0.35095800	2.24332100	-2.26169100
H	-1.52641700	-0.80700000	-1.67649100
C	-0.95394800	1.62631900	-0.36366200
C	-0.79620600	0.87476300	0.92269200
C	-1.87767400	0.85913800	1.83644100
H	-2.69774700	1.56125100	1.73461400
H	-1.71297500	0.49441500	2.84376500
C	-2.32840400	2.21164700	-0.69724600
C	-2.51172700	3.65201000	-0.17268600
H	-3.13796400	1.57629100	-0.32306000
H	-2.43975500	2.23095700	-1.78804700
C	-3.89115100	4.22923300	-0.50625300
H	-2.35674400	3.67316000	0.91306200

H	-1.72756800	4.28662400	-0.60343700
H	-3.99450400	5.25373000	-0.13383700
H	-4.06151300	4.25031800	-1.58891200
H	-4.69235500	3.63006700	-0.05852700

ts14

Sum of electronic and thermal Free Energies=-1358.814726

C	-0.11352800	-0.92042300	-0.46822300
C	-0.04786800	-1.41957400	-1.87017600
C	0.54334500	-1.47814300	0.56978000
C	1.44370100	-2.69554900	0.37242800
H	1.14971600	-3.48701600	1.07072100
H	1.36927100	-3.07345900	-0.64704800
C	2.89286200	-2.35602000	0.69498100
O	3.39404800	-2.43516000	1.79680400
O	3.55393800	-1.92447100	-0.39928100
C	4.91958400	-1.49470100	-0.18142300
C	5.48124700	-1.05391300	-1.51933200
H	5.48495200	-2.32689000	0.24932500
H	4.91565800	-0.68227000	0.55147600
H	6.51834700	-0.72658200	-1.39548900
H	5.46497200	-1.87530800	-2.24165200
H	4.90486000	-0.21997300	-1.93011000
C	0.51707100	-0.93460900	1.98848300
H	1.27054100	-0.14508000	2.07713600
H	0.83183400	-1.74051000	2.66566700
C	-0.82683900	-0.42215300	2.44834200
C	-0.95927300	0.69504300	3.17022000
H	-1.92492100	1.02040400	3.54882100
H	-0.10573000	1.32489600	3.40089300
C	1.01214900	-0.80697800	-2.76008100
H	2.00763200	-0.98452300	-2.33909100
H	0.97277600	-1.22532200	-3.77014000
H	0.89016300	0.28069800	-2.82694400
C	-0.88170700	-2.37340600	-2.31409800
H	-0.82487900	-2.74240600	-3.33484000
H	-1.63768900	-2.81243500	-1.67086600
C	-2.02281300	-1.28470000	2.08613500
H	-1.70335600	-2.33325000	1.97296900
H	-2.75512300	-1.27562500	2.90204100
C	-2.74634900	-0.87585300	0.81819900
C	-2.15088900	-0.27945100	-0.21305300
C	-2.32637400	0.61359900	-1.27026900
H	-2.10356900	0.30992500	-2.29050700
H	-3.05155900	1.41509500	-1.15810700
C	-4.21722900	-1.26857200	0.77498700
C	-4.96862600	-1.12885500	-0.55234700
H	-4.73844700	-0.69026600	1.55385700
H	-4.28011400	-2.31574100	1.10987100
C	-6.40229500	-1.66264100	-0.46066700
H	-4.99257600	-0.07730600	-0.85843100
H	-4.42194200	-1.66485700	-1.33769200
H	-6.92713600	-1.54914700	-1.41424200
H	-6.41556000	-2.72657400	-0.19829400
H	-6.97922800	-1.12688600	0.30167800
Pd	-0.46504500	1.19236400	-0.41774900
O	1.17448300	3.77143400	0.21538500
C	1.86588800	2.76444400	0.46703700
O	1.50274500	1.53751100	0.31962300
C	3.28774900	2.94887800	0.98515700
H	3.44109900	2.33753800	1.87870600
H	3.99458100	2.60053100	0.22507500
H	3.48318600	3.99806700	1.20767400
C	-0.79322500	3.19106400	-0.60039700
O	-1.31086400	4.19076200	-0.81754400

ts15

Sum of electronic and thermal Free Energies=-1245.522679

C	0.30947500	-1.39083000	-0.94596200
C	0.44052800	-1.44231300	-2.44960300
C	1.41702700	-1.48930500	-0.17302200
C	2.80963700	-1.60759000	-0.77027700
H	3.35946700	-2.40644600	-0.26262600
H	2.75808200	-1.83693500	-1.83433300
C	3.59298000	-0.30636000	-0.62750600
O	3.45401900	0.66425600	-1.34136900
O	4.46954700	-0.35938800	0.39763500
C	5.23474100	0.84907900	0.63278200
C	6.21895300	0.55674200	1.74906100
H	4.53970600	1.65321900	0.89329000
H	5.73693400	1.13230800	-0.29687600
H	6.81932100	1.44820600	1.95569500
H	5.69960300	0.27314600	2.66922500
H	6.89552200	-0.25677600	1.47159700
C	1.38683600	-1.45044900	1.34309500
H	2.38931100	-1.64916800	1.72962200
H	0.72840000	-2.24609900	1.71866900
C	0.89102300	-0.11656300	1.86355400
C	1.71127700	0.74909500	2.47817100
H	1.35925200	1.71597100	2.82421600

H	2.75455200	0.50609300	2.65411900
C	0.57746600	-0.11963200	-3.16437500
H	1.48147200	0.39887300	-2.82438300
H	0.62627500	-0.25626200	-4.24864800
H	-0.27070800	0.53843600	-2.93155300
C	0.46641400	-2.61474400	-3.09643400
Pd	-2.13338500	0.51202800	-0.99799100
O	-0.64570300	2.66075100	1.04480800
C	-1.43394500	3.21197200	0.20246800
O	-2.13102700	2.62150800	-0.66618700
C	-1.50538000	4.72623100	0.26913900
H	-2.24140000	5.10782200	-0.43883500
H	-1.75918400	5.04036900	1.28544500
H	-0.52022000	5.14264100	0.03697100
H	0.57256100	-2.66148500	-4.17732700
H	0.38713900	-3.56125500	-2.56884900
C	-0.57081900	0.13381400	1.72041400
H	-1.02685100	0.34826700	2.69134300
H	-0.66948800	1.40993600	1.22452300
C	-1.43805300	-0.67471400	0.90588900
C	-1.08192600	-1.26681500	-0.39829800
C	-2.17620500	-1.61601200	-1.23811900
H	-3.13298900	-1.91511900	-0.82661600
H	-1.96716600	-1.99696600	-2.23029600
C	-2.75276800	-1.04695500	1.58783300
C	-2.59082800	-2.30468200	2.47177000
H	-3.57428100	-1.21033100	0.88891600
H	-3.05526300	-0.20525000	2.22066900
C	-3.87825500	-2.65340700	3.22549100
H	-2.28991400	-3.14989100	1.83991300
H	-1.77452100	-2.14350100	3.18612200
H	-3.74447100	-3.54817800	3.84169800
H	-4.18362500	-1.83516800	3.88714100
H	-4.70556000	-2.84613300	2.53324000

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Sum of electronic and thermal Free Energies=-1358.847593

C	0.87157000	-1.05551900	0.56957700
C	1.27251500	-2.33395700	1.19422600
C	1.64715400	0.04143900	0.47209200
C	3.06843800	0.11090400	0.98536200
H	3.23524500	0.99218100	1.61828700
H	3.30184100	-0.75919600	1.60618000
C	4.08374900	0.14916600	-0.14981700
O	3.84588700	-0.07594300	-1.31965900
O	5.31328900	0.45024000	0.31513100
C	6.37705000	0.47086100	-0.66669700
C	7.66443200	0.80280500	0.06343300
H	6.13470100	1.21374900	-1.43324800
H	6.42196500	-0.50573100	-1.15884700
H	8.49708200	0.82941500	-0.64635400
H	7.59718500	1.77930900	0.55158700
H	7.88633200	0.05116800	0.82632600
C	1.13283900	1.30032100	-0.19688100
H	1.95026900	1.82493700	-0.71269400
H	0.75943200	2.00167000	0.55997700
C	0.03820600	1.03543700	-1.21920700
C	0.17198900	-0.00379600	-2.11240200
H	-0.52785300	-0.11183400	-2.93581800
H	1.08892700	-0.58333300	-2.14490500
C	1.49172400	-3.50025600	0.25536100
H	2.27952800	-3.26745800	-0.47121200
H	1.77299200	-4.40581300	0.79986800
H	0.58497600	-3.71395400	-0.32347200
C	1.41552200	-2.45716500	2.52395100
Pd	-0.93313000	-0.94285200	-0.38617800
H	1.69824700	-3.40326400	2.97786000
H	1.23539800	-1.62218800	3.19431500
C	-1.01271700	2.11190500	-1.46333200
H	-0.54712100	2.84051100	-2.14082500
H	-1.84966100	1.65484300	-2.00351300
C	-1.53760800	2.85850300	-0.24252800
C	-1.22669200	4.12250000	-0.06832000
C	-0.91884600	5.38524600	0.07971100
H	-1.52894900	6.17616400	-0.35282800
H	-0.04340400	5.69942400	0.64502800
C	-2.44790700	2.09324500	0.70330100
C	-3.02603600	2.89662800	1.87155000
H	-1.89113500	1.22706500	1.09318600
H	-3.26058500	1.65604700	0.10679200
C	-3.92590700	2.04766000	2.77501400
H	-2.20550800	3.32456600	2.46051500
H	-3.59180700	3.75027200	1.47833600
H	-4.33259300	2.64129100	3.60004100
H	-4.77142800	1.63057100	2.21646700
H	-3.37367700	1.20722600	3.21081200
O	-2.73984200	-0.67119900	-1.51371900
C	-3.73434500	-1.39914000	-1.14876100
O	-3.73455000	-2.19947700	-0.18866200

C	-4.99306500	-1.25787600	-1.99380900
H	-5.21576700	-0.20070200	-2.15940600
H	-4.81616200	-1.71326100	-2.97373100
H	-5.83677400	-1.75416800	-1.51409700
C	-1.85439900	-2.16620400	0.91311500
O	-2.06899600	-2.82918900	1.82189700

13

Sum of electronic and thermal Free Energies=-1358.853271

C	1.25116700	-1.57900400	0.79257200
C	2.12479100	-2.64617900	1.39482800
C	1.65587800	-0.29550500	0.64876200
C	3.04264000	0.12937100	1.07805500
H	3.01075800	1.06318700	1.65112300
H	3.51092300	-0.62034200	1.72060600
C	3.95449500	0.33506600	-0.12714700
O	3.74889100	-0.10447200	-1.24006300
O	5.04323000	1.04698900	0.21303800
C	6.02099800	1.25668000	-0.83801000
C	7.14297700	2.09365900	-0.25535300
H	5.52849100	1.75268500	-1.67980100
H	6.37166000	0.28114600	-1.18889300
H	7.90465400	2.27354800	-1.02023600
H	6.77003100	3.06122000	0.09241000
H	7.61647300	1.58290800	0.58788700
C	0.83895400	0.86443600	0.11302700
H	1.53784100	1.65297900	-0.20240900
H	0.29074500	1.31321400	0.95236200
C	-0.11674200	0.66365600	-1.04252400
C	0.08850100	-0.32724700	-2.00108700
H	-0.41890100	-0.26308400	-2.96058200
H	0.96637700	-0.96345300	-1.96029500
C	2.80629200	-3.56858500	0.41299900
H	3.41279400	-2.99677700	-0.29945800
H	3.44779100	-4.29020500	0.92603300
H	2.06010600	-4.12271100	-0.16685800
C	2.24797000	-2.76773000	2.72075100
Pd	-1.43828900	-1.05739400	-0.63967000
H	2.86161800	-3.54980200	3.15972600
H	1.72703100	-2.10684100	3.40718600
C	-0.97428800	1.88250400	-1.39908100
H	-0.33772500	2.53639800	-2.01009700
H	-1.80365500	1.55283500	-2.03483100
C	-1.52267400	2.69980900	-0.23412000
C	-1.02580400	3.89129700	0.00898600
C	-0.53123000	5.08303300	0.22575900
H	-0.94183300	5.96803900	-0.25702600
H	0.30631400	5.24301400	0.90249200
C	-2.66235900	2.10075900	0.57403700
C	-3.21539900	2.98134100	1.69799100
H	-2.32718000	1.13932600	0.99184800
H	-3.46253200	1.82991300	-0.12755000
C	-4.36489400	2.30751400	2.45396500
H	-2.40810800	3.23205600	2.39763600
H	-3.55575400	3.93557600	1.27736400
H	-4.74295800	2.94951600	3.25622100
H	-5.20324000	2.08469000	1.78405800
H	-4.04439500	1.36208600	2.90615500
O	-3.50637900	-0.43672600	-1.47506400
C	-4.02168400	-1.16724800	-0.57526700
O	-3.28913900	-1.78686900	0.27083400
C	-5.52285200	-1.31374100	-0.47089700
H	-5.86378700	-0.89141600	0.47987600
H	-6.01932200	-0.80394100	-1.29751300
H	-5.78968700	-2.37428000	-0.46828700
C	-0.06598600	-2.10192700	0.31649700
O	-0.39007200	-3.25931100	0.43590600

14

Sum of electronic and thermal Free Energies=-1358.863830

C	1.09089600	0.18738100	1.11563600
C	1.39724900	0.59389900	2.50896400
C	1.94772700	-0.18400000	0.12013300
C	3.44038400	-0.24409900	0.22408800
H	3.89447200	0.47589100	-0.46988500
H	3.77442000	0.04611400	1.22521900
C	4.02916500	-1.61726700	-0.08889100
O	3.40069900	-2.63975500	-0.25719800
O	5.37171600	-1.54020300	-0.13100200
C	6.07234000	-2.78616100	-0.37981800
C	7.55752200	-2.48101600	-0.37645700
H	5.73484000	-3.19109100	-1.33870900
H	5.79540500	-3.50424900	0.39796000
H	8.12319300	-3.39939600	-0.56105500
H	7.81131300	-1.75835800	-1.15718300
H	7.87136200	-2.07196100	0.58805100
C	1.23207600	-0.58567500	-1.15105900
H	1.35165100	-1.66454500	-1.29791200
H	1.66613700	-0.08770800	-2.02544900
C	-0.24746100	-0.20524700	-0.89924800

C	-1.32940400	-1.27727700	-1.15509500
H	-1.65881700	-1.31226100	-2.19729500
H	-0.99541800	-2.27318100	-0.84165600
C	0.73085800	-0.19877900	3.60918600
H	1.01387500	-1.25695700	3.55405500
H	1.01191500	0.18464300	4.59324000
H	-0.35779200	-0.15534200	3.50746700
C	2.21252800	1.62958800	2.75661400
Pd	-2.89419400	-0.82214600	0.05427800
H	2.44037900	1.93385300	3.77414300
H	2.65369600	2.21744600	1.95740300
C	-0.64347700	1.09912400	-1.68205400
H	-0.62687200	0.82691100	-2.74166300
H	-1.68488500	1.32788100	-1.42682500
C	0.20890200	2.33948300	-1.45488300
C	1.21286200	2.61345600	-2.25716200
C	2.19276800	2.88795000	-3.08038600
H	2.03342200	3.48100500	-3.97932300
H	3.21010900	2.54289900	-2.90342800
C	-0.19546100	3.26118100	-0.31223600
C	0.70251800	4.48009100	-0.08185200
H	-0.25500700	2.67673500	0.61615500
H	-1.22629000	3.59457600	-0.50462500
C	0.22396600	5.34448900	1.08848000
H	1.73056200	4.14300100	0.10222100
H	0.74312600	5.08040700	-0.99873000
H	0.87528900	6.21256000	1.23213500
H	-0.79278400	5.71645100	0.91917500
H	0.21545800	4.77475500	2.02452300
O	-4.45537400	-1.65025300	-1.01432900
C	-5.35841300	-1.32869700	-0.14768000
O	-5.03934000	-0.70313700	0.89555600
C	-6.78140800	-1.74791200	-0.42437000
H	-7.03851700	-1.54473500	-1.46704700
H	-6.87726400	-2.82703400	-0.26436900
H	-7.46471000	-1.22499300	0.24598000
C	-0.26371800	0.03828500	0.58686400
O	-1.33193100	0.02617700	1.23547100

15

Sum of electronic and thermal Free Energies=-1358.917089

C	-2.48788600	1.86404000	0.50165100
C	-3.24591100	3.12642900	0.66867000
C	-2.94379300	0.58810200	0.54601100
C	-4.36290800	0.15977400	0.77218200
H	-4.45478000	-0.39964900	1.71312800
H	-5.01745600	1.03113600	0.87538000
C	-4.93016600	-0.71973900	-0.33771100
O	-4.39546500	-0.96679200	-1.39774300
O	-6.14483300	-1.18089000	0.01666900
C	-6.82464600	-2.00238700	-0.96535900
C	-8.16141000	-2.40604900	-0.37397700
H	-6.19567800	-2.86828800	-1.19414100
H	-6.93836800	-1.42459600	-1.88772500
H	-8.70758100	-3.03051400	-1.08765400
H	-8.02536300	-2.97726600	0.54876300
H	-8.77170700	-1.52689800	-0.14879600
C	-1.84977900	-0.43757800	0.34486300
H	-2.09704900	-1.07693900	-0.50842600
H	-1.78800700	-1.09718600	1.22186100
C	-0.55515100	0.38072300	0.12888900
C	0.13852900	0.09166700	-1.22975500
H	-0.56248200	-0.29428300	-1.97746600
H	0.58315800	1.00745400	-1.63335500
C	-3.09023700	4.15625100	-0.42587900
H	-3.40784500	3.75064800	-1.39423100
H	-3.68317400	5.04955000	-0.21327000
H	-2.03795800	4.43904000	-0.52468400
C	-4.00245800	3.34348500	1.75467300
Pd	3.18537100	-0.14876800	-0.51494700
H	-4.55314800	4.27155400	1.87949800
H	-4.06880600	2.62237400	2.56375100
C	0.55776900	0.07141600	1.16975600
H	1.13806700	0.97824800	1.37534300
H	0.14404600	-0.27334500	2.12413400
C	1.44631900	-0.98880400	0.51061100
C	1.20982600	-0.94097800	-0.89907900
C	2.12750100	-1.46300600	-1.83999600
H	2.63398500	-2.40832800	-1.68184400
H	2.02971500	-1.16011300	-2.87929600
C	1.90114400	-2.12398100	1.41040200
C	2.72334500	-3.28402500	0.83539900
H	0.98441300	-2.54088100	1.86120200
H	2.45078500	-1.67557900	2.24906200
C	3.04819800	-4.33176500	1.90608300
H	2.16955700	-3.76305200	0.01865900
H	3.65626300	-2.89979600	0.40707200
H	3.63191300	-5.15666300	1.48606900
H	3.63148900	-3.89411800	2.72388600

H	2.13539700	-4.75673600	2.33961600
O	5.10922400	0.63419800	-1.21914800
C	5.28328100	1.20049600	-0.09159200
O	4.42206000	1.05584600	0.83628900
C	6.49371100	2.07371600	0.13290400
H	7.33848500	1.71061900	-0.45571200
H	6.26172200	3.09242900	-0.19667900
H	6.74845700	2.10644900	1.19372900
C	-1.02841100	1.84388800	0.21816800
O	-0.29552500	2.80739300	0.07245800

R-P2

Sum of electronic and thermal Free Energies=-1474.592292

C	-2.31891000	1.44743900	0.17466700
C	-2.69912100	2.87157300	0.32830000
C	-3.08356400	0.34495300	0.36244000
C	-4.51889400	0.31947200	0.79390000
H	-4.61648900	-0.15929800	1.77773600
H	-4.90467000	1.33720000	0.91485900
C	-5.44614000	-0.41984200	-0.16418500
O	-5.16019000	-0.81896500	-1.27262100
O	-6.66758700	-0.55597200	0.39022600
C	-7.66765000	-1.20794100	-0.43040600
C	-8.95315800	-1.25801600	0.37277200
H	-7.30776200	-2.20683800	-0.69595100
H	-7.78325600	-0.64207700	-1.36003600
H	-9.73777400	-1.74492600	-0.21459000
H	-8.81493400	-1.82433700	1.29822700
H	-9.29232300	-0.25109800	0.63215300
C	-2.33344700	-0.93183000	0.05917100
H	-2.75210900	-1.37748100	-0.85074800
H	-2.46321900	-1.67445800	0.85716000
C	-0.85935300	-0.51083000	-0.13601800
C	-0.12551100	-1.19058300	-1.32261400
H	-0.63807000	-2.13091300	-1.58363100
H	-0.14046800	-0.56572600	-2.22267400
C	-2.49184700	3.76296300	-0.87389800
H	-3.07342000	3.40296900	-1.73155500
H	-2.79272000	4.79154900	-0.65776700
H	-1.43968100	3.74914500	-1.17253100
C	-3.18280800	3.33590900	1.49005200
Pd	2.33342300	0.33491300	-0.46181900
H	-3.46193000	4.37945900	1.60605000
H	-3.28526500	2.70055600	2.36464300
C	0.04136000	-0.83186900	1.10918900
H	0.13457300	0.02158600	1.78921700
H	-0.41563900	-1.64485200	1.69646400
C	1.37889100	-1.32386000	0.55911600
C	1.28708000	-1.50590800	-0.83668800
C	2.00970300	-2.55031500	-1.67640500
H	1.50637900	-3.51696000	-1.51161800
H	1.87356500	-2.30737600	-2.74188900
C	2.27689300	-2.10923100	1.49550900
C	2.75458200	-1.35358700	2.74608000
H	3.13554700	-2.48821000	0.93624700
H	1.70695900	-2.99500700	1.83055200
C	3.61214600	-2.22565400	3.66872000
H	3.32622900	-0.47185200	2.43067400
H	1.89049200	-0.97175200	3.30547500
H	3.94543300	-1.66829900	4.55050400
H	3.05450900	-3.10172500	4.02027200
H	4.50488000	-2.59182700	3.14890600
O	5.18618300	0.67251500	0.36811800
C	4.80001200	1.90337700	0.06074400
O	3.66519300	2.15950800	-0.34674500
C	5.86168900	2.94882500	0.25680000
H	6.16423400	2.96992100	1.30804700
H	6.74706300	2.69238000	-0.33199400
H	5.48074800	3.92455200	-0.04126500
C	-0.97448900	1.01671700	-0.30328700
O	-0.10663000	1.74832900	-0.75591200
C	4.26646400	-2.03348500	-2.21576900
H	4.13673000	-2.28484300	-3.28013300
H	4.12320800	-0.95026800	-2.08638100
H	5.28242200	-2.29933700	-1.91200100
O	3.38143400	-2.77831800	-1.39949800
H	4.37848100	0.08772400	0.19354800

ts3coinsertion11fixopt-2ircf

Sum of electronic and thermal Free Energies=-1358.842803

C	-0.79032300	-1.68928800	-0.19027100
C	-1.20782400	-3.08785200	0.02117600
C	-1.49883800	-0.64996400	-0.65695000
C	-2.93001500	-0.83486800	-1.15835200
H	-3.02530900	-0.39597800	-2.15634000
H	-3.18018400	-1.89575400	-1.20371900
C	-3.93765100	-0.17292100	-0.22996600
O	-4.26879400	-0.60637000	0.85583000
O	-4.41155000	0.97621700	-0.75008400
C	-5.33036600	1.71970800	0.08707800

C	-5.77095900	2.94235200	-0.69470200
H	-4.81448700	1.98627600	1.01477200
H	-6.17161800	1.07114400	0.34951000
H	-6.46796900	3.53523400	-0.09426600
H	-4.91478600	3.57330700	-0.95010800
H	-6.27503200	2.65395900	-1.62163400
C	-0.93943500	0.75635300	-0.79700600
H	-1.51109900	1.28430200	-1.57365500
H	0.08518500	0.70759400	-1.18361200
C	-0.93680000	1.64507200	0.43884700
C	-1.44279400	1.29531800	1.62697200
H	-1.42169300	1.98440600	2.46709900
H	-1.90789000	0.33025200	1.79666100
C	-0.39769400	-4.16336400	-0.67230000
H	0.64651700	-4.15680100	-0.33713700
H	-0.81284000	-5.15586300	-0.47713500
H	-0.37900300	-3.99712300	-1.75554900
C	-2.25895700	-3.38876000	0.80614600
H	-2.56551800	-4.42233800	0.94827700
H	-2.84918400	-2.62100300	1.29565300
C	-0.30427500	3.01153800	0.21693300
H	-0.75441800	3.48142700	-0.66540900
H	-0.52390600	3.65438700	1.07807100
C	1.21372700	2.94700100	0.02471000
C	1.73395200	3.06300700	-1.17427500
C	2.22093700	3.18538300	-2.38334100
H	2.50648800	4.15341700	-2.79130800
H	2.35347800	2.32266600	-3.03391500
C	2.04324000	2.74595000	1.28180800
C	3.53375900	2.46571900	1.06789700
H	1.59295800	1.92590900	1.85848100
H	1.92107300	3.64290000	1.90991000
C	4.30144400	2.35660600	2.38917400
H	3.64673200	1.53471100	0.50087500
H	3.96808400	3.26275700	0.45193400
H	5.36193800	2.14919900	2.21447300
H	4.23423400	3.28408200	2.97011400
H	3.90590200	1.54636200	3.01273800
O	1.83723500	-1.10680300	-1.84430400
C	3.06369300	-0.93443200	-1.50256600
O	3.39123800	-1.01258700	-0.28020900
C	4.08573300	-0.60299300	-2.55710900
H	4.18188300	0.48666900	-2.61960300
H	5.05883400	-1.01237800	-2.27921200
H	3.77079300	-0.98190000	-3.53093900
Pd	1.20720100	-1.38087600	0.16727700
C	0.81344500	-1.53138200	2.01681600
O	0.60507000	-1.61053400	3.13700700

TS10

Sum of electronic and thermal Free Energies=-1358.824486

C	0.69741900	-1.80881800	0.25635900
C	1.06750700	-3.24952700	0.31669400
C	-0.42574700	-1.27419000	-0.29408000
C	-1.41670300	-2.13882400	-1.05880800
H	-1.64592900	-1.65285800	-2.01130600
H	-0.97619400	-3.11931100	-1.25313100
C	-2.72848200	-2.39356500	-0.31870000
O	-2.83629100	-3.04552600	0.69837200
O	-3.76748100	-1.83129200	-0.96309600
C	-5.06541200	-2.01279600	-0.34327000
C	-6.09448100	-1.34602000	-1.23521400
H	-5.03415500	-1.57029900	0.65722000
H	-5.25065800	-3.08464400	-0.22611400
H	-7.09186200	-1.46364300	-0.80038600
H	-5.88964500	-0.27669000	-1.33979800
H	-6.09934800	-1.79545200	-2.23231900
C	-0.74981500	0.20708000	-0.28514300
H	-0.89611900	0.52197400	-1.32606600
H	0.11402300	0.78455800	0.06449800
C	-1.97916800	0.60864200	0.52764300
C	-2.24972200	0.08016200	1.72607100
H	-3.10721400	0.41362600	2.30414000
H	-1.64067300	-0.70015100	2.17029400
C	2.40089400	-3.64524700	-0.27585300
H	3.23068000	-3.14141400	0.23597000
H	2.55820500	-4.72414500	-0.19542900
H	2.46672700	-3.35757900	-1.33135500
C	0.25661100	-4.14152300	0.90846700
H	0.53395000	-5.19153300	0.95500200
H	-0.69818300	-3.85883500	1.33838200
C	-2.84063100	1.69763800	-0.08526600
H	-3.22268300	1.35008700	-1.05226200
H	-3.70584100	1.87756200	0.56546200
C	-2.09090500	3.01455200	-0.29010800
C	-1.78757900	3.42363600	-1.49968400
C	-1.50269700	3.82000500	-2.71376300
H	-2.18386900	4.44944500	-3.28366600
H	-0.57056600	3.54303500	-3.20269600

C	-1.73229800	3.78955700	0.96702500
C	-0.89524500	5.05457100	0.75669800
H	-1.20845500	3.10894000	1.65354200
H	-2.67009400	4.05034700	1.48238400
C	-0.58793300	5.78028900	2.07010500
H	0.04146900	4.78697900	0.25273200
H	-1.42383400	5.73004000	0.07318300
H	0.01210400	6.67886400	1.89468300
H	-1.50768200	6.08975000	2.57988500
H	-0.02844600	5.13739400	2.75909700
O	3.55276800	-0.02734200	-1.70034600
C	4.31549900	0.73305800	-1.03001300
O	4.12173700	0.89064500	0.22553900
C	5.44494500	1.47908400	-1.69663900
H	5.17971400	2.53901800	-1.77181000
H	6.34982100	1.40950600	-1.08779700
H	5.62569600	1.08323100	-2.69681100
Pd	2.41551900	-0.44159800	0.17746000
C	1.39961300	-0.90608400	1.66165600
O	1.05565900	-0.97828200	2.77406200

TS11

Sum of electronic and thermal Free Energies=-1358.823054

C	-0.43085600	0.02620600	1.01356400
C	-0.49715500	0.05966900	2.49764000
C	-0.59719300	1.04672400	0.13607700
C	-0.84662700	2.47749800	0.51602600
H	-1.85731100	2.78779500	0.21745700
H	-0.80357600	2.60399000	1.60142900
C	0.13188900	3.47181100	-0.10485800
O	1.09824300	3.20210900	-0.78498300
O	-0.22495700	4.72648600	0.22940900
C	0.63955300	5.78360700	-0.25873400
C	0.07004300	7.10018600	0.23274600
H	0.67549700	5.73066400	-1.35121100
H	1.65304400	5.60649400	0.11371100
H	0.69710300	7.92651000	-0.11590000
H	-0.94425100	7.25493200	-0.14620300
H	0.03857800	7.12985500	1.32555200
C	-0.57493100	0.67180900	-1.32639300
H	0.20996200	1.24124300	-1.83161300
H	-1.53115800	0.97004200	-1.77756800
C	-0.37664600	-0.83151700	-1.49547300
C	0.78353100	-1.22036900	-2.30745800
H	0.74127400	-2.18915200	-2.80751600
H	1.26612000	-0.44506500	-2.90318500
C	0.64773100	-0.58296300	3.24406100
H	1.61527400	-0.19784400	2.90705600
H	0.54830800	-0.42064000	4.32039900
H	0.66517200	-1.66130900	3.05468800
C	-1.55365900	0.59937600	3.12423100
Pd	1.80445000	-1.33362100	-0.57013200
H	-1.61002600	0.62065300	4.20890100
H	-2.40127600	1.00637900	2.58162400
C	-1.64300000	-1.69507800	-1.80616500
H	-1.77768400	-1.62381400	-2.89042800
H	-1.39193600	-2.73524100	-1.57708900
C	-2.97013600	-1.33492500	-1.13624700
C	-3.70137500	-0.35787400	-1.62460100
C	-4.43455400	0.60059800	-2.13219000
H	-5.15966000	0.40731700	-2.92101700
H	-4.36065500	1.63018800	-1.78581500
C	-3.45922500	-2.19696800	0.02250700
C	-4.85362400	-1.85867300	0.55765100
H	-2.72970300	-2.15127700	0.83899400
H	-3.44075100	-3.24361500	-0.31677200
C	-5.27753400	-2.78542200	1.70143000
H	-4.86791700	-0.81680600	0.90142400
H	-5.58415700	-1.91650300	-0.25862600
H	-6.27509400	-2.52746000	2.07142400
H	-5.30413200	-3.83187800	1.37683200
H	-4.58150700	-2.72005600	2.54518800
O	3.89301900	-1.55476500	-0.94930700
C	4.18675700	-1.51715100	0.29929300
O	3.27951400	-1.38355000	1.16902800
C	5.63653600	-1.65891200	0.69929200
H	5.95365300	-2.69501400	0.54110600
H	6.26320400	-1.02285800	0.06900400
H	5.76829000	-1.40077200	1.75081500
C	-0.17673400	-1.26510200	0.33615900
O	-0.38283400	-2.38595100	0.75486200

TS12

Sum of electronic and thermal Free Energies=-1358.849474

C	2.20147400	-2.43973000	-0.20005100
C	3.32353100	-3.32443000	-0.59543800
C	2.21771300	-1.35384300	0.61361300
C	3.42541800	-0.77583500	1.29995100
H	3.27868000	-0.81573200	2.38621200
H	4.31730600	-1.34496000	1.03653500

C	3.65903900	0.67959800	0.89834300
O	4.36543800	1.02841500	-0.02042200
O	2.96216500	1.51738100	1.68863300
C	3.01950200	2.92428500	1.32921400
C	2.26971700	3.69158900	2.40085500
H	2.55426800	3.03787500	0.34692700
H	4.06930700	3.22367500	1.26123400
H	2.30192000	4.76311300	2.17857400
H	1.22207600	3.37933200	2.43923400
H	2.71607200	3.53438400	3.38732400
C	0.85766000	-0.71032500	0.77325900
H	0.88345700	0.33147300	0.43430200
H	0.57529800	-0.66731100	1.83337800
C	-0.11191700	-1.58009800	-0.05808600
C	-0.79538200	-0.82049700	-1.19100100
H	-0.08089800	-0.21941000	-1.76992200
H	-1.30308400	-1.48187200	-1.89222400
C	3.54162200	-3.50970800	-2.07858000
H	3.75555100	-2.54942300	-2.56324800
H	4.37670000	-4.18796800	-2.27196200
H	2.63771500	-3.91520900	-2.54341400
C	4.07858500	-3.93947700	0.32555400
Pd	-1.48286200	1.28090300	-0.81107200
H	4.89951300	-4.58957300	0.03660800
H	3.88854100	-3.83297400	1.38928000
C	-1.20960000	-2.29156900	0.76486400
H	-1.35633200	-3.30789400	0.37122200
H	-0.91926700	-2.40601200	1.81691500
C	-2.51903400	-1.55950400	0.62084200
C	-2.58397800	-0.52313500	-0.20999800
C	-3.37870000	0.50326900	-0.75877700
H	-3.77234100	0.38880200	-1.77010300
H	-3.97529400	1.13526800	-0.10316200
C	-3.71751800	-2.18747100	1.30519600
C	-5.07772000	-1.50297500	1.13808500
H	-3.48140400	-2.26020700	2.37786800
H	-3.78934700	-3.23068200	0.96043100
C	-6.19547500	-2.25563200	1.86760800
H	-5.02023400	-0.47606200	1.51775000
H	-5.32189400	-1.42664500	0.07192400
H	-7.15960500	-1.75480600	1.73648500
H	-6.29805400	-3.27915600	1.48973800
H	-5.99716900	-2.31840300	2.94362000
O	-1.63477500	3.42541400	-0.85978700
C	-0.36660200	3.57351400	-0.87464900
O	0.39895800	2.55934200	-0.83551300
C	0.20913900	4.96893400	-0.91390600
H	1.14950900	4.97421900	-1.46889700
H	-0.50344400	5.66323300	-1.36224700
H	0.41449000	5.30093500	0.10982500
C	0.81958600	-2.65742800	-0.68642700
O	0.42662100	-3.53639200	-1.43462900

TS13

Sum of electronic and thermal Free Energies=-1474.552839

C	-3.00932100	1.92256400	0.55630100
C	-3.90668900	3.07167200	0.29473100
C	-3.32699500	0.61620800	0.73008000
C	-4.69353500	0.00814000	0.63433600
H	-4.98544100	-0.46701900	1.58042200
H	-5.44823500	0.77500500	0.43316000
C	-4.79778500	-1.04691900	-0.46312700
O	-3.94331600	-1.30458400	-1.28509200
O	-5.99796800	-1.65390300	-0.41073700
C	-6.25112800	-2.65477900	-1.42857400
C	-7.64993500	-3.19332900	-1.19887500
H	-5.48906400	-3.43624600	-1.34881300
H	-6.14391100	-2.18860000	-2.41279400
H	-7.88115900	-3.95392000	-1.95092500
H	-7.73634700	-3.65085600	-0.20922200
H	-8.39409400	-2.39564400	-1.27634200
C	-2.12172800	-0.23860700	1.06072200
H	-2.11499300	-1.16237600	0.47534900
H	-2.17002700	-0.53227200	2.11973400
C	-0.90559000	0.67158000	0.77992000
C	-0.19915700	0.27717600	-0.55068200
H	-0.89302100	-0.21622400	-1.24157300
H	0.18534200	1.17115300	-1.05061500
C	-3.55327200	3.94890700	-0.88346400
H	-3.54638600	3.37062600	-1.81551900
H	-4.26567100	4.77087400	-0.99157100
H	-2.54851900	4.36176000	-0.75193400
C	-4.95510800	3.32890400	1.09081100
Pd	2.81655900	0.38773000	0.28019500
H	-5.60881900	4.17611700	0.90355700
H	-5.17133600	2.72759100	1.96860500
C	0.22967400	0.59052600	1.82471700
H	0.72754900	1.56807000	1.88828000
H	-0.14593400	0.35191400	2.82676600

C	1.20851000	-0.46782600	1.30334900
C	0.93618700	-0.65249300	-0.10589200
C	1.42919900	-1.67452300	-0.95727400
H	2.05253900	-2.46010100	-0.55565700
H	0.82038600	-1.96290000	-1.80847000
C	1.69972500	-1.44959500	2.35645100
C	2.62750000	-2.61169500	1.97508600
H	0.80894100	-1.86320700	2.85941800
H	2.19930500	-0.84610300	3.12891100
C	3.15442600	-3.34625600	3.21306900
H	2.08691700	-3.32828000	1.34451500
H	3.47066300	-2.23417300	1.38496200
H	3.79226900	-4.18952200	2.93095600
H	3.74756600	-2.67696200	3.84614300
H	2.33291700	-3.73905500	3.82366100
O	5.09757000	-0.55612900	-1.75885500
C	5.44717700	0.46317100	-1.10121900
O	4.69874200	1.16256100	-0.34398200
C	6.88856900	0.93360600	-1.23300000
H	7.48904400	0.20348600	-1.77678700
H	6.90670200	1.88827800	-1.76928400
H	7.31415800	1.11297800	-0.24199900
C	-1.53030800	2.07075900	0.64962700
O	-0.89328600	3.10927000	0.59820300
C	2.37472200	-0.23760000	-3.25500000
H	1.44146200	-0.54005300	-3.74041700
H	2.22455200	0.71640700	-2.73325400
H	3.14478600	-0.10258600	-4.02168700
O	2.78168400	-1.26794400	-2.36066000
H	3.71788500	-0.97546700	-1.97013200