

*Supporting Information*

**Mechanistic insight into the selective olefin-directed oxidative carbocyclization and borylation via palladium catalyst: a theoretical study**

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## Cartesian coordinates in MeOH and energies for all of the calculated structures in the two solvents

<b>R1</b>				H	2.24454100	-1.43563800	2.20152100
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.29168				C	3.63992500	-1.93661800	-0.98482500
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.227394				H	4.67412800	-1.63971400	-0.76674700
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-618.24556				H	3.62230100	-3.03434000	-0.99805900
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-618.309846				H	3.38090000	-1.57599500	-1.98358300
Sum of electronic Energies in MeOH at M06/BSII level =-618.2439385				<b>cat</b>			
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.291962				Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.114099			
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.227768				Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.063708			
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-618.237493				Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-583.637304			
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-618.301686				Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-583.687694			
Sum of electronic Energies in AcOH at M06/BSII level =-618.2355726				Sum of electronic Energies in MeOH at M06/BSII level =-584.780709			
C	1.70367400	-0.59716400	-0.22041800	Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.114246			
C	2.69793600	-1.40339900	0.07467900	Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.064052			
C	0.70026900	0.19471200	-0.52558000	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-583.626137			
C	-0.65687000	-0.37632400	-0.89459500	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-583.676331			
H	-0.99976400	0.01774100	-1.85916700	Sum of electronic Energies in AcOH at M06/BSII level =-584.7692953			
H	-0.60104000	-1.46558800	-1.00436000	Pd	0.00000000	0.00002600	-0.00348100
C	-1.73948500	-0.10011100	0.13444000	O	-1.77728900	-1.08724600	-0.00953100
O	-1.54880300	0.22705800	1.29481200	O	1.77726400	-1.08726100	-0.00955500
O	-2.95919900	-0.29742100	-0.38743200	C	-2.45862700	0.00008800	-0.00875100
C	-4.09746700	-0.13931100	0.50749400	O	-1.77722300	1.08732400	-0.00957100
C	-5.34510500	-0.43112400	-0.29809300	C	2.45862700	0.00004900	-0.00875400
H	-4.09241000	0.88254500	0.89829000	O	1.77724800	1.08730800	-0.00950700
H	-3.97913300	-0.83160700	1.34630100	C	-3.94612200	-0.00001200	0.02320800
H	-6.22619900	-0.31439000	0.34097400	H	-4.33342800	0.90364900	-0.45216300
H	-5.44031200	0.26004200	-1.14150300	H	-4.33336300	-0.89353600	-0.47117100
H	-5.33436600	-1.45562900	-0.68341600	H	-4.27385600	-0.01163000	1.06938600
C	0.81240000	1.71680400	-0.54936700	C	3.94612300	-0.00004300	0.02319500
H	0.15630100	2.13649300	0.22460800	H	4.33341700	0.90212200	-0.45504600
H	0.40302800	2.06165100	-1.51226600	H	4.27386000	-0.00816900	1.06940400
C	2.20866200	2.24902400	-0.38580600	H	4.33335700	-0.89511400	-0.46835600
C	2.59126300	3.10787200	0.56048500	<b>1</b>			
H	2.93880200	1.89952300	-1.11650800	Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.4081			
H	3.61362600	3.47394600	0.61788600	Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.316527			
H	1.89626500	3.48075600	1.31091800	Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1201.901052			
C	2.96823600	-1.85169900	1.49596600	Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1201.992625			
H	2.93243100	-2.94659300	1.56750600	Sum of electronic Energies in MeOH at M06/BSII level =-1203.0775129			
H	3.97429200	-1.54627400	1.81227900	Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.408751			

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.318045

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1201.877907

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1201.968614

Sum of electronic Energies in AcOH at M06/BSII level =-1203.0619842

C	-0.75146200	0.60015900	0.45310700
C	-0.29822600	1.86024100	0.21642500
C	-1.64683600	-0.32695900	0.75231300
C	-3.05835300	0.04422100	1.14545700
H	-3.36917500	-0.50743700	2.04159700
H	-3.13640900	1.10851500	1.38962600
C	-4.06047400	-0.25000400	0.04136500
O	-3.77553400	-0.62862900	-1.08374200
O	-5.31178200	-0.02223800	0.45517000
C	-6.37702900	-0.21764700	-0.52205600
C	-7.66594400	0.26103900	0.10992200
H	-6.41538200	-1.28059600	-0.77850900
H	-6.12825300	0.34777900	-1.42417700
H	-8.48816200	0.12115900	-0.59928800
H	-7.89820500	-0.30441400	1.01783000
H	-7.60953100	1.32451500	0.36301200
C	-1.26735800	-1.78873300	0.69340900
H	-2.12262000	-2.39660600	0.36840800
H	-1.00621600	-2.14448200	1.69741600
C	-0.11494300	-2.02940300	-0.25588500
C	-0.02561500	-1.45471100	-1.50938300
H	0.56280300	-2.84354000	-0.01194900
H	0.70653700	-1.81942300	-2.22305500
H	-0.81379400	-0.81424700	-1.89310900
C	-0.42822800	2.49902900	-1.14105800
H	-1.16610200	3.30882200	-1.05648700
H	0.51638900	2.95393600	-1.45270600
H	-0.76575900	1.79440800	-1.90214100
C	0.19990600	2.73005700	1.33556100
H	1.07012200	3.31936800	1.03774900
H	-0.61187400	3.43624500	1.56278300
H	0.42519100	2.16315400	2.23930400
Pd	1.22433000	-0.19909000	-0.15969600
O	4.50922300	-2.72441400	-0.25865700
O	3.09653200	1.73192500	-1.48358200
C	3.56419600	-2.04310300	0.16008400
O	2.80955300	-1.38801800	-0.68908800
C	3.30890500	1.78397000	-0.26059900
O	2.60383300	1.16052900	0.63723500
C	3.25960700	-1.94797900	1.64043200

H	2.23872300	-2.28736200	1.84438600
H	3.96479400	-2.55961500	2.20603700
H	3.33260100	-0.90672600	1.96766800
C	4.46897400	2.58285900	0.30546600
H	4.18437200	3.09453600	1.22842200
H	5.28587700	1.89270200	0.54682200
H	4.82756900	3.30600900	-0.42966400

### TS1

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.402379

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.311801

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1201.886524

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1201.977101

Sum of electronic Energies in MeOH at M06/BSII level =-1203.0544698

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.402971

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.314268

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1201.861646

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1201.950348

Sum of electronic Energies in AcOH at M06/BSII level =-1203.0393408

C	-0.61374400	0.51680100	0.21537500
C	-0.56476500	1.94043500	0.00369200
C	-1.59471500	-0.29517200	0.62941000
C	-2.96124900	0.19015400	1.05412900
H	-3.27891900	-0.29315700	1.98490700
H	-2.95994300	1.26936500	1.24796800
C	-4.02382200	-0.06268200	-0.00256500
O	-3.80368900	-0.22287000	-1.19331100
O	-5.25085000	-0.05505800	0.52987100
C	-6.37303600	-0.22244800	-0.38553500
C	-7.63547400	-0.20745000	0.44880600
H	-6.24486600	-1.16797700	-0.92017700
H	-6.35030300	0.59354100	-1.11403600
H	-8.50431600	-0.33900500	-0.20380200
H	-7.63065200	-1.02022800	1.18202100
H	-7.74559900	0.74333400	0.97987400
C	-1.33387300	-1.78288200	0.69502700
H	-2.19976600	-2.34625300	0.31723000
H	-1.20967900	-2.09127800	1.74066700
C	-0.10479400	-2.16638900	-0.10797600
C	0.05652800	-1.79911500	-1.43521700
H	0.54142400	-2.94002900	0.30054400
H	0.82601200	-2.26610700	-2.04235200
H	-0.71931700	-1.24856200	-1.95974900
C	-0.95877700	2.46527300	-1.34118700
H	-0.45962800	1.90847100	-2.14084700

H	-2.03535900	2.28686200	-1.46860000
H	-0.75222500	3.53212500	-1.44659300
C	0.04535200	2.76989200	0.95776200
H	1.21520400	2.32199500	0.65436700
H	0.01859200	3.84488400	0.79067800
H	0.02397900	2.44268200	1.99893400
Pd	1.19477000	-0.36825600	-0.22104000
O	4.77019200	-2.63717800	-0.07028600
O	4.09489900	1.27635200	-0.87628600
C	3.79431600	-1.93531700	0.25112800
O	2.92536600	-1.53713700	-0.62767000
C	3.37770200	1.91607000	-0.11433300
O	2.22094700	1.45044200	0.35039900
C	3.61163800	-1.50540900	1.69829100
H	2.57197400	-1.62274500	2.01938500
H	4.26722200	-2.08393300	2.35270300
H	3.86703900	-0.44434800	1.79486500
C	3.73192800	3.30007200	0.38056300
H	4.71948600	3.58533700	0.01569400
H	2.98910000	4.02173200	0.02374400
H	3.71692600	3.32563300	1.47446700

## 2

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.408726

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.316157

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1201.902022

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1201.99459

Sum of electronic Energies in MeOH at M06/BSII level =-1203.0803437

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.724488

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.603715

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.064222

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.184995

Sum of electronic Energies in AcOH at M06/BSII level =-1796.2802849

C	-0.51452700	0.53355600	0.30702600
C	-0.48184100	2.00550700	0.23273500
C	-1.55822400	-0.25147100	0.63060200
C	-2.92279700	0.26707400	1.02355600
H	-3.27110100	-0.18514300	1.95892400
H	-2.89670500	1.35079600	1.18363100
C	-3.96047900	0.00709400	-0.05481500
O	-3.71884200	-0.07434100	-1.24991000
O	-5.19361600	-0.09462300	0.45767000
C	-6.28650900	-0.30322600	-0.48370800
C	-7.56462800	-0.39044200	0.32247700
H	-6.08965100	-1.22375800	-1.04106300

H	-6.30190600	0.53152300	-1.19063900
H	-8.40898400	-0.56163700	-0.35278700
H	-7.52438400	-1.21846700	1.03731700
H	-7.74855000	0.53778800	0.87270100
C	-1.37937100	-1.75305200	0.58789600
H	-2.26947500	-2.25002000	0.17398100
H	-1.26499200	-2.14780200	1.60565500
C	-0.16975400	-2.12466400	-0.24777600
C	0.02215300	-1.62053800	-1.53162000
H	0.41343700	-2.98890800	0.06341600
H	0.76197800	-2.06808100	-2.18931200
H	-0.72369500	-0.98131700	-1.99510300
C	-0.48382300	2.60663100	-1.15438700
H	-1.37774300	2.28726400	-1.70480500
H	-0.46606400	3.69989500	-1.11908500
H	0.38337400	2.26499100	-1.73232900
C	-0.43813000	2.76102100	1.34581900
H	2.23661300	1.78678300	1.40343600
Pd	1.20012500	-0.42044900	-0.15630800
O	4.78339100	-2.78674900	-0.11210300
O	3.46329500	1.73376800	-1.37272800
C	3.78989700	-2.11101300	0.22245900
O	2.99936900	-1.55930800	-0.63933900
C	3.21500200	2.14610600	-0.26135200
O	2.52239600	1.32991800	0.59227700
C	3.47980100	-1.90837300	1.70103800
H	2.46941900	-2.26323900	1.93152700
H	4.19916700	-2.44351200	2.32486400
H	3.51577100	-0.84197400	1.94779800
C	3.60298000	3.48183300	0.29988000
H	2.69880600	4.04400900	0.55931400
H	4.18724000	3.34771800	1.21587600
H	4.18374800	4.03417000	-0.43831600
H	-0.42796200	3.84753000	1.29157800
H	-0.43055200	2.31648200	2.33767700

## HOAC

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.066136

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.035401

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-229.031233

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-229.061968

Sum of electronic Energies in MeOH at M06/BSII level =-229.0423987

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.066256

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.035535

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-229.024668

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-229.055389

Sum of electronic Energies in AcOH at M06/BSII level =-229.0355543

H	1.73472500	-0.81811700	0.00030900
O	0.63534800	1.20871000	0.00001700
C	0.08950000	0.11772200	-0.00011500
O	0.78477800	-1.03643100	-0.00002600
C	-1.39310400	-0.11723700	-0.00004500
H	-1.92109600	0.83623200	-0.00449800
H	-1.67612600	-0.70378600	-0.87992000
H	-1.67689000	-0.69547500	0.88513600

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Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.338957

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.257996

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-972.877798

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-972.958758

Sum of electronic Energies in MeOH at M06/BSII level =-974.0392709

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.339324

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.259405

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-972.861571

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-972.94149

Sum of electronic Energies in AcOH at M06/BSII level =-974.022934

C	-0.28445200	0.54850300	0.39160900
C	0.15067200	1.88717100	0.23744100
C	-1.22462200	-0.37686400	0.56369000
C	-2.60473200	-0.06494000	1.08915100
H	-2.89920800	-0.76378600	1.87952700
H	-2.63521400	0.94028000	1.52519600
C	-3.65878500	-0.09638700	-0.00674300
O	-3.42976900	0.01575500	-1.20054900
O	-4.88779600	-0.22740000	0.50498600
C	-6.00129200	-0.19795800	-0.43660500
C	-7.27729200	-0.32180100	0.36815800
H	-5.87829800	-1.02519400	-1.14151900
H	-5.95719600	0.74158500	-0.99496100
H	-8.13566700	-0.30404000	-0.31098300
H	-7.30312700	-1.26221400	0.92753900
H	-7.38165200	0.50901300	1.07301300
C	-0.87591100	-1.79569100	0.16816900
H	-1.41615100	-2.05274700	-0.75323600
H	-1.22290500	-2.49783800	0.93669600
C	0.62295200	-1.98573400	-0.03957700
C	1.25161600	-1.91149200	-1.25069700
H	1.18815200	-2.33665900	0.82275900
H	2.28506500	-2.22439300	-1.36344600

H	0.69322600	-1.70467000	-2.16091100
C	-0.44578000	2.79518900	-0.80874200
H	-1.19947600	3.42836200	-0.32357700
H	0.31072800	3.45069300	-1.24867600
H	-0.94654600	2.22901300	-1.59715500
C	1.37194200	2.15950000	0.87574300
Pd	1.60187600	0.16868200	-0.17155400
O	3.73827700	0.13252000	-0.65845600
C	4.46337800	-0.39360700	0.26714600
O	4.02388700	-0.84253100	1.34915700
C	5.96097900	-0.41870400	-0.00892400
H	6.46212800	-1.14589700	0.63384300
H	6.16385000	-0.64708400	-1.05877100
H	6.37966100	0.57308400	0.19963800
H	1.94967600	3.03407200	0.58889600
H	1.60783900	1.70922100	1.83758800

### R2

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.383492

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.315828

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-822.202222

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-822.269886

Sum of electronic Energies in MeOH at M06/BSII level =-822.2501875

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.383803

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.316182

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-822.192827

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-822.260447

Sum of electronic Energies in AcOH at M06/BSII level =-822.2402307

C	-3.01424900	0.74069600	-0.26630600
C	-3.01431800	-0.74067500	0.26634900
B	-0.85263400	-0.00020500	-0.00038200
O	-1.61355600	1.14229000	-0.06855200
O	-1.61371400	-1.14259300	0.06809800
C	-3.90425300	-1.70757900	-0.50746700
H	-3.81619700	-2.71231900	-0.08203600
H	-4.95395200	-1.40483100	-0.43722200
H	-3.62853000	-1.76078900	-1.56288900
C	-3.28539100	-0.85437300	1.76960000
H	-4.33032100	-0.63227800	2.00475800
H	-3.07323300	-1.87782000	2.09413100
H	-2.64758600	-0.17694600	2.34529800
C	-3.28584900	0.85446100	-1.76947200
H	-4.33077000	0.63201500	-2.00435300
H	-3.07418700	1.87802900	-2.09395900
H	-2.64800000	0.17735900	-2.34550300

C	-3.90381100	1.70769900	0.50783100	O	-7.29063700	-0.59449600	-0.91809000
H	-3.81542000	2.71252300	0.08267800	C	-8.14165800	0.17599200	-1.81657500
H	-4.95360800	1.40530900	0.43748700	C	-9.56249500	-0.30419100	-1.61557900
H	-3.62802900	1.76050600	1.56325600	H	-7.79446300	0.01581800	-2.84160600
C	3.01416400	0.74065000	0.26649900	H	-8.02919900	1.23682600	-1.57561500
C	3.01436300	-0.74057700	-0.26643400	H	-10.22939900	0.25390900	-2.28058800
B	0.85258500	-0.00012000	-0.00047600	H	-9.65746600	-1.36929300	-1.84911000
O	1.61346700	1.14235100	0.06832200	H	-9.89098300	-0.14036100	-0.58442500
O	1.61372400	-1.14247900	-0.06894300	C	-2.96209900	-1.38835800	-1.13164800
C	3.90392000	-1.70759100	0.50769300	H	-3.12246300	-0.68654700	-1.96012100
H	3.81581800	-2.71233000	0.08226900	H	-3.33102900	-2.36370600	-1.47388000
H	4.95368500	-1.40500600	0.43775100	C	-1.47268300	-1.50064700	-0.82595900
H	3.62785600	-1.76070600	1.56303700	C	-0.53837300	-0.55378400	-1.14755100
C	3.28631300	-0.85394100	-1.76957100	H	-1.13294400	-2.47002100	-0.46251700
H	4.33141500	-0.63196700	-2.00407400	H	0.52111400	-0.77625200	-1.08133200
H	3.07415900	-1.87726900	-2.09448500	H	-0.82647600	0.36314900	-1.65572000
H	2.64895900	-0.17625400	-2.34546700	C	-3.48058500	1.84309700	2.29349600
C	3.28522300	0.85398100	1.76977700	H	-4.50603100	1.81717100	2.68340200
H	4.33017500	0.63192700	2.00490000	H	-2.87798100	2.46157200	2.96385400
H	3.07297600	1.87731500	2.09460500	H	-3.51480100	2.30278600	1.30313000
H	2.64750400	0.17632300	2.34529800	C	-2.06198000	-0.08442500	3.17891000
C	3.90396200	1.70781900	-0.50711300	Pd	-1.05153200	-0.25162800	1.13036100
H	3.81551400	2.71252600	-0.08169100	O	0.83752000	1.83142400	2.54355600
H	4.95373800	1.40538700	-0.43661000	C	1.48752100	0.77554500	2.37332800
H	3.62846000	1.76094300	-1.56259800	O	1.07561100	-0.23639100	1.68759400
<b>4</b>				C	2.85167000	0.61055200	3.02913100
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.724958				H	3.58231000	0.21533700	2.32002600
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.59733				H	3.20665500	1.55965300	3.43567000
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.085958				H	2.76557300	-0.11370600	3.84796300
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.213585				H	-1.67707400	0.55421800	3.96852500
Sum of electronic Energies in MeOH at M06/BSII level =-1796.3018502				H	-1.94968700	-1.15828800	3.31357500
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.726				C	3.61345400	-2.97912700	-1.23487900
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.599983				C	4.34088600	-2.70244200	0.13584400
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.062007				B	3.54315400	-0.72721600	-0.74795300
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.188024				O	2.92408200	-1.70551200	-1.48937400
Sum of electronic Energies in AcOH at M06/BSII level =-1796.2779658				O	4.46651500	-1.23698200	0.13360900
C	-3.05152500	-0.35164800	1.05401900	C	5.74111700	-3.29630700	0.26011800
C	-2.95936100	0.42952600	2.23552800	H	6.17738900	-3.00156600	1.21964100
C	-3.74888000	-0.92217700	0.07361300	H	5.70231900	-4.39005800	0.23187600
C	-5.24437000	-1.11643400	0.12792900	H	6.40701500	-2.95178800	-0.53389400
H	-5.50877600	-2.16617200	-0.05083600	C	3.50314500	-3.06626100	1.36579800
H	-5.63770500	-0.86018500	1.11769700	H	3.37455500	-4.14914100	1.45193100
C	-5.99297200	-0.26790500	-0.88655600	H	4.01691000	-2.71580700	2.26629100
O	-5.49975300	0.61184900	-1.57366700	H	2.51767500	-2.59429800	1.33550900

C	4.57214400	-3.18639900	-2.41125300	H	-5.16381700	-1.85449100	0.11582800
H	5.09198900	-4.14622900	-2.33836100	H	-4.77969500	-0.67437000	1.35839900
H	4.00000700	-3.17920900	-3.34415000	C	-5.33585000	0.18189900	-0.49150400
H	5.31910700	-2.38891800	-2.46548700	O	-4.77798000	1.10367500	-1.06779200
C	2.56849300	-4.08994300	-1.20380000	O	-6.66757200	0.03569500	-0.45456000
H	2.10333500	-4.18565100	-2.19024400	C	-7.46155500	1.05915000	-1.12196300
H	3.03318600	-5.05037800	-0.95910800	C	-8.91929100	0.71979500	-0.89756900
H	1.78045300	-3.89009600	-0.47423500	H	-7.19987400	1.06096200	-2.18425000
C	2.30117500	2.92708100	-1.63524300	H	-7.19850300	2.03330400	-0.69982500
C	3.50125900	3.21334600	-0.65003800	H	-9.54497800	1.47224600	-1.38836900
B	3.22969100	0.94046900	-0.91448700	H	-9.16637800	-0.25966100	-1.31909200
O	2.44248800	1.48663000	-1.89949200	H	-9.16371200	0.71472600	0.16939000
O	3.77128800	1.88705200	-0.07992400	C	-2.82347700	-1.55367200	-1.41536500
C	3.18501500	4.16549200	0.49959900	H	-3.53199600	-1.18423600	-2.17079100
H	4.07614600	4.29388400	1.12239500	H	-2.91852800	-2.64740200	-1.42624900
H	2.89745500	5.15131600	0.12043000	C	-1.41561600	-1.15743400	-1.81392000
H	2.38232900	3.78288400	1.13353100	C	-0.95905500	0.14733700	-1.72389700
C	4.79201500	3.64421800	-1.35383400	H	-0.84346100	-1.87301000	-2.40014000
H	4.70720700	4.65561200	-1.76191200	H	-0.03644300	0.44093300	-2.21595300
H	5.61077600	3.63859500	-0.62777800	H	-1.61840400	0.94992600	-1.40675300
H	5.05578400	2.96088600	-2.16638400	C	-1.87894500	1.31303900	2.34723900
C	0.91991500	3.12489200	-1.00467500	H	-2.49166800	1.97751500	1.72473200
H	0.71947900	4.18461600	-0.81931000	H	-1.97886400	1.62509200	3.39104100
H	0.15560500	2.75497700	-1.69521800	H	-0.83804000	1.46099300	2.03780600
H	0.82207100	2.58312800	-0.06076800	C	-2.73928100	-0.88553300	3.17543800
C	2.37416300	3.66216000	-2.97104800	Pd	-0.30024300	-0.90224900	0.08772900
H	1.51593000	3.38489700	-3.59163100	O	0.43586800	-1.33095900	2.05290600
H	2.33951800	4.74530500	-2.81662500	C	1.59907600	-1.01584800	2.48541900
H	3.28397200	3.42004200	-3.52477200	O	2.54310800	-0.52151500	1.81280100
<b>TS2</b>				C	1.84364900	-1.30538600	3.95621400
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.723982				H	0.96898500	-1.02825500	4.55076500
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.603383				H	2.00361300	-2.38258300	4.08370300
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.084812				H	2.72819100	-0.77632100	4.31566700
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.20541				H	-2.84270200	-0.47955100	4.17949400
Sum of electronic Energies in MeOH at M06/BSII level =-1796.3017366				H	-3.01135600	-1.92800800	3.03389100
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.724488				C	2.45884200	-2.38431600	-1.29804400
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.603715				C	3.92788100	-2.29606300	-0.71757200
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.064222				B	2.80825300	-0.31600700	-0.20331600
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.184995				O	1.81633800	-1.19232700	-0.72015700
Sum of electronic Energies in AcOH at M06/BSII level =-1796.2802849				O	4.06509100	-0.88585300	-0.38300000
C	-2.17108800	-0.67764700	0.79542400	C	5.02758600	-2.63827400	-1.72400100
C	-2.29442200	-0.12744900	2.15818000	H	6.00503600	-2.52283900	-1.24453400
C	-3.16749900	-1.02255800	-0.04136300	H	4.94235500	-3.67554500	-2.06343500
C	-4.63616200	-0.91029300	0.29857800	H	5.00319900	-1.98227300	-2.59680900

C	4.14935900	-3.11365200	0.56191300	C	-2.11927400	-0.44384300	0.91520900
H	4.15022500	-4.18750900	0.35243500	C	-2.18455700	0.44120100	2.09226000
H	5.12681500	-2.85117100	0.97901500	C	-3.14536100	-0.99455400	0.24050600
H	3.39393400	-2.90650000	1.32124100	C	-4.60069100	-0.80875400	0.60381500
C	2.38894200	-2.20914700	-2.81841700	H	-5.10712700	-1.77296800	0.73299000
H	2.83251000	-3.06239300	-3.33976100	H	-4.70479800	-0.27266800	1.55302800
H	1.34168000	-2.13622700	-3.12715600	C	-5.36229900	-0.00961900	-0.43874000
H	2.90226800	-1.29870600	-3.14078600	O	-4.85495300	0.73496700	-1.26408900
C	1.68101500	-3.62722300	-0.87431700	O	-6.68492000	-0.19276100	-0.32692900
H	0.67348000	-3.60072400	-1.30080200	C	-7.53425500	0.56135200	-1.23968000
H	2.17612200	-4.53089700	-1.24467600	C	-8.97156700	0.28420100	-0.85490300
H	1.59026800	-3.70282400	0.21120300	H	-7.31323500	0.23751900	-2.26127100
C	3.07221500	3.58251200	-0.74479600	H	-7.28455100	1.62257700	-1.15259700
C	1.86613000	3.51121400	0.26131100	H	-9.63838600	0.83457600	-1.52643500
B	2.63406700	1.38228800	-0.20309900	H	-9.20575200	-0.78190100	-0.93730700
O	3.62273100	2.22493900	-0.66372400	H	-9.17368800	0.60919100	0.17053000
O	1.52312700	2.08180500	0.22840700	C	-2.84514300	-1.86353100	-0.96005600
C	0.63584600	4.31623800	-0.14466700	H	-3.58469600	-1.70989800	-1.75895100
H	-0.15228000	4.19513500	0.60545600	H	-2.91956000	-2.92296600	-0.68195400
H	0.87696600	5.38245600	-0.20482200	C	-1.45934700	-1.57334100	-1.50090500
H	0.23747600	3.99583600	-1.10996500	C	-1.01793300	-0.28185900	-1.75073100
C	2.25931400	3.83059100	1.70711200	H	-0.90675000	-2.40720800	-1.92702100
H	2.48283700	4.89398300	1.83512900	H	-0.12177200	-0.10959700	-2.33850900
H	1.42698100	3.57777800	2.37108300	H	-1.68050300	0.56703400	-1.61172000
H	3.13267700	3.25157100	2.02162100	C	-1.73046600	1.86950700	1.89987700
C	2.64674100	3.79002700	-2.20232000	H	-2.30507800	2.35727700	1.10259200
H	2.28985800	4.80947600	-2.37601400	H	-1.84867400	2.45065000	2.81920200
H	3.50955600	3.61675700	-2.85297200	H	-0.67622600	1.90684900	1.60374000
H	1.85724500	3.09078100	-2.49374000	C	-2.61263500	-0.01832200	3.28119400
C	4.17402900	4.56935200	-0.37153000	Pd	-0.27379000	-0.86482800	0.22619100
H	4.97599700	4.52279300	-1.11535600	O	0.56596000	-0.72173400	2.23210500
H	3.78957200	5.59439600	-0.35807800	C	1.77270400	-0.66542600	2.58660600
H	4.60640300	4.34723300	0.60644300	O	2.79229000	-0.59554200	1.80549800
<b>5</b>				C	2.09308000	-0.65718000	4.06035100
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.724391				H	1.21425100	-0.91840100	4.65082700
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.6025				H	2.91079000	-1.35225700	4.26971800
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.088722				H	2.43202100	0.34623000	4.34223600
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.210613				H	-2.67980600	0.63570900	4.14792300
Sum of electronic Energies in MeOH at M06/BSII level =-1796.3058702				H	-2.90650900	-1.05490800	3.42182500
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.725155				C	2.53906300	-2.33961100	-1.19822000
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.604075				C	4.01228000	-2.23780900	-0.64978900
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.068543				B	2.80588500	-0.41094400	0.22522400
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.189623				O	1.84202000	-1.38685300	-0.34463000
Sum of electronic Energies in AcOH at M06/BSII level =-1796.2854536				O	4.10047800	-0.85954100	-0.23366600



C	5.09546300	-2.48073000	-1.70310100	Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.604508			
H	6.08385700	-2.39592500	-1.23872300	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.050518			
H	5.01372300	-3.48402500	-2.13430400	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.169885			
H	5.04244000	-1.74739500	-2.51113500	Sum of electronic Energies in AcOH at M06/BSII level =-1796.2717914			
C	4.27349300	-3.15269000	0.56032300	C	-2.10856400	-0.66960100	0.49049700
H	4.35136500	-4.20379400	0.26411200	C	-2.47779400	-1.55984000	1.60337400
H	5.22370400	-2.86087900	1.01957200	C	-2.92991700	-0.21396800	-0.47179700
H	3.49267100	-3.06639600	1.31952800	C	-4.38546600	-0.60068900	-0.62052500
C	2.40842600	-1.85838300	-2.64958900	H	-4.62146100	-0.90380400	-1.64762700
H	2.90248400	-2.54289800	-3.34582900	H	-4.63428700	-1.44809000	0.02906900
H	1.35044800	-1.81449800	-2.92572600	C	-5.33133100	0.52096900	-0.23126600
H	2.83686500	-0.86016000	-2.77924900	O	-5.05441500	1.44838900	0.51522700
C	1.90111600	-3.71884400	-1.04535000	O	-6.54300100	0.36037800	-0.78341800
H	0.88086400	-3.71132500	-1.44135800	C	-7.56593700	1.33434500	-0.42649400
H	2.46761700	-4.46846800	-1.60844100	C	-8.84513600	0.92322200	-1.12360800
H	1.85634400	-4.03404300	-0.00040800	H	-7.22662700	2.32507600	-0.74355900
C	2.27134600	3.19965800	-1.36929900	H	-7.67590400	1.33937600	0.66181700
C	2.25291200	3.54502400	0.16541100	H	-9.63856700	1.63529600	-0.87468500
B	2.51023500	1.26083700	-0.11891300	H	-8.71841200	0.91793800	-2.21084700
O	2.74472800	1.81254000	-1.36633100	H	-9.16676900	-0.07300800	-0.80361800
O	2.07172500	2.22296700	0.77738500	C	-2.37749200	0.74547000	-1.50307600
C	1.11270300	4.45439600	0.61306500	H	-3.11241900	1.52638200	-1.75424000
H	1.15399700	4.59142100	1.69856300	H	-2.18024500	0.21687200	-2.44564500
H	1.20367200	5.44200700	0.14903800	C	-1.10646100	1.40569700	-1.00819100
H	0.13336900	4.04386800	0.35921300	C	-1.02555800	1.97848900	0.26650600
C	3.58953500	4.08302600	0.68867400	H	-0.38312600	1.71360300	-1.75816400
H	3.78174800	5.09835200	0.32946700	H	-0.26611500	2.71995800	0.49066500
H	3.56021500	4.10955400	1.78262200	H	-1.88842500	1.97320400	0.92616900
H	4.42446500	3.44277900	0.38863200	C	-1.92055700	-2.96684600	1.58091700
C	0.88060200	3.18961900	-2.01153600	H	-0.82773800	-2.96487700	1.52235200
H	0.47927600	4.20217700	-2.11585100	H	-2.21977300	-3.53065600	2.46997600
H	0.95155400	2.75051200	-3.01177000	H	-2.28139400	-3.50651700	0.69550600
H	0.17464400	2.59439400	-1.42564300	C	-3.27087800	-1.13447300	2.60674900
C	3.23354400	4.03312000	-2.21126900	Pd	-0.11819700	0.00559300	0.37058500
H	3.20035300	3.69462500	-3.25202000	O	0.52683700	-0.78262000	2.47950400
H	2.94890200	5.09024800	-2.19461000	C	1.71226000	-1.09192600	2.64434700
H	4.26414200	3.94566700	-1.86032900	O	2.56174400	-1.23608700	1.64383500
<b>TS3</b>				C	2.31766100	-1.30335400	3.99866900
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.722943				H	1.54604100	-1.27916900	4.76798900
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.603379				H	2.85403300	-2.25604100	4.02759500
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.069673				H	3.04785800	-0.50783400	4.18535500
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.189237				H	-3.52941500	-1.78517100	3.43971200
Sum of electronic Energies in MeOH at M06/BSII level =-1796.2907777				H	-3.68243100	-0.12881000	2.61890500
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.723876				C	1.45951600	-2.45289500	-1.56449700

C	3.02605400	-2.28333500	-1.58154300	Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.084136			
B	2.16220900	-1.16135500	0.24257600	Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.208865			
O	1.12949700	-2.02884100	-0.18922800	Sum of electronic Energies in MeOH at M06/BSII level =-1796.3010226			
O	3.24044800	-1.17808600	-0.64751800	Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.725411			
C	3.61360700	-1.89512400	-2.93434000	Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.601039			
H	4.69984600	-1.79140100	-2.84592800	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.06401			
H	3.41049000	-2.66999200	-3.68038100	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.188382			
H	3.21166700	-0.94671700	-3.29686700	Sum of electronic Energies in AcOH at M06/BSII level =-1796.2812209			
C	3.77287900	-3.49434400	-1.00984500	C	2.14725200	0.47721700	0.79668100
H	3.72237000	-4.35257400	-1.68645300	C	2.52213900	1.08913000	2.08169300
H	4.82625800	-3.23043300	-0.87437500	C	2.99257000	0.37263600	-0.24960500
H	3.37079200	-3.79404700	-0.03737200	C	4.42190500	0.88339100	-0.29008300
C	0.74047800	-1.53166300	-2.55120000	H	4.62590600	1.48422600	-1.18464400
H	0.91275900	-1.85926700	-3.58086700	H	4.62544600	1.51859100	0.58098200
H	-0.33549800	-1.57151400	-2.36120500	C	5.44350600	-0.23622300	-0.23017900
H	1.07397700	-0.49621000	-2.45563900	O	5.28145200	-1.30535800	0.34142900
C	0.96525300	-3.88659600	-1.73077000	O	6.58638400	0.08675500	-0.85733600
H	-0.12853300	-3.90792600	-1.69300000	C	7.66754100	-0.88633300	-0.79181700
H	1.27359900	-4.28538100	-2.70257900	C	8.83846300	-0.32011500	-1.56669000
H	1.34657900	-4.54576300	-0.94817700	H	7.31283800	-1.82920000	-1.21868800
C	3.04174400	2.81066400	-0.88682900	H	7.91715800	-1.05799900	0.25968300
C	3.50928800	2.61856500	0.61003700	H	9.66889600	-1.03295400	-1.53850500
B	1.84971600	1.07138600	0.10447400	H	8.57201300	-0.14571700	-2.61400300
O	2.18876800	1.63540300	-1.10945100	H	9.18213600	0.62357300	-1.13124200
O	2.49066200	1.70689800	1.15044600	C	2.51291500	-0.28922700	-1.52939800
C	3.50435100	3.88715000	1.45877200	H	3.31753200	-0.87986900	-1.99799000
H	3.79403000	3.64076700	2.48527500	H	2.25007500	0.47440000	-2.27488800
H	4.22482700	4.61626400	1.07406200	C	1.32511000	-1.20907800	-1.31382500
H	2.51821100	4.35589300	1.48908300	C	1.32841400	-2.23414600	-0.36875000
C	4.85288400	1.89538200	0.75479700	H	0.60684700	-1.27885400	-2.12818800
H	5.68186000	2.51926900	0.40732100	H	0.66835000	-3.08691900	-0.48389800
H	5.02365900	1.66613800	1.81155000	H	2.18443700	-2.37176700	0.28679000
H	4.86587700	0.95474300	0.19800500	C	1.91491500	2.44406300	2.38540300
C	2.16711700	4.04618700	-1.11651300	H	0.82375000	2.42540600	2.29124000
H	2.74942700	4.96774200	-1.02201400	H	2.17134900	2.79077200	3.39192700
H	1.75657600	4.01043200	-2.13056300	H	2.27451800	3.19231900	1.66607600
H	1.33159200	4.09449000	-0.41332100	C	3.33057800	0.48332100	2.97808400
C	4.16314100	2.77237600	-1.92240800	Pd	0.22409200	-0.54832000	0.46134500
H	3.73920100	2.88197000	-2.92588500	O	-0.78728600	0.27160100	2.25501000
H	4.86775800	3.59557200	-1.76592400	C	-1.88601700	0.71361000	2.57271100
H	4.71409700	1.83012200	-1.88935100	O	-2.76345300	1.23627900	1.70636700
<b>6</b>				C	-2.39826300	0.69772900	3.97689800
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.724399				H	-1.66283700	0.25056000	4.64472300
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.59967				H	-2.62774000	1.72054600	4.29274100

H	-3.33267300	0.12730500	4.00995200
H	3.54577700	0.93102100	3.94654900
H	3.79185300	-0.47881900	2.76853300
C	-1.58795500	2.79651500	-1.36613800
C	-3.15233300	3.02533500	-1.35782300
B	-2.53114400	1.82102200	0.46177400
O	-1.33802200	2.28925600	0.00268700
O	-3.60499400	2.05724000	-0.34342500
C	-3.86055800	2.70535600	-2.66813800
H	-4.93713300	2.86189500	-2.54885600
H	-3.51120600	3.36911000	-3.46498500
H	-3.69750800	1.67121800	-2.97836300
C	-3.56619900	4.40654700	-0.84465800
H	-3.31676000	5.18944800	-1.56614700
H	-4.64888000	4.41978100	-0.68750200
H	-3.08146600	4.64354300	0.10732300
C	-1.13974400	1.70121900	-2.33345100
H	-1.26929900	2.02090200	-3.37141200
H	-0.07764900	1.49564600	-2.17590000
H	-1.69824700	0.77397600	-2.17985100
C	-0.75163900	4.05572700	-1.55615700
H	0.31156100	3.79895500	-1.51930200
H	-0.95452500	4.50466700	-2.53351200
H	-0.95047000	4.80025400	-0.78263600
C	-2.98705200	-3.03051300	-1.12300600
C	-3.62366600	-2.57927700	0.24308300
B	-1.51167800	-1.63927100	0.00681300
O	-1.84237500	-2.11454200	-1.25026400
O	-2.47037800	-1.98827300	0.94237800
C	-4.17418500	-3.71029500	1.10637700
H	-4.56349800	-3.30273900	2.04505600
H	-4.99844800	-4.22081400	0.59740500
H	-3.40765900	-4.44885100	1.35051500
C	-4.66962500	-1.46979000	0.09988200
H	-5.59110900	-1.84793100	-0.35335300
H	-4.91779300	-1.08051800	1.09215100
H	-4.29993500	-0.63909600	-0.50660600
C	-2.40645800	-4.44831000	-1.09375100
H	-3.19647700	-5.20510100	-1.06961700
H	-1.81165900	-4.60929700	-1.99835500
H	-1.75563300	-4.59860400	-0.22737000
C	-3.87897200	-2.85143600	-2.34754500
H	-3.34242400	-3.17439600	-3.24562600
H	-4.78427800	-3.46113700	-2.26167400

H	-4.17572900	-1.80956800	-2.48689500
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### Bpin-OAC

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.248298

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.192772

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-639.582982

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-639.638508

Sum of electronic Energies in MeOH at M06/BSII level =-639.6091496

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.248525

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.193083

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-639.573348

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-639.628789

Sum of electronic Energies in AcOH at M06/BSII level =-639.599083

O	2.84353800	1.32046800	-0.13827900
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C	2.96289400	0.11758600	-0.03229200
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O	1.90346100	-0.74116700	-0.07145100
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C	4.25767400	-0.62095100	0.12899700
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H	5.08986000	0.08280000	0.14200800
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H	4.23989900	-1.19758800	1.05958200
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H	4.38112800	-1.33278400	-0.69366900
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C	-1.37386500	0.81140000	0.09321600
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C	-1.68029800	-0.72979600	-0.06778400
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B	0.56344100	-0.36674800	-0.04269500
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O	0.06169800	0.81077700	0.42597000
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O	-0.37104800	-1.26547500	-0.47144600
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C	-2.69134000	-1.07763700	-1.15372700
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H	-2.82209400	-2.16333100	-1.20091900
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H	-3.66499700	-0.63149700	-0.92861500
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H	-2.36743900	-0.73055800	-2.13714300
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C	-2.04385100	-1.42288000	1.24773100
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H	-3.04054600	-1.13004700	1.59006500
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H	-2.04249500	-2.50601500	1.09207300
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H	-1.32326300	-1.19106000	2.03785900
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C	-1.51166900	1.60195600	-1.21032300
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H	-2.56037700	1.71045900	-1.50113200
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H	-1.09218800	2.60241200	-1.06753900
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H	-0.97099900	1.12065900	-2.03088900
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C	-2.12129600	1.50701300	1.22433500
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H	-1.81459900	2.55641300	1.27598000
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H	-3.20044100	1.48137800	1.04320400
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H	-1.91933700	1.04553200	2.19334500
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### 7

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.473939

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.382738

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.512845

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.604046	C	5.59651400	-0.04415900	-1.40744700
Sum of electronic Energies in MeOH at M06/BSII level =-1156.6939153	H	5.97381400	0.98254800	-1.35716100
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.474434	H	6.45638500	-0.71931400	-1.34478900
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.383647	H	5.11832100	-0.18038700	-2.37998700
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.499097	C	5.27052700	0.11636500	1.07417900
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.589883	H	6.19568100	-0.43678900	1.26271000
Sum of electronic Energies in AcOH at M06/BSII level =-1156.6806303	H	5.51572400	1.18271300	1.03998800
C	H	4.59027800	-0.04749700	1.91519400
C	C	3.81812900	-2.35837900	-1.61075000
C	H	4.78309800	-2.67506800	-2.01816100
C	H	3.18127800	-3.24458900	-1.52648200
H	H	3.34962100	-1.67054900	-2.32080100
H	C	4.61545200	-2.71101900	0.73988100
C	H	4.06534600	-3.65754800	0.71734500
O	H	5.65089300	-2.91967100	0.45057900
O	H	4.61073000	-2.34261200	1.76824000
C	<b>TS7</b>			
C	Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.472902			
H	Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.386169			
H	Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.50184			
H	Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.588573			
H	Sum of electronic Energies in MeOH at M06/BSII level =-1156.6858537			
H	Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.473492			
C	Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.386421			
H	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.488882			
H	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.575953			
C	Sum of electronic Energies in AcOH at M06/BSII level =-1156.6728949			
C	C	0.44711900	-0.27560000	-0.24365600
H	C	0.38689800	-1.52272800	-1.04849900
H	C	1.44804000	-0.00129200	0.63436000
H	C	2.63602200	-0.92141100	0.86409900
C	H	2.85617500	-1.03100900	1.93108100
H	H	2.43758500	-1.92295500	0.47043500
H	C	3.89141600	-0.44384000	0.15572900
H	O	3.90973600	0.12569500	-0.92573900
C	O	5.00200400	-0.76499000	0.83496900
Pd	C	6.27552600	-0.43936000	0.20626200
H	C	7.37280600	-0.84690300	1.16623000
H	H	6.29396100	0.63372900	-0.00414300
C	H	6.33953700	-0.97850200	-0.74360200
C	H	8.34632900	-0.61243300	0.72384200
B	H	7.28836900	-0.30617300	2.11411500
O	H	7.34044000	-1.92156500	1.37162800
O	C	1.59863300	1.33143800	1.36801700

H	2.50238600	1.82043500	0.97623600	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.530705			
H	1.80724200	1.13346000	2.43030900	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.618875			
C	0.43635300	2.30236500	1.26018500	Sum of electronic Energies in AcOH at M06/BSII level=-1156.7226855			
C	0.48421300	3.50154200	0.59400300	C	0.46117300	0.81372500	-0.55698800
H	-0.39474600	2.12637300	1.94218200	C	0.76537800	2.26102000	-0.25531200
H	-0.29933300	4.24364500	0.72043000	C	1.43414800	-0.02583600	-0.97032100
H	1.36735800	3.80270800	0.03397300	C	2.87207500	0.43936300	-1.11181600
C	0.48818700	-1.34365000	-2.54485400	H	3.33690300	0.02515300	-2.01431500
H	1.44011900	-0.86670400	-2.81092600	H	2.94715500	1.52832300	-1.19475400
H	0.41949800	-2.30038800	-3.07173800	C	3.74185000	0.04647900	0.07005300
H	-0.31033400	-0.68670600	-2.91181900	O	3.33888900	-0.39449900	1.13530300
C	0.22357100	-2.73707200	-0.49404400	O	5.03898100	0.27050600	-0.18771900
Pd	-0.43449100	1.58345100	-0.68551000	C	5.98219500	-0.01684500	0.88445000
H	0.16850700	-3.63624500	-1.10354700	C	7.35838300	0.37943000	0.39458100
H	0.12901200	-2.86647600	0.58083500	H	5.92345200	-1.08373500	1.12020300
C	-3.48404600	-0.54321300	1.20257000	H	5.68480000	0.54896500	1.77205700
C	-3.69184600	-1.05051700	-0.27978700	H	8.09561600	0.16579700	1.17522800
B	-1.69411000	0.12203400	-0.09680600	H	7.63649000	-0.18313700	-0.50227300
O	-2.07479600	-0.13030400	1.20885300	H	7.40227600	1.44877300	0.16526600
O	-2.62035200	-0.35028500	-1.00762300	C	1.28599900	-1.50425200	-1.29191900
C	-5.02153400	-0.65399900	-0.91678600	H	1.91074500	-2.06262000	-0.58065300
H	-5.05357000	-1.01405300	-1.95017600	H	1.75749100	-1.66478800	-2.27595200
H	-5.86057200	-1.10687000	-0.37864900	C	-0.09131500	-2.12004500	-1.33421400
H	-5.16231400	0.42904600	-0.93147500	C	-0.39118400	-3.35232300	-0.73068800
C	-3.45229300	-2.55018300	-0.46506000	H	-0.72050200	-1.78320400	-2.15914800
H	-4.24471200	-3.13758400	0.00841900	H	-1.20522900	-3.96529000	-1.11494700
H	-3.45229600	-2.78366700	-1.53455300	H	0.38040000	-3.89217700	-0.18157800
H	-2.49083000	-2.86340600	-0.05148400	C	0.50640300	3.24347000	-1.37371300
C	-4.30402200	0.70413400	1.54921800	H	-0.52422500	3.16069500	-1.73851800
H	-5.37258000	0.47799100	1.61115000	H	0.68073600	4.27575500	-1.05444100
H	-3.98165600	1.08374300	2.52397100	H	1.15597600	3.03235100	-2.23319200
H	-4.15964800	1.49961600	0.81219100	C	1.18840100	2.64963400	0.95567700
C	-3.66849200	-1.60700200	2.28104200	Pd	-1.19773800	-1.76854600	0.45436500
H	-3.46142100	-1.17267800	3.26434700	H	1.37552300	3.69781200	1.18095100
H	-4.69905400	-1.97615600	2.28887600	H	1.36884200	1.93546700	1.75492300
H	-2.99632700	-2.45543400	2.13644000	C	-3.36533700	0.85977800	-0.57340600
<b>12</b>				C	-3.00759400	0.92600300	0.96725100
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.474826				B	-1.07597300	0.53902100	-0.29803100
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.387212				O	-2.04955200	0.89893000	-1.21416800
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.543254				O	-1.61466300	0.43980400	1.00390200
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.630868				C	-3.84673900	0.02537800	1.86545600
Sum of electronic Energies in MeOH at M06/BSII level=-1156.7355463				H	-3.50802300	0.11792600	2.90232200
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.475287				H	-4.90123900	0.31669700	1.82918400
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.387117				H	-3.76363100	-1.02461700	1.57029700

C	-2.95730400	2.34807700	1.53250600
H	-3.95716800	2.78777700	1.58892500
H	-2.54408200	2.31506900	2.54520900
H	-2.32300800	3.00270600	0.92862600
C	-4.04558500	-0.44335400	-1.00495100
H	-5.05921300	-0.51813100	-0.60003900
H	-4.11382500	-0.46353900	-2.09734200
H	-3.47063200	-1.31971500	-0.68316500
C	-4.16856800	2.05322800	-1.08799400
H	-4.34244800	1.94051500	-2.16280900
H	-5.14433500	2.10487000	-0.59470000
H	-3.64653500	2.99881700	-0.92644000

#### TS4

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.337543  
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.259868  
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-972.841611  
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-972.935286  
Sum of electronic Energies in MeOH at M06/BSII level =-974.0119755  
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.337907  
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.260767  
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-972.825507  
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-972.902647  
Sum of electronic Energies in AcOH at M06/BSII level =-973.9920109

C	0.01268000	-1.21091800	0.52463000
C	0.18645000	-0.88300500	1.95797400
C	-1.09411800	-1.43384600	-0.23705700
C	-2.54658800	-1.22262700	0.07578600
H	-3.16567900	-1.93809400	-0.47494800
H	-2.76275300	-1.38115300	1.13909500
C	-3.03465300	0.17806000	-0.26664500
O	-2.32391600	1.12937000	-0.54494800
O	-4.36978500	0.24408600	-0.20144500
C	-4.97454500	1.54410600	-0.46726900
C	-6.46844700	1.39880600	-0.27201800
H	-4.72075100	1.83933500	-1.48956600
H	-4.54023000	2.27438600	0.22126600
H	-6.95098600	2.36412700	-0.45642500
H	-6.89037100	0.66648300	-0.96752700
H	-6.70406000	1.08834900	0.75086000
C	-0.56178200	-2.26060800	-1.36926900
H	-0.53694600	-1.79098800	-2.35852300
H	-1.09731100	-3.21511100	-1.45604300
C	0.80784500	-2.45966000	-0.72239400
C	2.00512100	-1.96885900	-1.34590600

H	0.89354300	-3.31829400	-0.05923500
H	2.95895100	-2.40529600	-1.04807800
H	1.94026200	-1.67574000	-2.39510400
C	-0.65345000	0.23736000	2.53436700
H	-1.71230600	-0.03760200	2.58951800
H	-0.31833900	0.48318300	3.54612400
H	-0.58708600	1.13800000	1.91556400
C	1.08388600	-1.55143700	2.70540900
Pd	1.74243800	-0.24085200	-0.28155400
O	3.35722300	1.05774000	-0.88294800
C	3.01325400	2.05492400	-0.14767500
O	2.00109400	1.98652300	0.60524400
C	3.83806400	3.31564700	-0.23009300
H	3.63940800	3.81369100	-1.18608200
H	3.58701800	3.99863600	0.58346600
H	4.90434400	3.07387300	-0.20029400
H	1.21818300	-1.31804200	3.75816100
H	1.69370800	-2.34995600	2.29297500

#### 8

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.339463  
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.263639  
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-972.868399  
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-972.944223  
Sum of electronic Energies in MeOH at M06/BSII level =-974.0271525  
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.339926  
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.264442  
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-972.853756  
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-972.929239  
Sum of electronic Energies in AcOH at M06/BSII level =-974.0097337

C	1.27408800	-1.69312500	0.08965300
C	1.99375900	-1.92581100	1.34537500
C	-0.06312400	-1.47867100	-0.30018800
C	-1.35411900	-1.39443700	0.45333900
H	-1.78084600	-2.39992800	0.57079000
H	-1.20588000	-1.00326700	1.46524100
C	-2.39501100	-0.51937800	-0.21860000
O	-2.18026200	0.27402000	-1.12166900
O	-3.60064000	-0.70920300	0.33013600
C	-4.69445500	0.11331900	-0.17210600
C	-5.95337000	-0.32073000	0.54715700
H	-4.76954800	-0.03419700	-1.25306100
H	-4.45239400	1.16284300	0.01966400
H	-6.79675900	0.28032300	0.19237200
H	-6.17700000	-1.37406000	0.35045400

H	-5.86120500	-0.17686300	1.62832600	C	6.76748000	0.86728600	-0.20285100
C	0.18373200	-2.00533600	-1.71204600	C	8.11646200	0.94412400	-0.88450900
H	-0.19097300	-1.43436700	-2.56550400	H	6.85939300	0.65571600	0.86625100
H	-0.14952100	-3.04721800	-1.79317200	H	6.19267500	1.79032300	-0.32454900
C	1.70867300	-1.90410400	-1.38688400	H	8.69973200	1.75613700	-0.43859000
C	2.20221700	-0.51517500	-1.72219700	H	8.67540800	0.01151400	-0.75858900
H	2.34514700	-2.75368800	-1.65304300	H	8.00783500	1.14709600	-1.95459300
H	3.24818900	-0.31848100	-1.47299200	C	3.08972300	-3.02537800	0.98098800
H	1.92576900	-0.12663300	-2.70694500	H	3.28164300	-2.39112000	1.85319900
C	1.30097700	-1.61243600	2.65055700	H	3.74876400	-3.90178600	1.02838700
H	0.40077400	-2.22458100	2.77955100	C	1.55337500	-3.32073300	0.74086300
H	1.96522100	-1.80460100	3.49748000	C	0.50323600	-2.65501300	1.61730600
H	0.98833200	-0.56249600	2.68989400	H	1.34238500	-4.38590500	0.59163600
C	3.23930500	-2.43264400	1.29898300	H	-0.07186100	-3.33378000	2.25420800
Pd	1.06440700	0.47386400	-0.34309800	H	0.91220700	-1.83164700	2.21075000
O	1.61895400	2.56396100	-0.53127100	C	0.74674000	-1.03450300	-2.38450300
C	0.81941500	2.97794100	0.38759700	H	1.34390900	-1.40826900	-3.22689300
O	0.08005700	2.16664200	1.01649700	H	-0.22352800	-0.72029400	-2.77560000
C	0.78804600	4.45603400	0.68539900	H	1.26362700	-0.16588000	-1.97178400
H	0.48304000	5.00284700	-0.21314200	C	-0.55024800	-2.91523100	-1.29174000
H	0.09579500	4.67779000	1.49924300	Pd	-0.88494300	-1.64412600	0.47884900
H	1.79262100	4.79957700	0.95263400	O	-2.89655000	0.73894700	1.82711900
H	3.79665300	-2.63592300	2.20932000	C	-2.34671000	-0.01750400	2.66204300
H	3.73418800	-2.66085800	0.35962500	O	-1.54555400	-0.98608900	2.39848700
<b>TS5</b>				C	-2.62117100	0.19711200	4.14162900
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.72395				H	-2.96535600	-0.73532000	4.59999900
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.60436				H	-1.69189200	0.48599600	4.64477400
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.072927				H	-3.36791600	0.97905100	4.29084500
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.192517				H	-1.36180400	-2.72944100	-1.98544700
Sum of electronic Energies in MeOH at M06/BSII level =-1796.292427				H	-0.52172700	-3.90271300	-0.83882800
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.72395				C	0.71171100	3.07182500	1.03171300
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.60436				C	0.84821400	3.16628800	-0.53150800
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.072927				B	-0.97003700	1.85641100	0.01780400
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.192517				O	-0.62890600	2.49721000	1.18825800
Sum of electronic Energies in AcOH at M06/BSII level =-1796.292427				O	-0.04428900	2.08879300	-0.98217800
C	1.72723100	-2.52533200	-0.53032400	C	2.24729200	2.90847500	-1.08008800
C	0.59830400	-2.13219000	-1.36642300	H	2.22450400	2.92969100	-2.17457400
C	3.04408500	-2.27719600	-0.34457000	H	2.93813100	3.68959500	-0.74559200
C	4.12293000	-1.59151800	-1.11512800	H	2.64533500	1.94228500	-0.76453900
H	4.89155800	-2.31131500	-1.42434700	C	0.28153300	4.46348700	-1.11909100
H	3.72773600	-1.14400800	-2.03527300	H	0.91506000	5.32267500	-0.88053500
C	4.80703300	-0.48179100	-0.33765500	H	0.23168100	4.37082500	-2.20854100
O	4.31274600	0.12502400	0.60054000	H	-0.72874200	4.66156000	-0.74894500
O	6.02611800	-0.22244200	-0.82533300	C	1.68953500	2.08331200	1.67481900

H	2.71334200	2.46779000	1.66187100	H	3.74029300	-1.11509600	-2.02042000
H	1.40022500	1.92336500	2.71850800	C	4.79976500	-0.39627100	-0.33264500
H	1.67734600	1.11573800	1.16574600	O	4.27354500	0.22263200	0.57999100
C	0.74721700	4.40673300	1.76955400	O	6.02426500	-0.12486800	-0.79940600
H	0.61348400	4.23707800	2.84277600	C	6.73253800	0.98923900	-0.18096200
H	1.71291000	4.90289400	1.62732100	C	8.09021500	1.08547200	-0.84203500
H	-0.04330900	5.08143800	1.43346900	H	6.81157000	0.79318900	0.89218900
C	-4.41689200	0.82084300	-1.43536000	H	6.14051300	1.89810200	-0.32403200
C	-3.85550500	-0.62481200	-1.14802600	H	8.65035200	1.91304900	-0.39504400
B	-2.42570200	0.99793700	-0.24856900	H	8.66539300	0.16554600	-0.69766400
O	-3.58851800	1.67685600	-0.59654000	H	7.99501600	1.27593700	-1.91567800
O	-2.46639400	-0.32419800	-0.74325600	C	3.16707800	-2.94805400	1.03756900
C	-3.83362300	-1.53664100	-2.37254800	H	3.33372200	-2.27843200	1.88821800
H	-3.50583400	-2.54135000	-2.09147800	H	3.85842600	-3.79704200	1.11423200
H	-4.84264100	-1.62842700	-2.78762300	C	1.64330100	-3.30668700	0.80471900
H	-3.17310000	-1.16015500	-3.15644100	C	0.56421000	-2.64339800	1.64757400
C	-4.55058100	-1.34794800	0.00931300	H	1.47051200	-4.38326900	0.69461000
H	-5.55428600	-1.67032300	-0.28437200	H	0.00653500	-3.31667300	2.30633600
H	-3.97411900	-2.24319300	0.26623500	H	0.94367100	-1.78558900	2.21262500
H	-4.62876200	-0.72337400	0.89980600	C	0.75952800	-1.16104200	-2.39660200
C	-4.19309600	1.28630700	-2.87991400	H	1.38317400	-1.54112000	-3.21668400
H	-4.83267400	0.74940100	-3.58655400	H	-0.21893800	-0.90612700	-2.80898500
H	-4.43330000	2.35207100	-2.94784900	H	1.23288600	-0.25415500	-2.01402300
H	-3.15045900	1.15625200	-3.18471300	C	-0.47849200	-3.03586700	-1.22292200
C	-5.87795700	1.02637600	-1.04092800	Pd	-0.84867100	-1.70392400	0.47574800
H	-6.16898400	2.06146700	-1.24760200	O	-3.00125600	0.66961000	1.69218900
H	-6.53573600	0.37135300	-1.62148500	C	-2.41860000	-0.05025900	2.58237700
H	-6.04394300	0.83396900	0.02119700	O	-1.52174700	-0.90652000	2.36583600
<b>9</b>				C	-2.87058400	0.18764200	4.00094400
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.724593				H	-2.55431300	1.18996700	4.31055100
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.605704				H	-3.96303100	0.15912200	4.05029200
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.077966				H	-2.44527300	-0.55332200	4.67863100
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.205855				H	-1.29352700	-2.90944800	-1.92617300
Sum of electronic Energies in MeOH at M06/BSII level =-1796.3024978				H	-0.41382000	-4.00357300	-0.73235800
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.725813				C	0.64346000	3.13425000	1.02996400
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.610086				C	0.67376600	3.10684600	-0.54215200
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.057949				B	-1.07052100	1.79531400	0.22721700
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.173676				O	-0.66070400	2.53471500	1.32271900
Sum of electronic Energies in AcOH at M06/BSII level =-1796.2770902				O	-0.21480000	1.97905600	-0.84851600
C	1.79176400	-2.54953900	-0.49224000	C	2.04235400	2.83848800	-1.16006300
C	0.64845000	-2.22165000	-1.33652400	H	1.95197600	2.78512000	-2.24999400
C	3.09758600	-2.24492400	-0.31151100	H	2.73505000	3.65325000	-0.92386100
C	4.15219000	-1.53741100	-1.09584300	H	2.48087700	1.90351900	-0.80572600
H	4.94217900	-2.23709800	-1.39694700	C	0.03694200	4.34312700	-1.18808100



H	0.66104900	5.23242400	-1.05949000	C	1.49028300	-0.61740800	-1.65349300
H	-0.08320800	4.16482600	-2.26135800	C	3.75740000	-1.75519800	-0.94425900
H	-0.95182500	4.54806600	-0.76699300	C	4.99086200	-0.99001500	-1.29396800
C	1.69789300	2.23290000	1.68063400	H	5.77158800	-1.65742300	-1.67585100
H	2.70544900	2.64169700	1.56169700	H	4.79231900	-0.24999600	-2.07885800
H	1.48860700	2.15545000	2.75245100	C	5.55243000	-0.22245000	-0.10749400
H	1.68126500	1.22485400	1.25787400	O	4.89362700	0.17985600	0.83851300
C	0.68159700	4.52580100	1.65561100	O	6.86664600	-0.00618900	-0.23925900
H	0.63120900	4.44085000	2.74606000	C	7.51442600	0.77085800	0.81075300
H	1.61446100	5.04077400	1.40357500	C	8.98110000	0.88039700	0.45374100
H	-0.15638100	5.14456500	1.32664700	H	7.36138900	0.25595500	1.76367000
C	-4.22934600	0.84311500	-1.48691400	H	7.03044800	1.75032400	0.86544400
C	-3.78697300	-0.62788800	-1.15862000	H	9.49936000	1.45260100	1.22999600
B	-2.54544000	0.89394500	0.17829500	H	9.44684200	-0.10807200	0.38854900
O	-3.67819900	1.60522200	-0.39735000	H	9.11790500	1.39692600	-0.50152900
O	-2.48022100	-0.38865200	-0.55003900	C	3.58885800	-3.04637600	-0.15651900
C	-3.63251800	-1.52195600	-2.38706900	H	3.88541600	-2.98081200	0.89609300
H	-3.41766900	-2.55193000	-2.08620400	H	4.04567700	-3.94335600	-0.59633100
H	-4.56648800	-1.54122200	-2.95922400	C	2.02837800	-2.84157200	-0.37945800
H	-2.83375500	-1.18009500	-3.04928200	C	1.14594800	-2.42710400	0.78439900
C	-4.70005200	-1.32588500	-0.13937200	H	1.57082000	-3.63688800	-0.98095200
H	-5.64771100	-1.62559800	-0.59827800	H	0.52717500	-3.23167600	1.20075300
H	-4.20190700	-2.23305000	0.22028500	H	1.73125900	-1.96063300	1.58700800
H	-4.91915600	-0.69124600	0.72172100	C	1.99964600	0.73449500	-2.06873400
C	-3.61203700	1.37332400	-2.79242100	H	2.59010000	0.61731400	-2.98758900
H	-4.04419600	0.90130300	-3.68040000	H	1.18236400	1.42392200	-2.28162200
H	-3.80324700	2.44971400	-2.85718000	H	2.66192800	1.16648900	-1.31289500
H	-2.52827400	1.22500500	-2.80847600	C	0.16838600	-1.00567400	-1.87677000
C	-5.74457400	1.05255100	-1.51363800	Pd	-0.18316800	-0.79992900	0.28380100
H	-5.96754000	2.10071600	-1.74071400	O	-2.68893300	-0.05546300	2.06698100
H	-6.21690800	0.43612800	-2.28614500	C	-1.67330700	-0.32623000	2.84662500
H	-6.20218500	0.81398300	-0.55071300	O	-0.58024700	-0.74619400	2.42612900
<b>TS6</b>				C	-1.91107200	-0.06942600	4.30260300
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.722439				H	-2.13414400	0.99363000	4.44314100
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.601997				H	-2.78364000	-0.63682500	4.64009100
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.055153				H	-1.03357800	-0.34348100	4.88776100
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.186595				H	-0.48418600	-0.33153000	-2.41919700
Sum of electronic Energies in MeOH at M06/BSII level=-1796.2891				H	-0.07143700	-2.06546700	-1.93647300
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.723973				C	-0.89971100	3.43726700	0.47303100
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.606794				C	-1.46597000	3.25908700	-0.98578900
Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.034893				B	-1.10244000	1.16849100	-0.01970700
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.152072				O	-1.02383800	2.08421000	1.02163700
Sum of electronic Energies in AcOH at M06/BSII level=-1796.2629323				O	-1.25401800	1.82622100	-1.23151900
C	2.42582800	-1.60483400	-1.14387200	C	-0.72857800	4.04362200	-2.06799200

H	-1.15665500	3.80844900	-3.04790900	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1795.044274			
H	-0.83755100	5.12124000	-1.90678600	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1795.16675			
H	0.33687800	3.80659100	-2.09762200	Sum of electronic Energies in AcOH at M06/BSII level=-1796.26614694			
C	-2.97216700	3.51679300	-1.09656500	C	2.61187300	-1.23507000	-1.51025400
H	-3.20331400	4.57690500	-0.95487900	C	1.81254300	-0.04970600	-1.80623900
H	-3.31373500	3.23037700	-2.09632500	C	3.90153600	-1.55621900	-1.24834600
H	-3.53834300	2.93522600	-0.36539300	C	5.21210100	-0.83703300	-1.25204700
C	0.58949800	3.79700500	0.52174600	H	6.01213900	-1.47757600	-1.63885800
H	0.76751200	4.81933700	0.17417900	H	5.17785900	0.05219400	-1.89440800
H	0.94094400	3.72629400	1.55606300	C	5.61683800	-0.34246900	0.12846700
H	1.18890600	3.11333700	-0.08599500	O	4.83871800	-0.04219800	1.02069600
C	-1.69323800	4.38586600	1.36825100	O	6.94676000	-0.23272000	0.24331100
H	-1.25278500	4.39780100	2.37061800	C	7.45577200	0.30220900	1.50032300
H	-1.66217200	5.40863100	0.97849700	C	8.96316000	0.37332500	1.38590400
H	-2.73774800	4.08113500	1.46236100	H	7.13683100	-0.35971900	2.31083500
C	-4.39173700	-0.69113400	-0.97453200	H	7.00996500	1.28759900	1.66388900
C	-4.00432900	-2.09468300	-0.36563000	H	9.37749000	0.76959700	2.31859500
B	-2.75920200	-0.42732400	0.64663200	H	9.39403900	-0.61814600	1.21438100
O	-3.79188800	0.23727900	-0.01890500	H	9.26621400	1.03445400	0.56785600
O	-2.75145200	-1.79921700	0.33612400	C	3.56451000	-2.98701400	-0.85129200
C	-3.73831000	-3.19567900	-1.38720400	H	3.75976500	-3.22881300	0.20013900
H	-3.43907200	-4.11328900	-0.87004200	H	4.00259700	-3.77771200	-1.47767000
H	-4.64321400	-3.41737700	-1.96223100	C	2.05018300	-2.58331600	-1.12463700
H	-2.94248400	-2.92292300	-2.08359500	C	1.06984800	-2.38077000	0.02653100
C	-4.99300000	-2.58738800	0.69783500	H	1.60265400	-3.15103300	-1.95196900
H	-5.94581000	-2.88872900	0.25209300	H	0.34032200	-3.19683400	0.12887500
H	-4.56644000	-3.45800700	1.20592900	H	1.61015000	-2.28691900	0.98090200
H	-5.19065800	-1.81796800	1.45001600	C	2.48879500	1.29803100	-1.81593800
C	-3.77660700	-0.43540100	-2.35352100	H	3.18506000	1.33974200	-2.66433900
H	-4.26156600	-1.04904500	-3.11858100	H	1.77158000	2.11222800	-1.92960400
H	-3.91943400	0.61500700	-2.62261700	H	3.07350500	1.45964100	-0.90598100
H	-2.70647700	-0.64944400	-2.36692800	C	0.51099100	-0.21910000	-2.30828800
C	-5.89138500	-0.40422300	-1.01609200	Pd	0.14310800	-0.35519800	-0.18379200
H	-6.06315200	0.59434700	-1.43098500	O	-2.61330300	-0.26419600	2.31151100
H	-6.40586200	-1.12581100	-1.65882400	C	-1.33486600	-0.26683200	2.71773700
H	-6.34240500	-0.43981800	-0.02188500	O	-0.37800400	-0.42553800	1.96860600
<b>10</b>				C	-1.18832700	-0.01414900	4.18430900
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.724586				H	-1.68849900	0.92506200	4.44267500
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.602624				H	-1.68740500	-0.81407600	4.74136400
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1795.065373				H	-0.13435800	0.03253100	4.45650800
Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1795.205336				H	0.01405600	0.62441700	-2.77670900
Sum of electronic Energies in MeOH at M06/BSII level=-1796.2957391				H	0.18778800	-1.20090500	-2.64688200
Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.602838				C	-2.42069200	3.17067400	-0.37572900
Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.602838				C	-1.02783800	3.87898300	-0.21167100

B	-0.72848900	1.56786700	-0.29690900	Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.601657			
O	-2.02915400	1.79885800	-0.73388400	Sum of electronic Energies in MeOH at M06/BSII level =-1156.6873464			
O	-0.14373000	2.75329700	0.12669100	Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.475768			
C	-0.95016200	4.90365300	0.91624600	Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.38715			
H	0.06217500	5.31740900	0.96985700	Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.498979			
H	-1.64094200	5.73393100	0.73549300	Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.587597			
H	-1.18588400	4.46227100	1.88709500	Sum of electronic Energies in AcOH at M06/BSII level =-1156.6734574			
C	-0.48944000	4.48870100	-1.51061000	C	1.91834300	-1.53418500	0.64548800
H	-1.05560200	5.37929400	-1.80051500	C	1.53120500	-2.37044400	-0.49101700
H	0.55285200	4.78774800	-1.36096500	C	3.00490700	-0.82854800	1.03636800
H	-0.52484000	3.77314000	-2.33729100	C	4.39807100	-0.63631300	0.52967800
C	-3.22205200	3.07304700	0.92719800	H	5.12533200	-0.70183000	1.34599300
H	-3.61396500	4.04859500	1.23140400	H	4.66482100	-1.41054200	-0.20023000
H	-4.07060500	2.39898500	0.77459900	C	4.58042500	0.69681000	-0.17846900
H	-2.61581900	2.67305300	1.74494500	O	3.70868000	1.27506000	-0.80840100
C	-3.30196900	3.72501700	-1.49117600	O	5.83447900	1.15067800	-0.06175400
H	-4.23136600	3.14919700	-1.54850900	C	6.15628700	2.38971500	-0.75950100
H	-3.56782400	4.76873500	-1.29315300	C	7.61529000	2.69013100	-0.49260700
H	-2.80985000	3.67202000	-2.46470700	H	5.49850100	3.17876100	-0.38369100
C	-4.82775400	-1.50460100	-0.23802200	H	5.95451900	2.24910600	-1.82541800
C	-3.68448500	-2.60213400	-0.23236500	H	7.89498900	3.61474500	-1.00777400
B	-3.18686200	-0.94321600	1.23712300	H	7.80181900	2.82501200	0.57746700
O	-4.49122700	-0.68928300	0.94150200	H	8.25772800	1.88485800	-0.86262300
O	-2.59616200	-1.92870100	0.50630500	C	2.32474300	-0.23980300	2.25735900
C	-3.15976400	-2.98651800	-1.60905700	H	2.19924300	0.84968500	2.24777000
H	-2.35447400	-3.72038800	-1.50593500	H	2.74414000	-0.53660500	3.22743600
H	-3.95538000	-3.44481800	-2.20480900	C	1.04207400	-1.04204800	1.79588100
H	-2.77107300	-2.12282800	-2.15214700	C	-0.16422000	-0.20867600	1.36851900
C	-4.03267800	-3.85134400	0.57918300	H	0.74811000	-1.82439100	2.50650700
H	-4.80069300	-4.44740500	0.07859600	H	-0.86463000	-0.03726800	2.18959000
H	-3.13550000	-4.46897500	0.68382100	H	0.14637400	0.76243500	0.96728600
H	-4.38905300	-3.59467900	1.58133400	C	2.30022900	-2.23918000	-1.78311500
C	-4.78369100	-0.56731700	-1.44547900	H	3.29353800	-2.69415400	-1.68083300
H	-5.06112600	-1.09232300	-2.36380600	H	1.78538500	-2.74510300	-2.60467900
H	-5.50213500	0.24373400	-1.29091200	H	2.45592600	-1.18898500	-2.05013000
H	-3.79485900	-0.12199100	-1.57796300	C	0.49123100	-3.23808900	-0.36432600
C	-6.23817400	-2.05049000	-0.04256200	Pd	-1.04173000	-1.20388700	-0.19459900
H	-6.95231100	-1.22128100	-0.02384900	H	0.18011100	-3.86255700	-1.19783700
H	-6.51184000	-2.71016200	-0.87187100	H	0.03432400	-3.44284300	0.60161100
H	-6.33656900	-2.60665700	0.89200600	C	-4.07147100	1.79588100	0.27726300
<b>11</b>				C	-4.81061700	0.64411800	-0.49735900
Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.475142				B	-2.62013300	0.02757100	-0.05917900
Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.385987				O	-2.85801400	1.11980500	0.75368100
Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.512501				O	-3.68801400	-0.21036500	-0.91402000

C	-5.56863700	1.08075600	-1.74705600
H	-6.01185900	0.20570400	-2.23367800
H	-6.38210600	1.76623400	-1.48750500
H	-4.91540900	1.57507100	-2.46941900
C	-5.70917900	-0.21629300	0.39682800
H	-6.60674400	0.32842200	0.70518200
H	-6.02632500	-1.10368300	-0.16011600
H	-5.17938500	-0.54906100	1.29440400
C	-3.60721300	2.94247600	-0.62684800
H	-4.45036500	3.54853800	-0.97179700
H	-2.93271400	3.59278500	-0.06102300
H	-3.06548600	2.56949500	-1.50107800
C	-4.81600000	2.34805600	1.48927800
H	-4.20602800	3.11498000	1.97754500
H	-5.75902700	2.81426900	1.18586000
H	-5.03440000	1.57027000	2.22441700

### TS8

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.473443

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.38662

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.499119

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.585942

Sum of electronic Energies in MeOH at M06/BSII level =-1156.6865829

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.473984

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.387669

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.485888

Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.572204

Sum of electronic Energies in AcOH at M06/BSII level =-1156.6731081

C	-1.54120500	0.87374100	0.97358200
C	-1.43302300	2.21978700	0.39746800
C	-2.55048000	0.01126400	1.24004100
C	-4.04232300	0.05843300	1.16780900
H	-4.49341700	-0.37622200	2.06749900
H	-4.41070400	1.08906500	1.10160200
C	-4.59546600	-0.68016100	-0.04051500
O	-3.95878600	-0.96236200	-1.04338500
O	-5.89578800	-0.96297500	0.11405000
C	-6.56304000	-1.62579100	-0.99924700
C	-8.02660500	-1.75780300	-0.63592400
H	-6.08960200	-2.60017400	-1.15291400
H	-6.41625100	-1.02409500	-1.90075100
H	-8.55644700	-2.26467000	-1.44891700
H	-8.15472700	-2.34795500	0.27697400
H	-8.48672500	-0.77579700	-0.48714400
C	-1.63644100	-1.11524900	1.67854600

H	-1.65737900	-2.01000800	1.04389600
H	-1.73024000	-1.42800100	2.72702700
C	-0.44705600	-0.12840700	1.35630300
C	0.48566400	-0.56249200	0.21214500
H	0.13281600	0.14161800	2.24717200
H	1.03939600	-1.44579100	0.55993300
H	-0.09293300	-0.91624500	-0.64971800
C	-2.53958800	2.68854500	-0.51982100
H	-3.44033800	2.92900300	0.05915400
H	-2.24753600	3.59151300	-1.06377300
H	-2.81966100	1.91321600	-1.24029900
C	-0.37827200	3.02941500	0.69960400
Pd	1.03496600	1.39024300	-0.54602600
H	-0.31830600	4.03328800	0.28587400
H	0.32336100	2.78268100	1.49344200
C	4.31529600	-1.14701900	-0.83707400
C	4.31001400	-0.95087200	0.72349300
B	2.34669100	-0.11139700	-0.18637800
O	2.91190200	-0.91223300	-1.18196100
O	3.20619500	-0.00326800	0.90904500
C	5.57746100	-0.33130800	1.30470200
H	5.46769300	-0.21229700	2.38761100
H	6.44328200	-0.97712200	1.12541100
H	5.78346300	0.65180300	0.87556100
C	3.93976200	-2.22200600	1.49622300
H	4.74915600	-2.95807400	1.46955500
H	3.75213800	-1.96352300	2.54323700
H	3.03664000	-2.69152700	1.09493800
C	5.14163000	-0.08942100	-1.57929400
H	6.21514700	-0.23894800	-1.42994000
H	4.93615900	-0.16265800	-2.65195600
H	4.88254700	0.92241200	-1.25308800
C	4.69970600	-2.54444200	-1.31585900
H	4.65235600	-2.58584100	-2.40903300
H	5.72432200	-2.78975900	-1.01748100
H	4.02951000	-3.31068100	-0.91989700

### 13

Thermal correction to Enthalpy in MeOH at B3LYP/BSI level=0.475202

Thermal correction to Gibbs Free Energy in MeOH at B3LYP/BSI level=0.38792

Sum of electronic and thermal Enthalpies in MeOH at B3LYP/BSI level=-1155.542511

Sum of electronic and thermal Free Energies in MeOH at B3LYP/BSI level=-1155.629793

Sum of electronic Energies in MeOH at M06/BSII level =-1156.7356772

Thermal correction to Enthalpy in AcOH at B3LYP/BSI level=0.475609

Thermal correction to Gibbs Free Energy in AcOH at B3LYP/BSI level=0.388184

Sum of electronic and thermal Enthalpies in AcOH at B3LYP/BSI level=-1155.530371	C	-4.74539800	-2.18858800	-0.66639400			
Sum of electronic and thermal Free Energies in AcOH at B3LYP/BSI level=-1155.617795	H	-5.75710600	-2.26998500	-0.25819600			
Sum of electronic Energies in AcOH at M06/BSII level =-1156.7228896	H	-4.80173100	-2.35024900	-1.74732300			
C	1.18043100	0.19871300	-1.24862500	H	-4.13218300	-2.98649200	-0.23693900
C	0.71094800	1.55765400	-0.95033800	C	-3.74243000	0.90667600	1.53160500
C	2.39420000	-0.39977300	-1.35259400	H	-4.74658800	1.34091400	1.54846500
C	3.82479100	0.01388700	-1.20040000	H	-3.31984400	0.99328200	2.53694500
H	4.45195000	-0.46952500	-1.95706400	H	-3.13905100	1.52389400	0.83960900
H	3.95045100	1.09505400	-1.33418500	C	-4.58775400	-1.36799900	2.12097500
C	4.39900000	-0.30330100	0.17180100	H	-4.23074100	-1.16293200	3.13537700
O	3.75544400	-0.34665300	1.20887600	H	-5.64247400	-1.07888000	2.07253200
O	5.72499600	-0.49050300	0.11976600	H	-4.51473000	-2.44343100	1.94744200
C	6.40697500	-0.73055800	1.38514100				
C	7.88186600	-0.87853900	1.08035200				
H	5.98814100	-1.63397700	1.83824800				
H	6.20796300	0.11382300	2.05163100				
H	8.42948800	-1.05529200	2.01162400				
H	8.06343200	-1.72453900	0.40990400				
H	8.28038200	0.02894500	0.61571100				
C	1.82784400	-1.75568300	-1.72013700				
H	2.02327400	-2.56952100	-1.00933700				
H	2.07561700	-2.11168000	-2.72917900				
C	0.41288100	-1.09236300	-1.56491500				
C	-0.44481800	-1.69253800	-0.43874900				
H	-0.15415200	-1.06146000	-2.50456200				
H	-0.66024000	-2.74259100	-0.70395600				
H	0.15454900	-1.74005000	0.48042100				
C	1.73325100	2.55800200	-0.43735300				
H	2.44824200	2.82132900	-1.22900100				
H	1.24883100	3.48329300	-0.11295900				
H	2.30775100	2.15462900	0.40205600				
C	-0.50897400	2.01677900	-1.48900500				
Pd	-0.97832900	1.30360100	0.45357600				
H	-0.68791700	3.08886800	-1.56024800				
H	-1.06330900	1.40651000	-2.19958000				
C	-3.76080900	-0.56848900	1.11598000				
C	-4.13667600	-0.80703700	-0.40043300				
B	-1.85217500	-1.04704200	-0.11512000				
O	-2.37974300	-1.05005900	1.17796300				
O	-2.83381000	-0.80122000	-1.06558000				
C	-5.00529200	0.28018100	-1.02714000				
H	-5.19222100	0.04110600	-2.07904400				
H	-5.97393700	0.34354600	-0.52081700				
H	-4.52518200	1.26030500	-0.98327900				