

Effect of Alkoxy Substituents on the Regioselectivity of Catalytic C-H Activation in Benzoic Acids: Experimental and DFT Study

Vladimir B. Kharitonov ¹, Dmitry V. Muratov ¹, Yulia V. Nelyubina ¹ and Dmitry A. Loginov

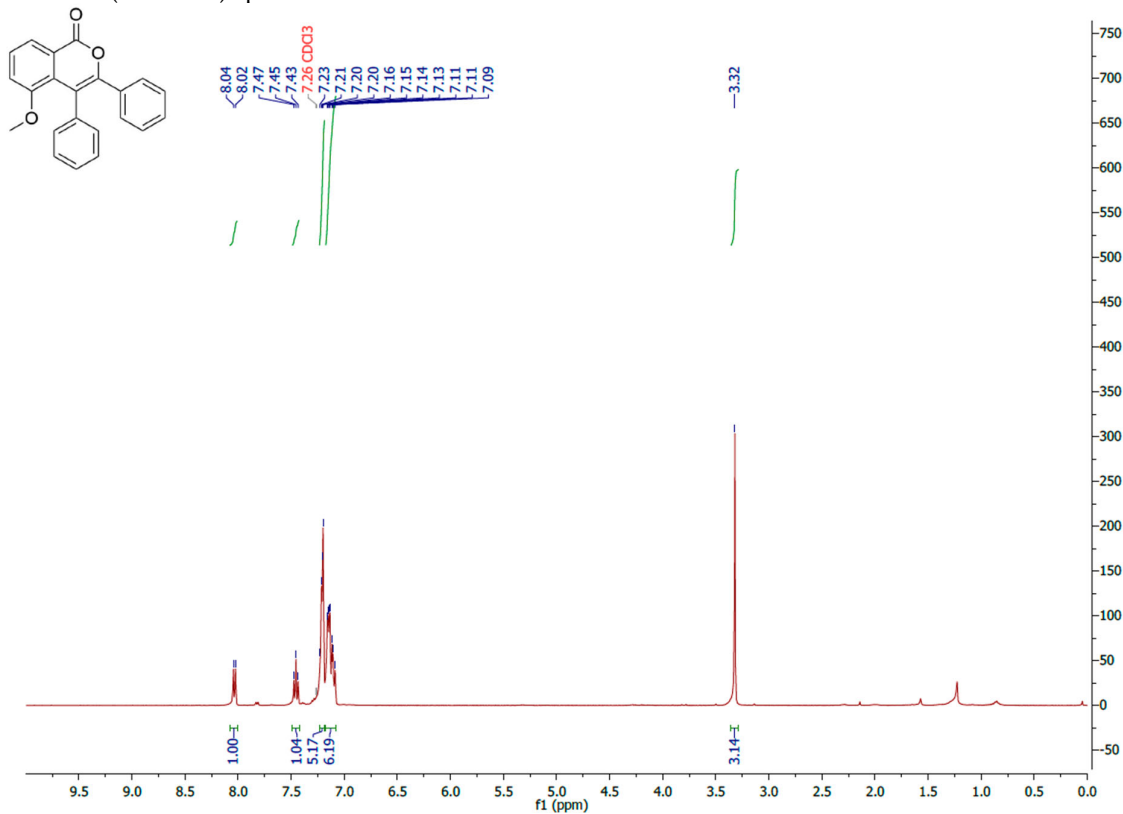
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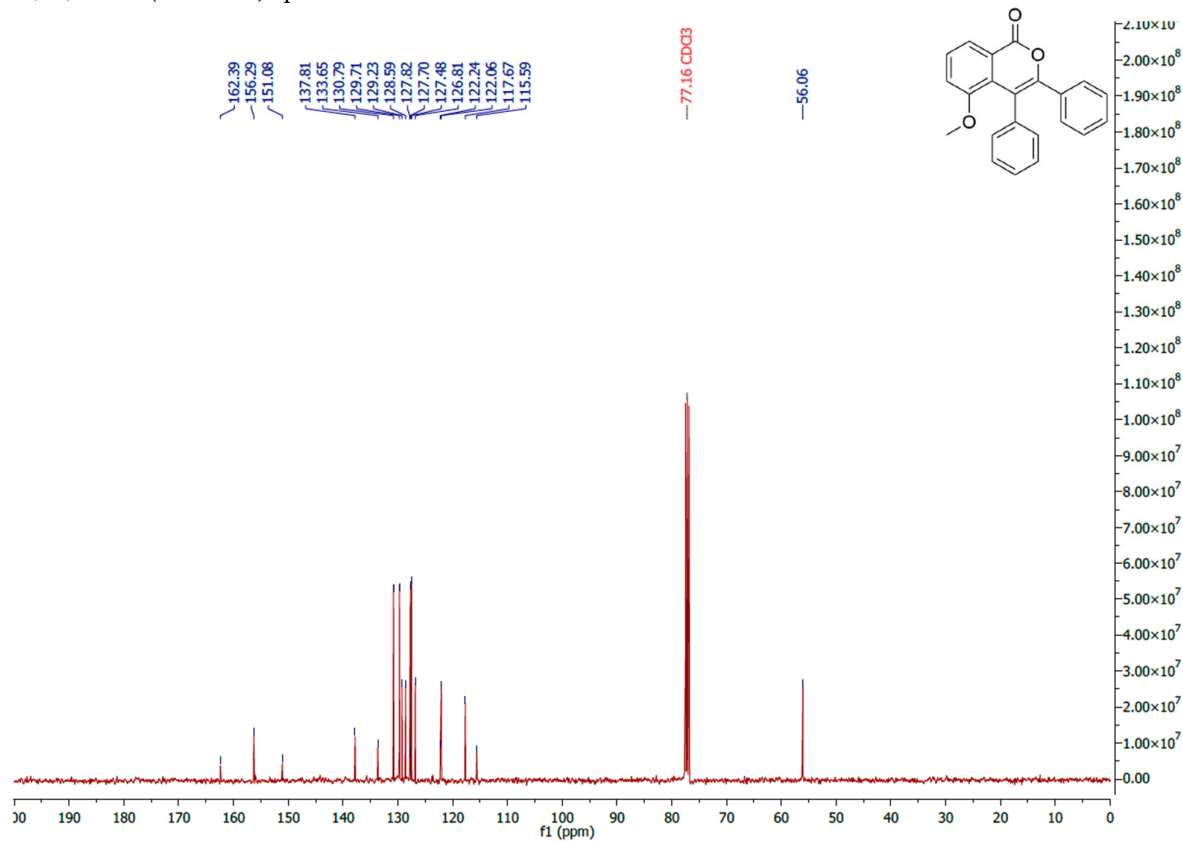
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1. Copies of NMR spectra

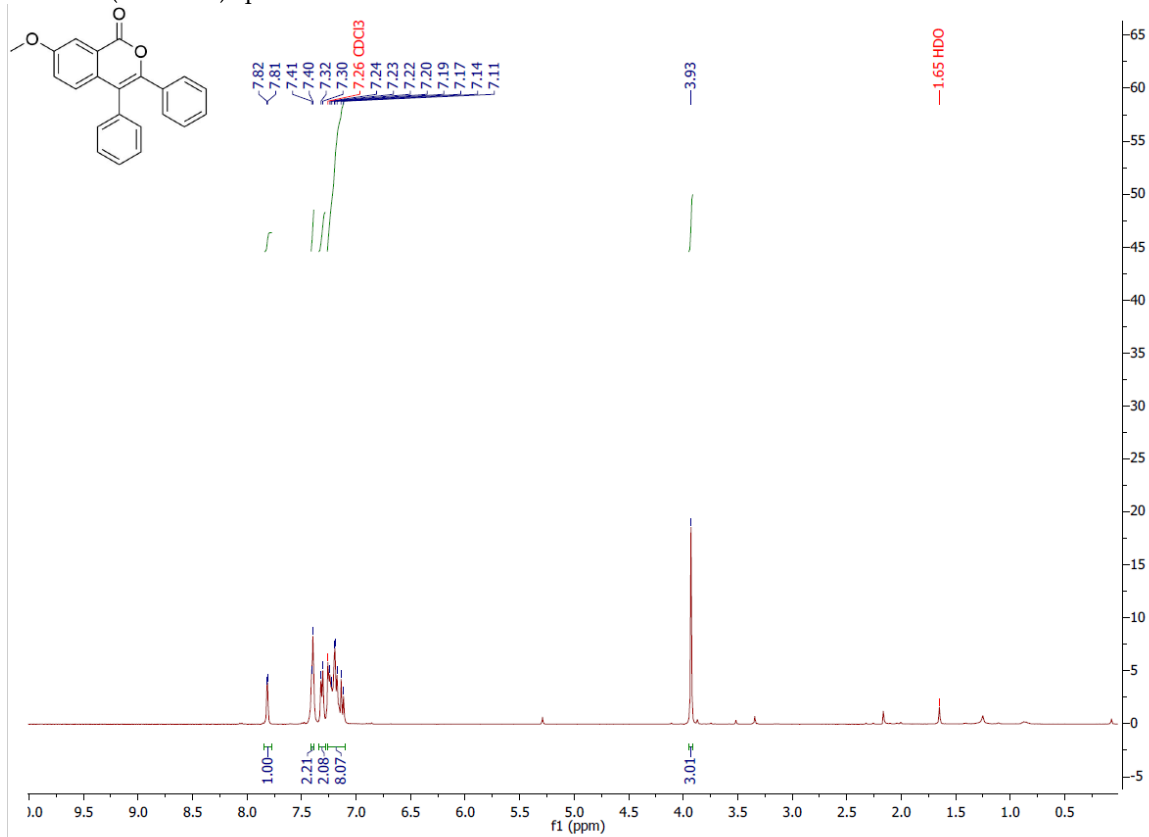
^1H NMR (400 MHz) spectrum of **3aa** in CDCl_3



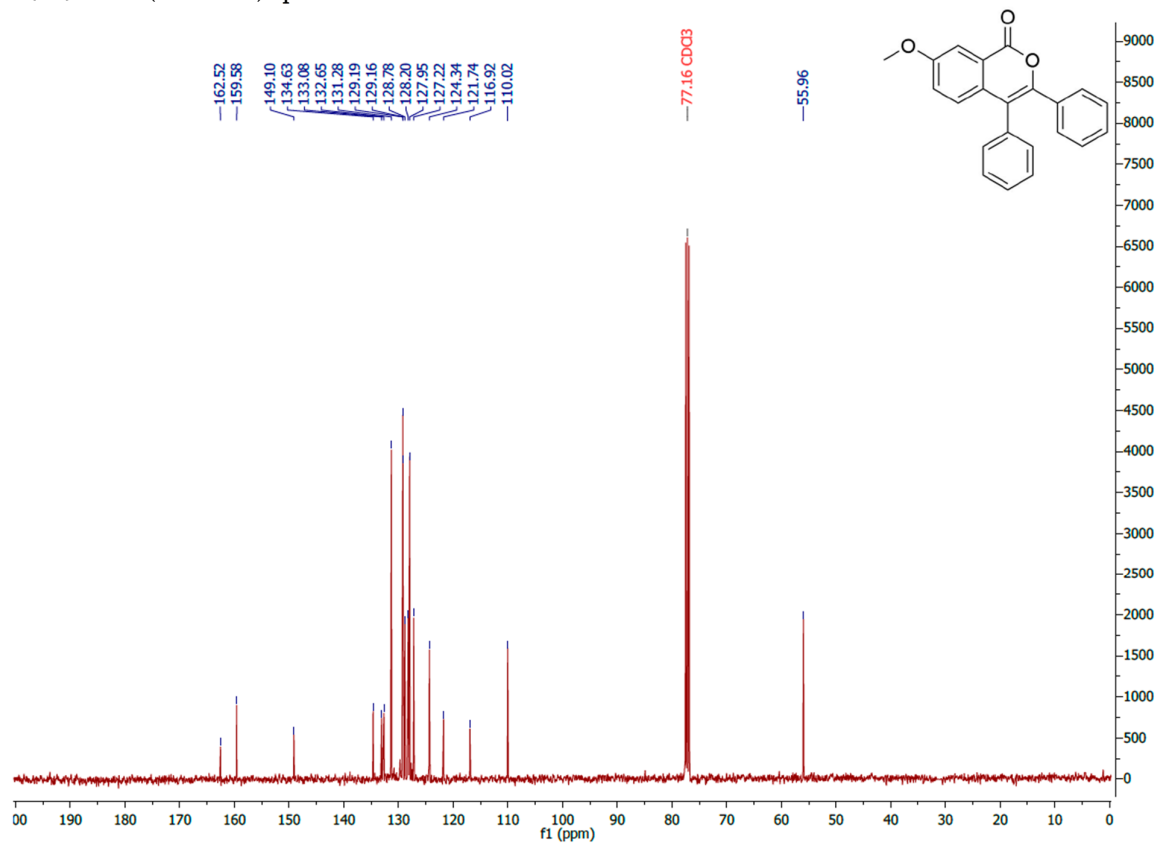
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3aa** in CDCl_3



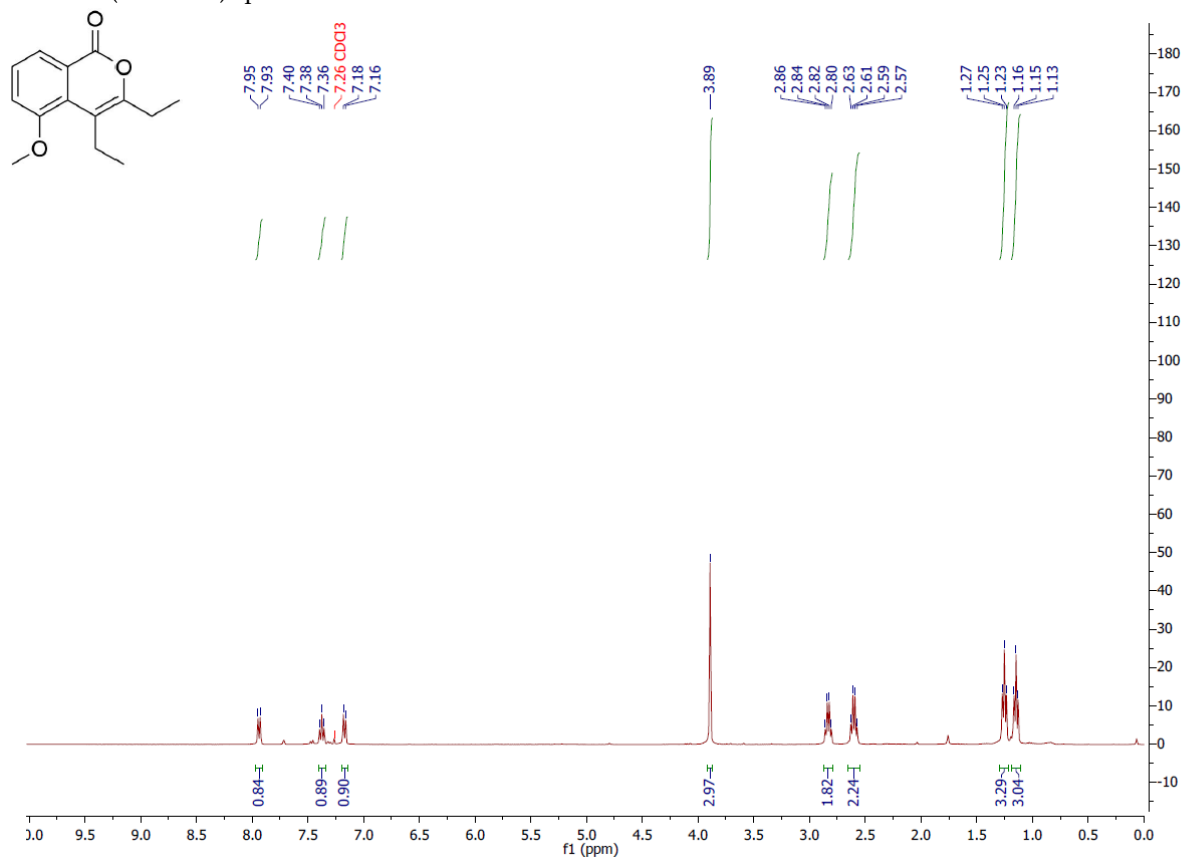
^1H NMR (400 MHz) spectrum of **3aa'** in CDCl_3



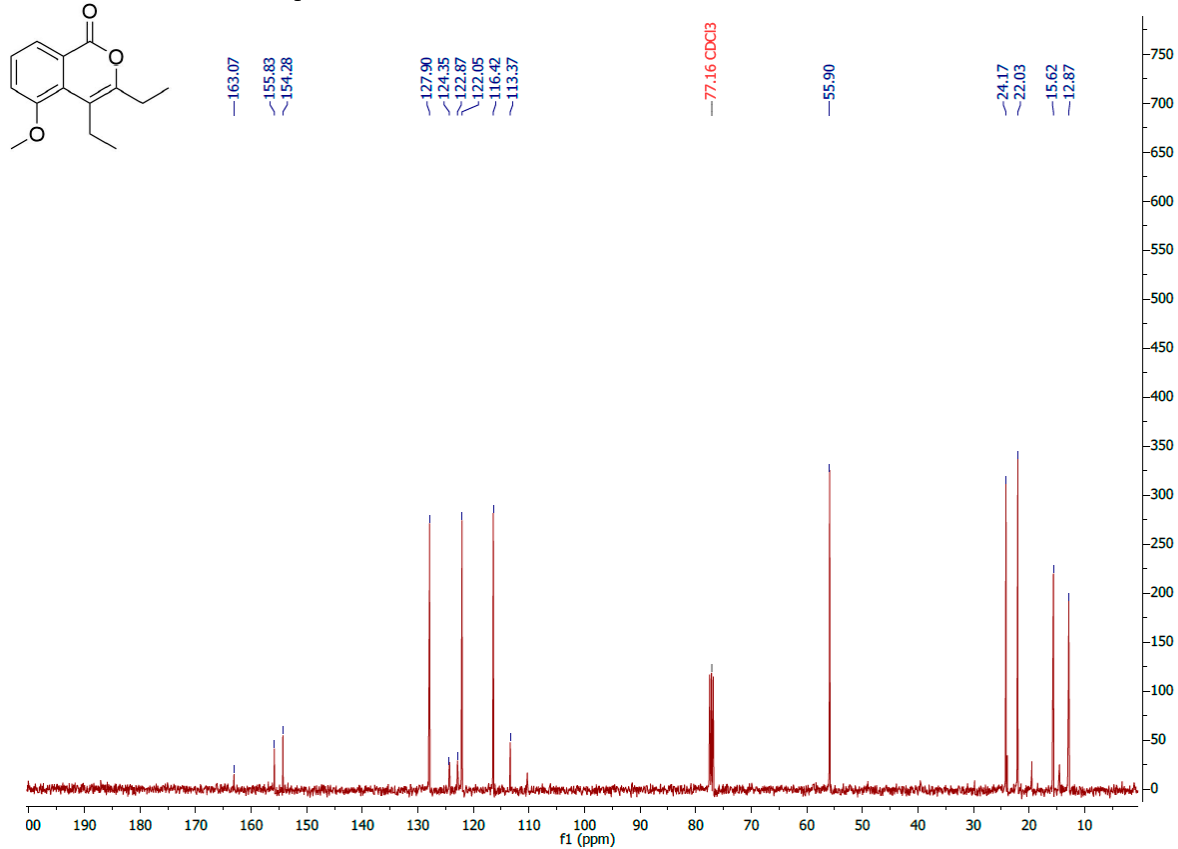
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3aa'** in CDCl_3



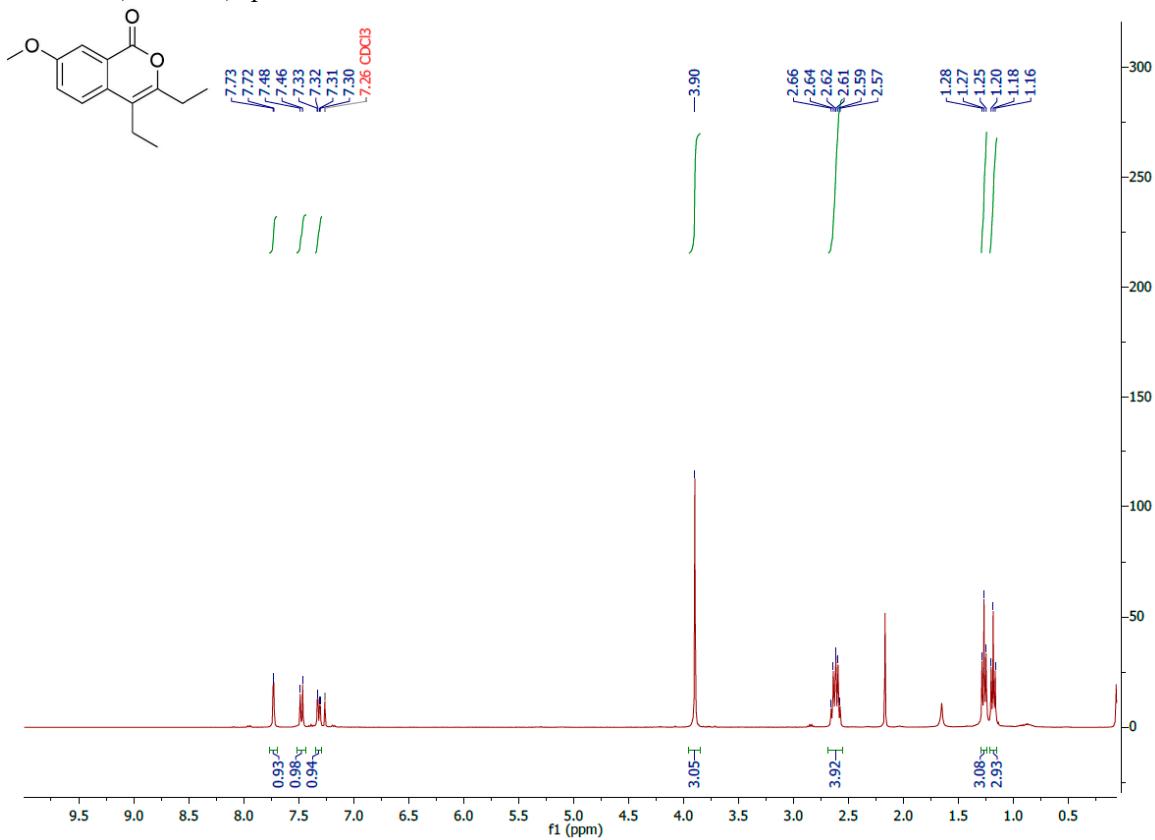
^1H NMR (400 MHz) spectrum of **3ab** in CDCl_3



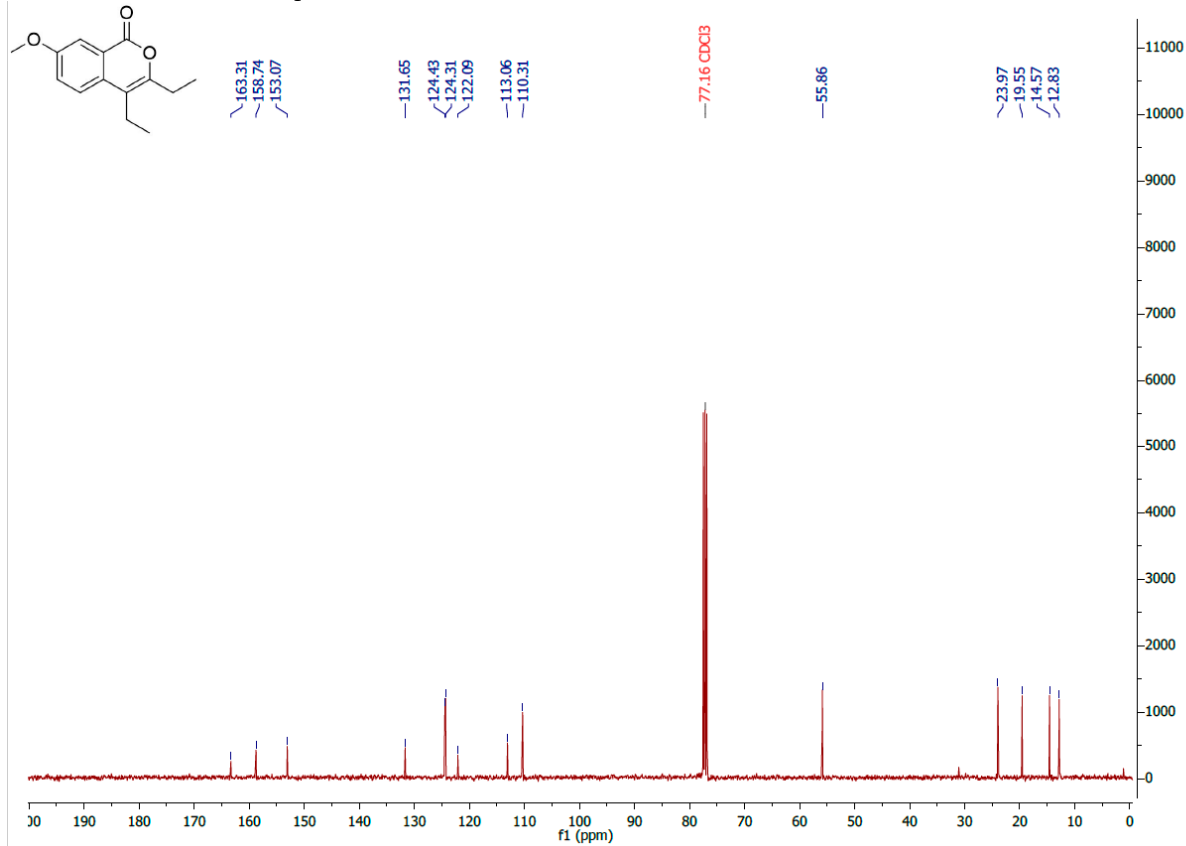
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3ab'** in CDCl_3



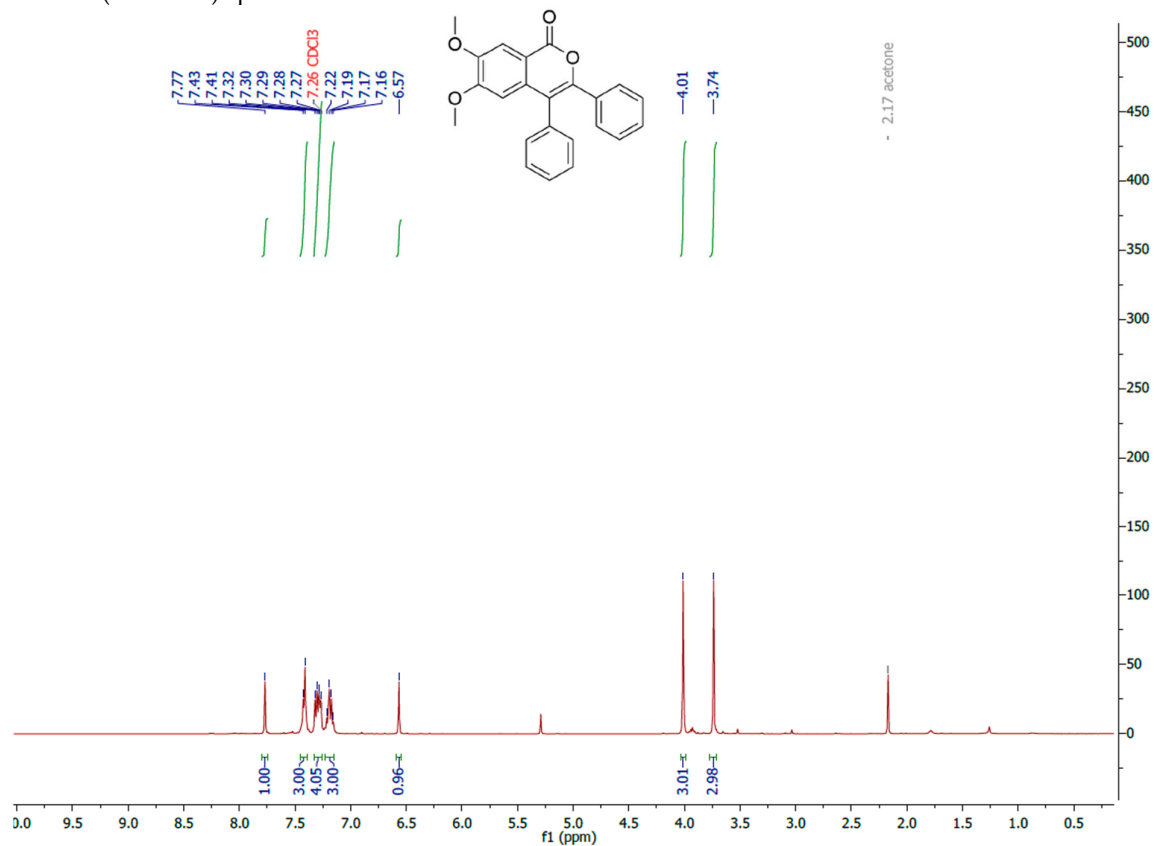
^1H NMR (400 MHz) spectrum of **3ab'** in CDCl_3



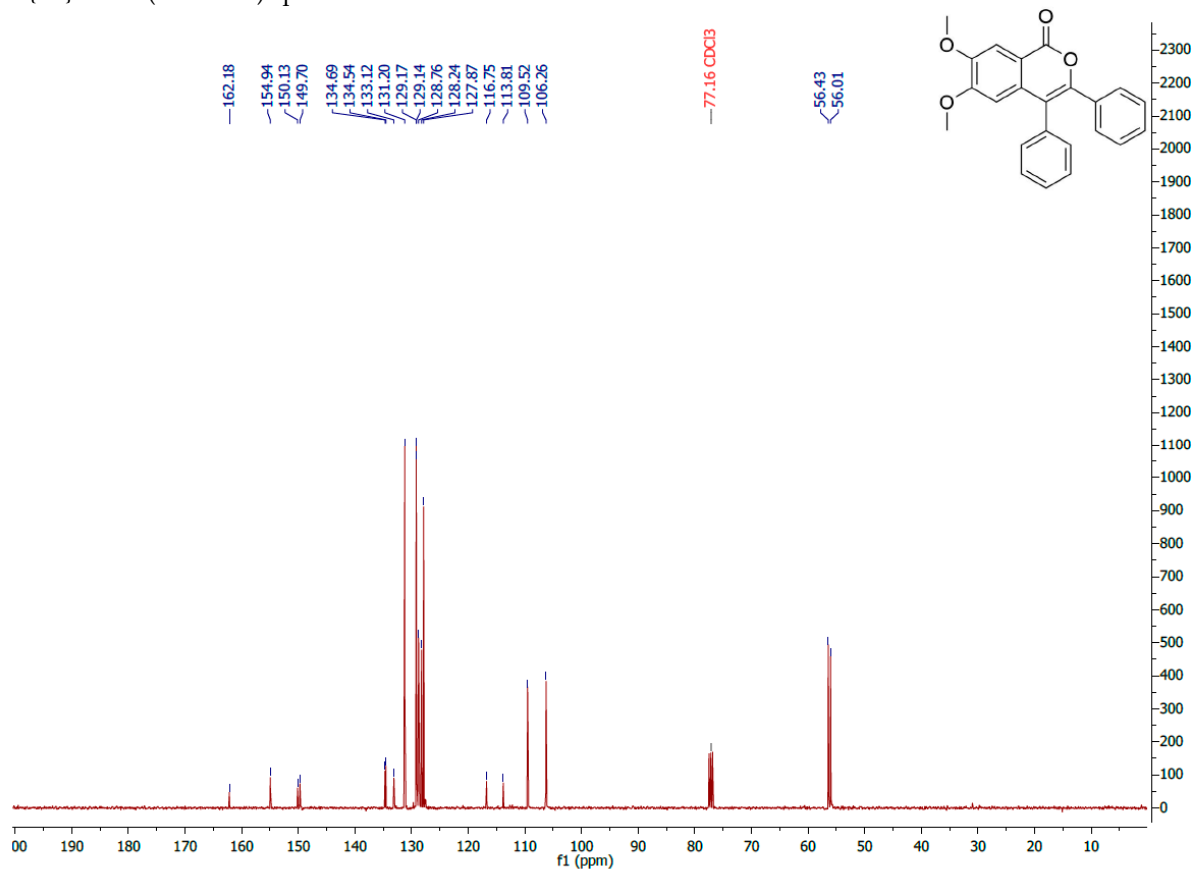
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3ab'** in CDCl_3



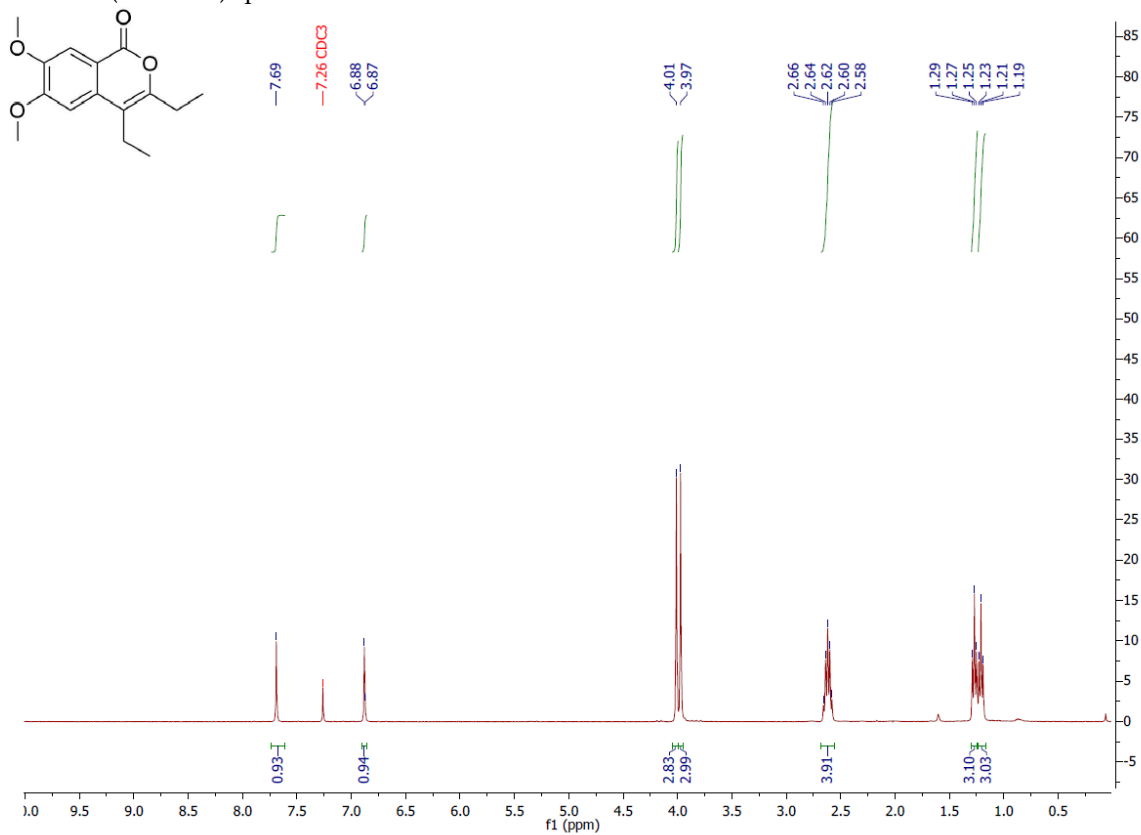
^1H NMR (400 MHz) spectrum of **3ba'** in CDCl_3



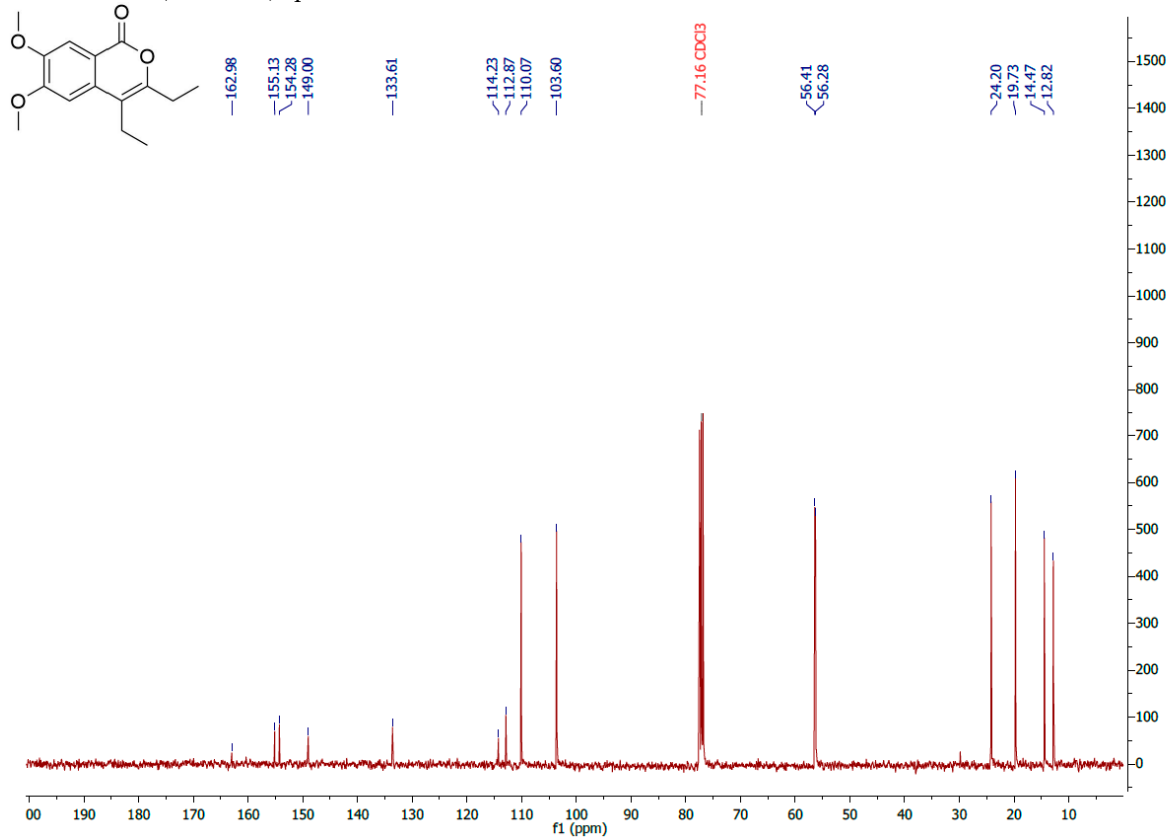
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3ba'** in CDCl_3



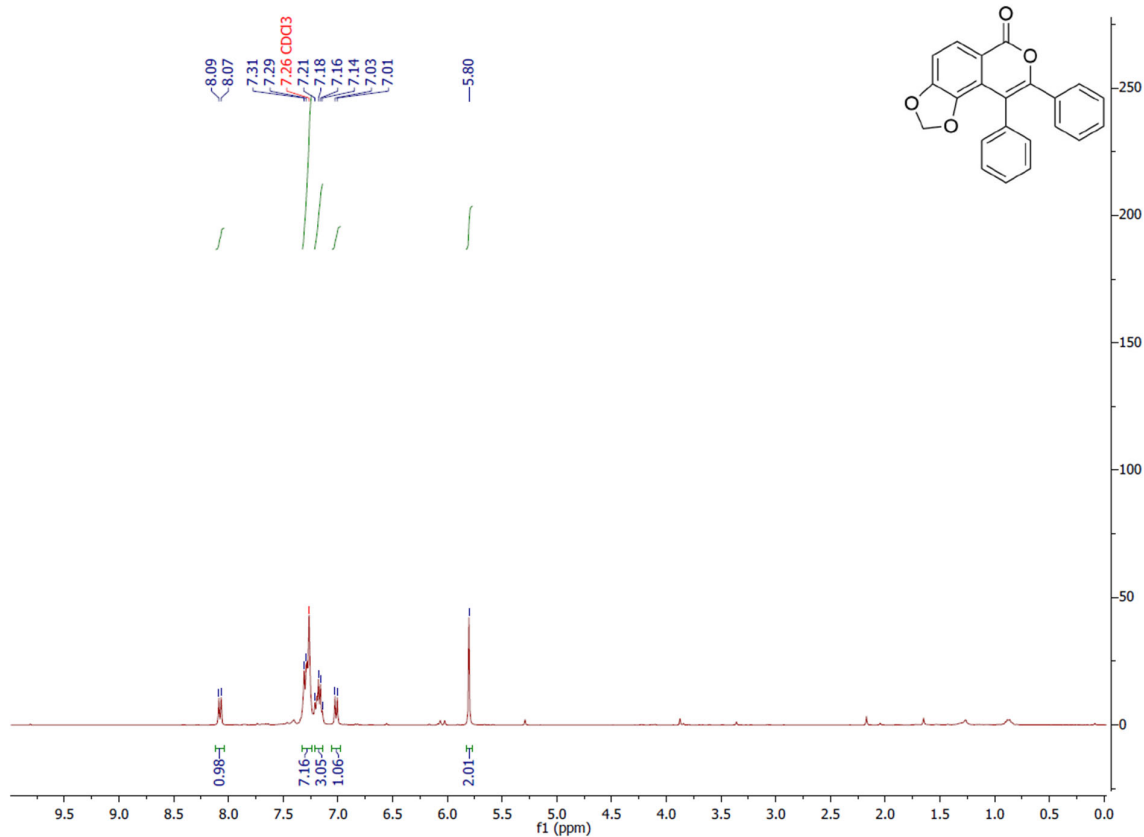
^1H NMR (400 MHz) spectrum of **3bb'** in CDCl_3



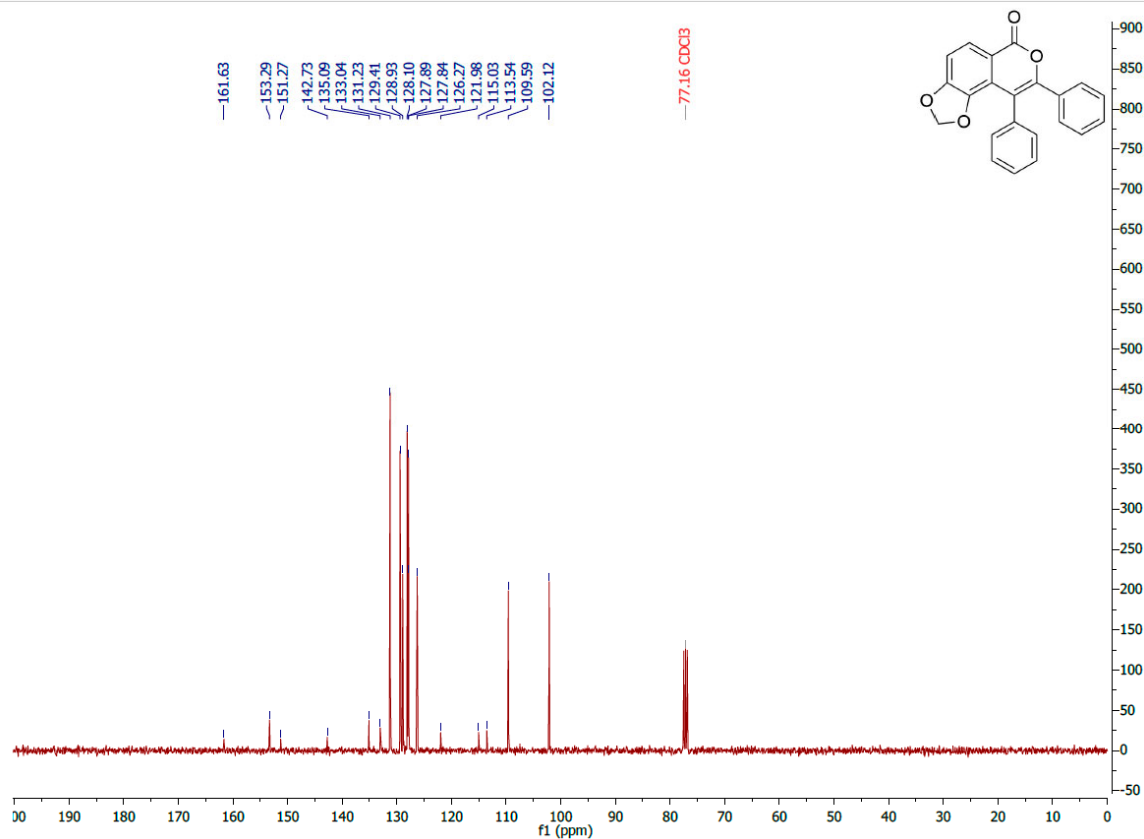
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3bb'** in CDCl_3



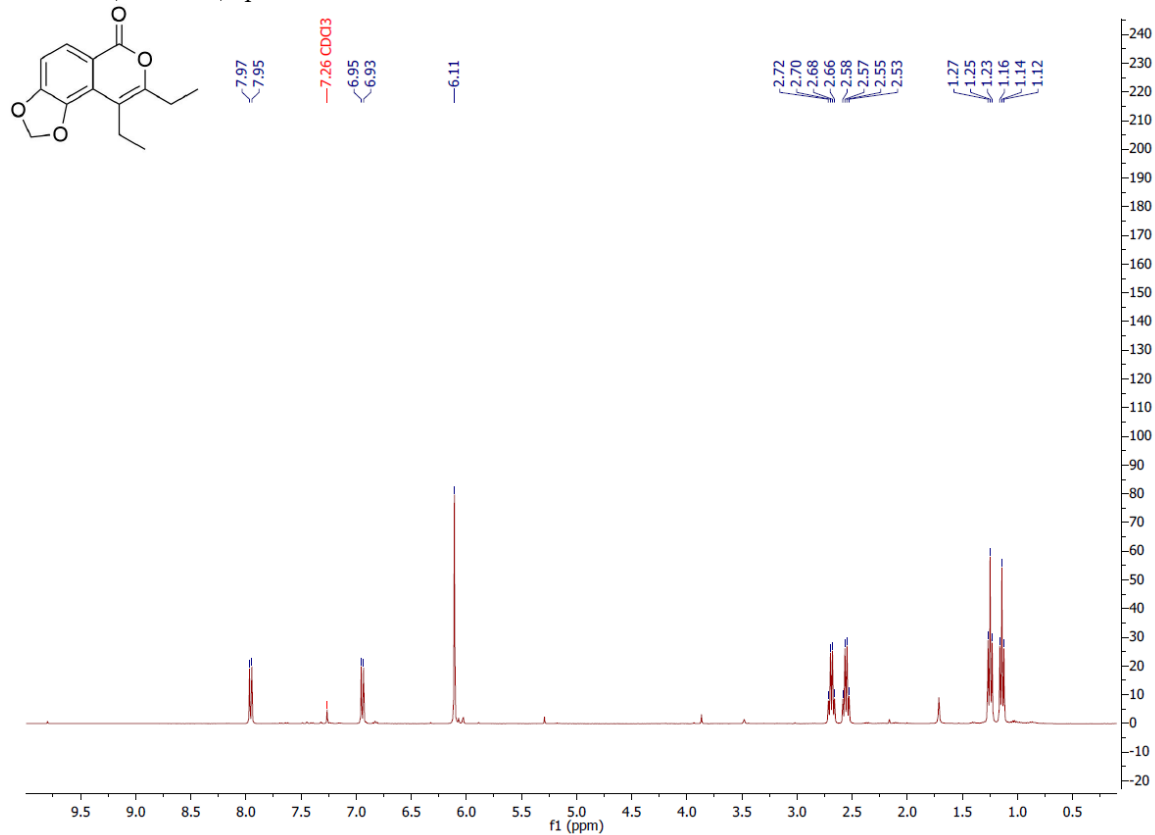
^1H NMR (400 MHz) spectrum of **3ca** in CDCl_3



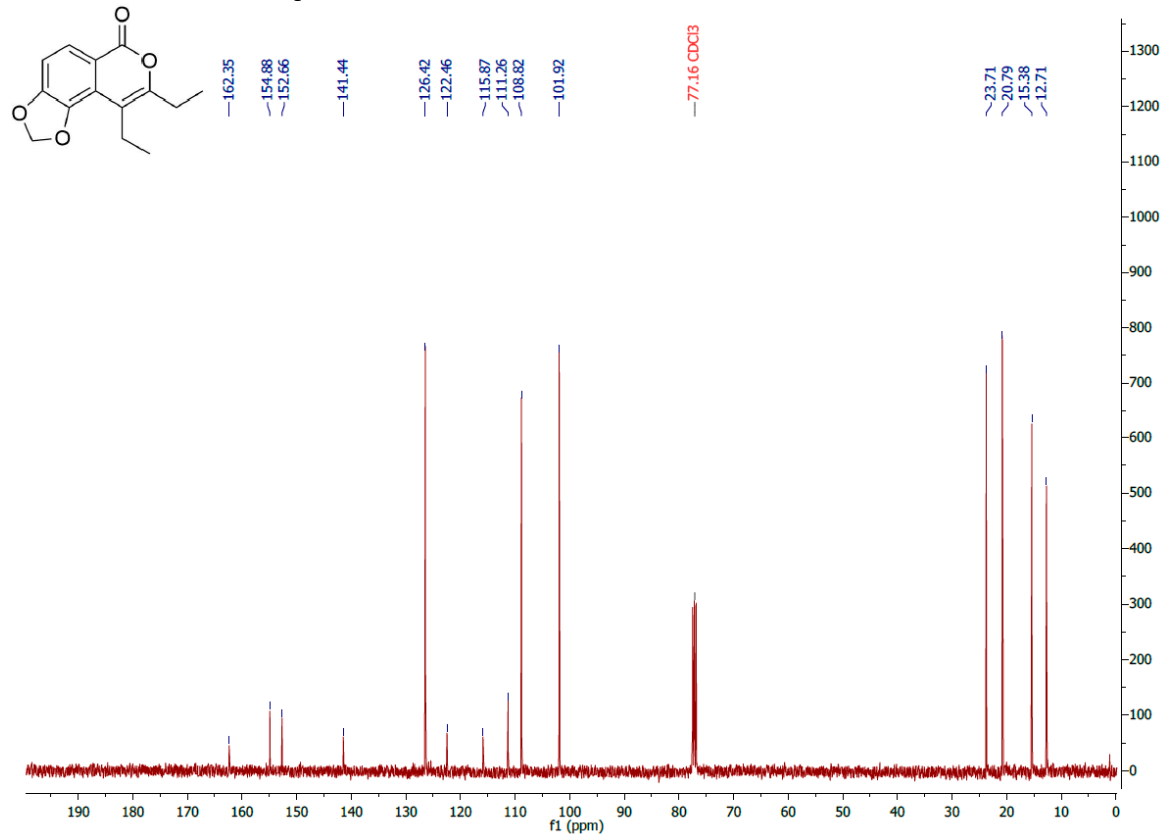
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3ca** in CDCl_3



^1H NMR (400 MHz) spectrum of **3cb** in CDCl_3



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **3cb'** in CDCl_3



2. Calculated energy profiles

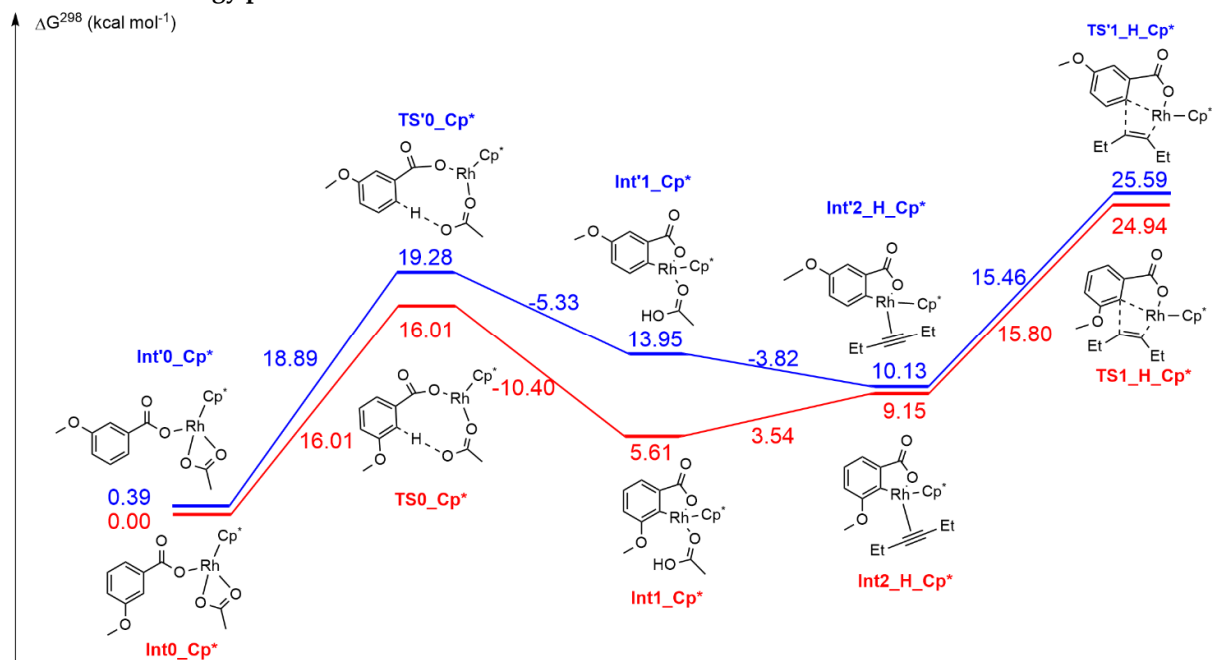


Figure S1. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diethylacetylene catalyzed by $[\text{Cp}^*\text{RhCl}_2]_2$. The calculated Gibbs free energies are given relative to intermediate **Int0_Cp*** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in kcal·mol⁻¹, at 298 K).

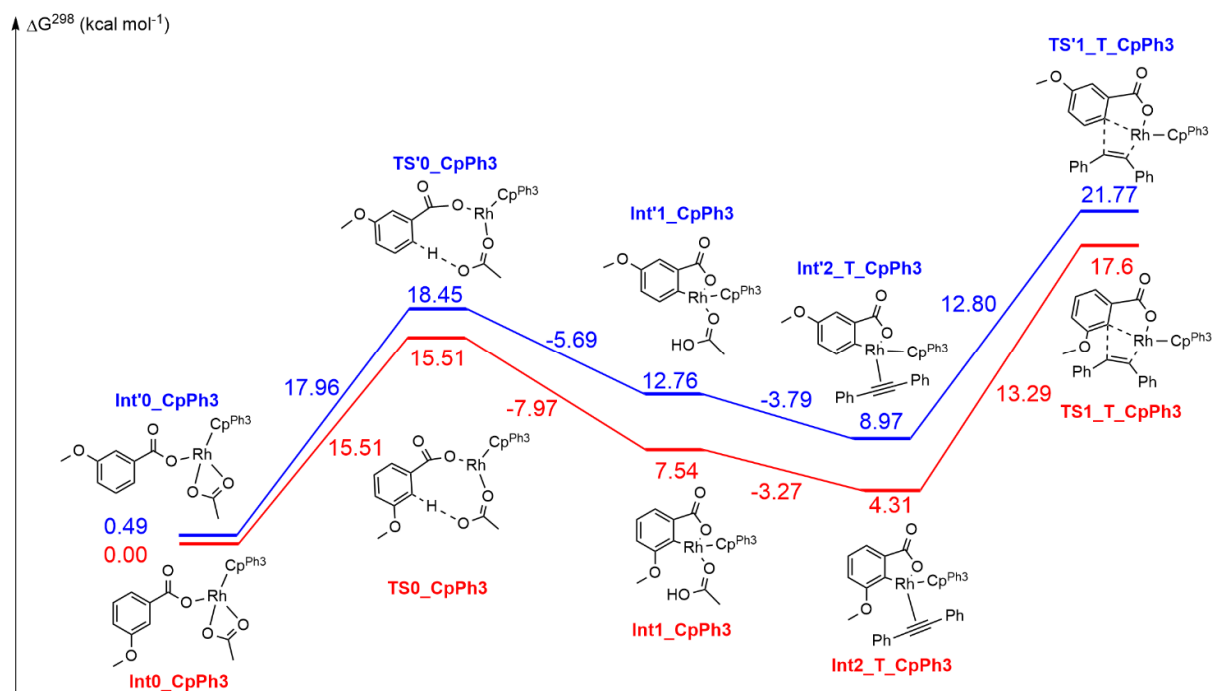


Figure S2. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diphenylacetylene catalyzed by $[\text{Cp}^{\text{Ph}_3}\text{RhI}_2]_2$. The calculated Gibbs free energies are given relative to intermediate **Int0_CpPh3** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in kcal·mol⁻¹, at 298 K).

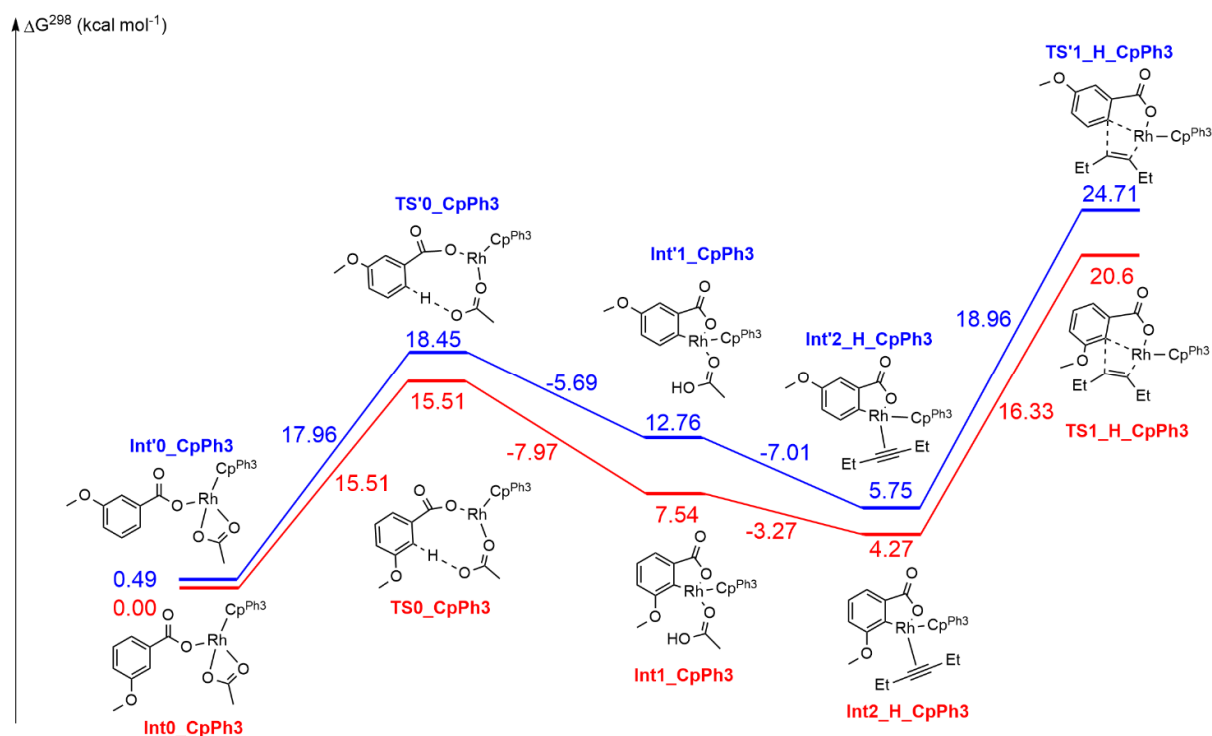


Figure S3. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diethylacetylene catalyzed by $[\text{Cp}^{\text{Ph}_3}\text{RhI}_2]_2$. The calculated Gibbs free energies are given relative to intermediate **Int0_CpPh3** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in $\text{kcal}\cdot\text{mol}^{-1}$, at 298 K).

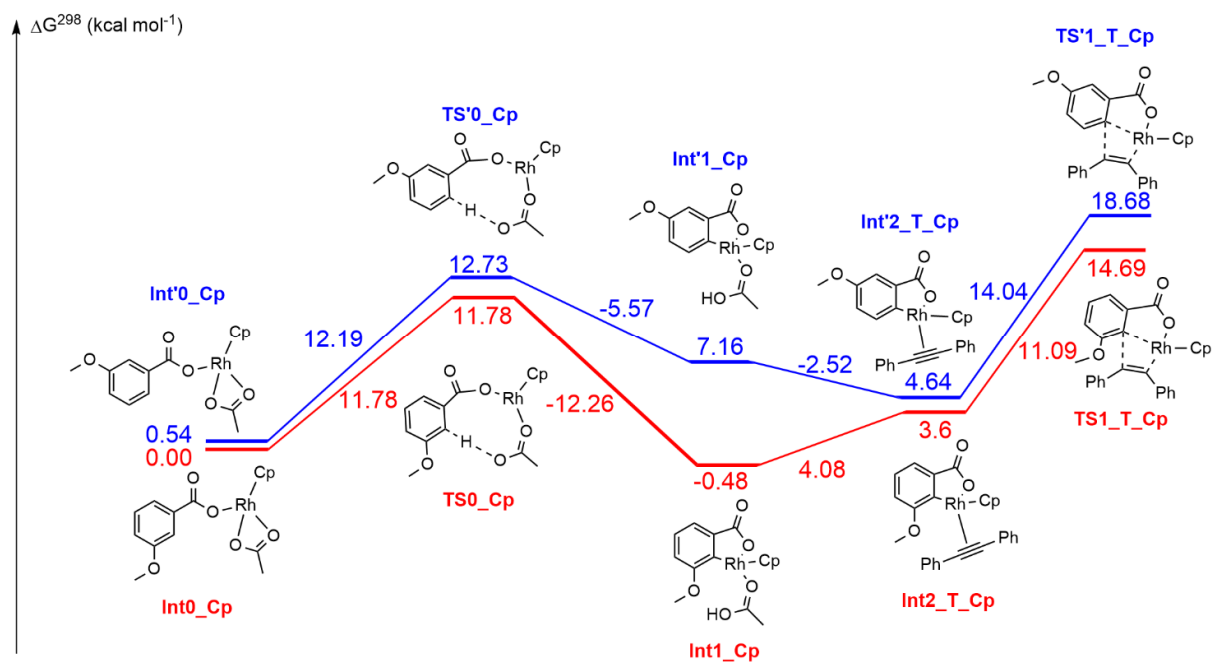


Figure S4. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diphenylacetylene catalyzed by $[\text{CpRhI}_2]_n$. The calculated Gibbs free energies are given relative to intermediate **Int0_Cp** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in $\text{kcal}\cdot\text{mol}^{-1}$, at 298 K).

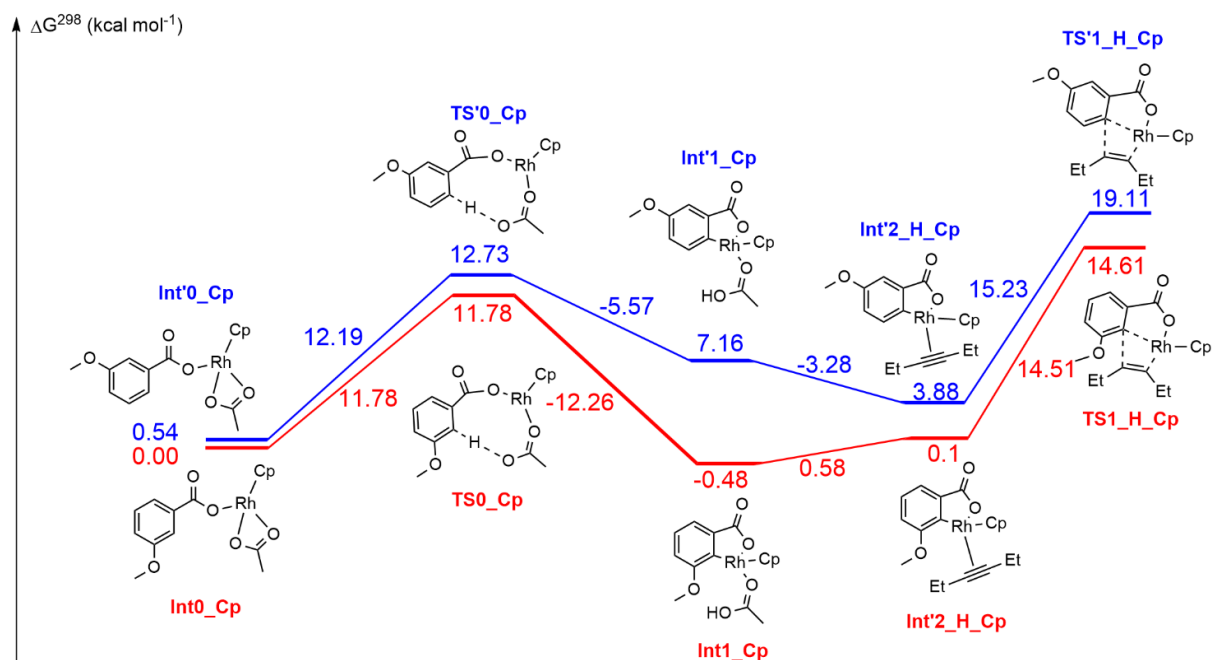


Figure S5. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diethylacetylene catalyzed by $[\text{CpRhI}_2]_n$. The calculated Gibbs free energies are given relative to intermediate **Int0_Cp** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in kcal·mol⁻¹, at 298 K).

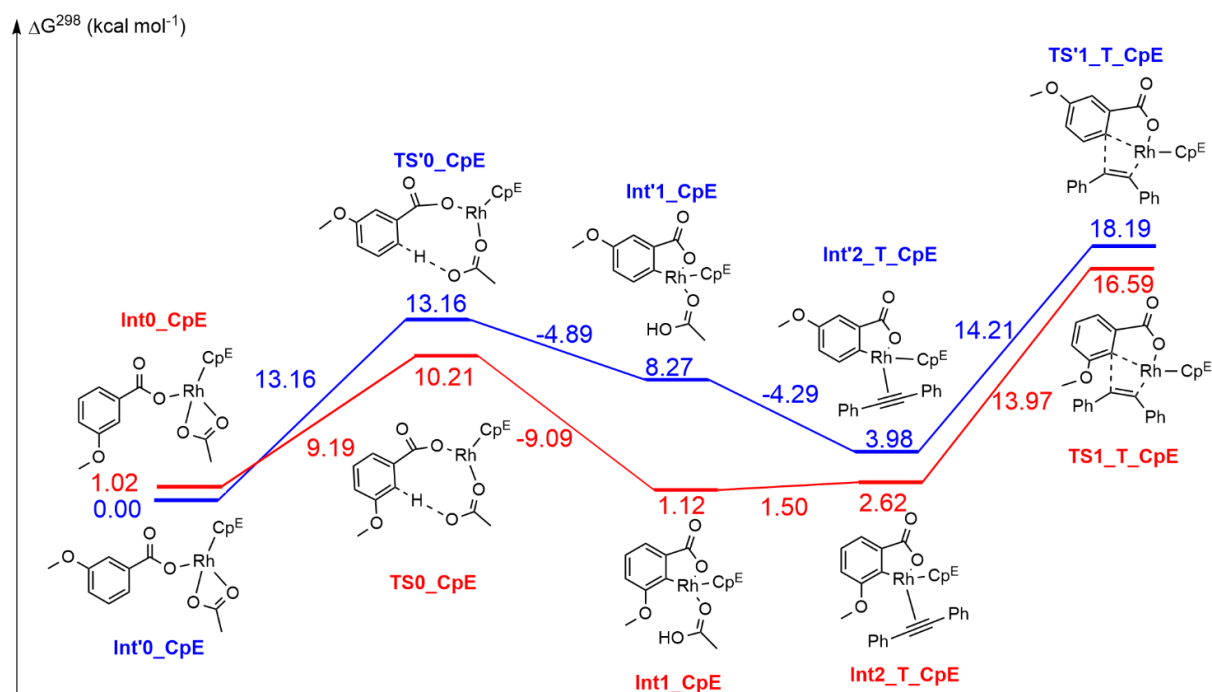


Figure S6. Energy profiles of C-H activation and alkyne insertion steps for the annulation of **1a** with diphenylacetylene catalyzed by $[\text{Cp}^*\text{RhCl}_2]_2$. The calculated Gibbs free energies are given relative to intermediate **Int'0_CpE** at the M06L(D3)/LANL2DZ level with CPCM correction for methanol solvation (in kcal·mol⁻¹, at 298 K).

3. Optimized geometries at the M06L(D3)/LANL2DZ level

AcOH; Gibbs free energy ... -228.99874000 Eh

6	-2.898171000	2.102487000	-4.780182000
8	-3.170532000	3.040446000	-4.006404000
8	-2.609631000	0.833762000	-4.310681000
1	-2.648719000	0.796312000	-3.328086000
6	-2.833797000	2.158932000	-6.272076000
1	-1.838258000	1.869552000	-6.611413000
1	-3.541980000	1.448538000	-6.700568000
1	-3.063245000	3.161768000	-6.620274000

3-Hexyne; Gibbs free energy ... -234.42175293 Eh

6	0.102298000	0.147095000	-1.317254000
6	0.859854000	1.106022000	-1.203494000
6	-0.833148000	-0.977473000	-1.461590000
1	-0.409645000	-1.715731000	-2.150616000
1	-0.941367000	-1.484287000	-0.496844000
6	-2.220218000	-0.539603000	-1.968386000
1	-2.144529000	-0.071936000	-2.952840000
1	-2.674331000	0.179649000	-1.282893000
1	-2.882047000	-1.405003000	-2.047226000
6	1.786389000	2.238731000	-1.068724000
1	1.610491000	2.947659000	-1.884709000
1	1.565259000	2.779851000	-0.142537000
6	3.266014000	1.812080000	-1.071860000
1	3.514633000	1.272835000	-1.988886000
1	3.485994000	1.159635000	-0.223616000
1	3.910292000	2.691723000	-1.005694000

Diphenylacetylene; Gibbs free energy ... -539.16093857 Eh

6	0.049291000	-0.066919000	-2.163337000
6	0.754143000	0.538402000	-1.081822000
6	0.086560000	0.843988000	0.130516000
6	2.132741000	0.845180000	-1.201416000
6	0.780841000	1.441886000	1.188544000
6	2.818406000	1.442957000	-0.137652000
6	2.147321000	1.744533000	1.059953000
1	-0.967413000	0.611623000	0.228709000
1	2.650458000	0.612421000	-2.124563000
1	0.258757000	1.673116000	2.109226000
1	3.872020000	1.673304000	-0.240790000
1	2.680227000	2.211950000	1.879193000
6	-0.559176000	-0.588713000	-3.095526000
6	-1.264027000	-1.194035000	-4.177041000
6	-0.596443000	-1.499620000	-5.389379000
6	-2.642625000	-1.500815000	-4.057448000
6	-1.290722000	-2.097520000	-6.447406000
6	-3.328288000	-2.098594000	-5.121212000
6	-2.657202000	-2.400170000	-6.318815000
1	0.457529000	-1.267254000	-5.487572000
1	-3.160343000	-1.268056000	-3.134300000
1	-0.768638000	-2.328751000	-7.368088000

1	-4.381901000	-2.328943000	-5.018074000
1	-3.190107000	-2.867588000	-7.138056000

Int0_Cp; Gibbs free energy ... -1065.89797110 Eh

45	1.165220000	-0.396720000	-0.244518000
8	2.946564000	0.353533000	0.814439000
6	2.473979000	1.573968000	0.850479000
6	-1.821382000	0.691038000	0.371995000
6	3.160295000	2.664275000	1.595282000
8	1.347348000	1.770285000	0.212321000
6	-1.911883000	-0.391396000	1.258776000
6	-2.897676000	0.983627000	-0.481963000
6	2.069314000	-1.644915000	-1.813154000
6	1.087756000	-2.416478000	-1.068992000
6	-0.202700000	-1.792128000	-1.272182000
6	-0.009058000	-0.623151000	-2.087884000
6	1.403946000	-0.533446000	-2.431148000
6	-3.090636000	-1.162454000	1.316657000
6	-4.152740000	-0.865130000	0.455238000
6	-4.068305000	0.203700000	-0.452609000
1	-3.153562000	-1.988534000	2.014795000
1	-4.900927000	0.419707000	-1.110253000
1	-5.053202000	-1.466744000	0.479152000
1	2.731541000	2.740261000	2.597603000
1	4.223102000	2.451545000	1.692885000
1	3.011652000	3.620229000	1.095247000
6	-0.764477000	-0.734015000	2.155892000
8	-0.963507000	-1.242489000	3.300713000
8	0.475731000	-0.469889000	1.735550000
1	1.284560000	-3.308570000	-0.499589000
1	3.129695000	-1.836642000	-1.832673000
1	1.863589000	0.232413000	-3.031905000
1	-0.772220000	0.083062000	-2.373550000
1	-1.137317000	-2.112521000	-0.839706000
1	-0.933013000	1.314486000	0.341890000
8	-2.700635000	2.065322000	-1.338592000
6	-3.796113000	2.409426000	-2.246545000
1	-4.690478000	2.685306000	-1.681698000
1	-3.437697000	3.259691000	-2.818983000
1	-4.021965000	1.573714000	-2.914517000

Int'0_Cp; Gibbs free energy ... -1065.89711718 Eh

45	1.505884000	0.437578000	-0.175296000
8	3.226389000	-0.877911000	-0.580229000
6	3.025996000	-1.560736000	0.518848000
6	-1.236002000	-0.687031000	1.239304000
6	3.792297000	-2.799995000	0.823561000
8	2.091888000	-1.103849000	1.314223000
6	-1.684098000	-0.874645000	-0.079759000
6	-2.122997000	-0.182577000	2.205150000
6	2.285884000	2.422116000	-0.720523000
6	1.022533000	2.182363000	-1.394875000
6	0.003777000	2.037383000	-0.374267000

6	0.643265000	2.143065000	0.909988000
6	2.062397000	2.386146000	0.698072000
6	-3.017836000	-0.585833000	-0.429407000
6	-3.885926000	-0.068531000	0.543269000
6	-3.440271000	0.138783000	1.863410000
1	-3.340266000	-0.761375000	-1.449199000
1	-4.132635000	0.538036000	2.594384000
1	3.304784000	-3.648449000	0.336792000
1	4.805708000	-2.726058000	0.432185000
1	3.813621000	-2.985831000	1.895588000
6	-0.779399000	-1.416903000	-1.141823000
8	-1.248429000	-2.099147000	-2.103585000
8	0.534474000	-1.200567000	-1.044061000
1	0.867675000	2.149116000	-2.459628000
1	3.242812000	2.535127000	-1.203389000
1	2.806861000	2.516079000	1.464412000
1	0.162590000	2.021810000	1.867167000
1	-1.040018000	1.827973000	-0.545939000
1	-0.217268000	-0.948818000	1.506384000
1	-1.784750000	-0.039327000	3.224302000
8	-5.214774000	0.270724000	0.299319000
6	-5.718506000	0.073165000	-1.060082000
1	-5.151137000	0.678458000	-1.772271000
1	-5.664003000	-0.981610000	-1.342681000
1	-6.754117000	0.399165000	-1.032178000

TS0_Cp; Gibbs free energy ... -1065.87918399 Eh

45	-0.682231000	-0.575605000	-0.330978000
8	-1.982838000	1.116543000	-0.115149000
6	-1.552968000	2.298752000	0.191635000
6	1.170675000	0.378560000	0.213082000
6	-2.529375000	3.429701000	0.305160000
8	-0.287982000	2.544152000	0.411316000
6	1.977879000	0.452751000	-0.957997000
6	1.828200000	0.161997000	1.453966000
6	-2.307783000	-2.129031000	-0.003421000
6	-1.504061000	-2.535099000	-1.107396000
6	-0.129107000	-2.675208000	-0.639445000
6	-0.122396000	-2.399720000	0.778228000
6	-1.453343000	-2.013397000	1.170496000
6	3.371736000	0.386667000	-0.900221000
6	3.989224000	0.199632000	0.349781000
6	3.233219000	0.090630000	1.526187000
1	3.956035000	0.458666000	-1.810378000
1	3.734846000	-0.057281000	2.474643000
1	5.068406000	0.129491000	0.412548000
1	-2.415650000	3.915607000	1.274759000
1	-2.316025000	4.174902000	-0.463097000
1	-3.547560000	3.068648000	0.186916000
1	0.380842000	1.424627000	0.313135000
6	1.227692000	0.624976000	-2.237214000
8	1.770477000	0.990786000	-3.320478000
8	-0.087208000	0.377705000	-2.138860000

1	-1.839877000	-2.667540000	-2.122646000
1	-3.358162000	-1.889339000	-0.037576000
1	-1.766705000	-1.734540000	2.162441000
1	0.744127000	-2.413882000	1.419021000
1	0.717212000	-2.980859000	-1.232219000
8	0.994924000	0.065017000	2.554315000
6	1.610354000	-0.103981000	3.876308000
1	2.249107000	0.749516000	4.114457000
1	0.775852000	-0.155990000	4.568500000
1	2.189796000	-1.029703000	3.909775000

TS'0_Cp; Gibbs free energy ... -1065.87769695 Eh

45	1.261582000	-0.449414000	0.086952000
8	2.445475000	1.315202000	-0.241483000
6	1.929090000	2.425970000	-0.656188000
6	-0.657739000	0.299117000	-0.564505000
6	2.807276000	3.624546000	-0.844695000
8	0.654185000	2.541721000	-0.929328000
6	-1.464557000	0.444862000	0.601563000
6	-1.313990000	-0.099374000	-1.761959000
6	2.958471000	-1.966249000	0.282686000
6	1.863908000	-2.380943000	1.096814000
6	0.694578000	-2.556518000	0.250213000
6	1.110016000	-2.301272000	-1.116994000
6	2.484943000	-1.892485000	-1.093361000
6	-2.849714000	0.278379000	0.583144000
6	-3.463037000	-0.100895000	-0.626807000
6	-2.693330000	-0.291205000	-1.797179000
1	-3.413018000	0.425447000	1.498386000
1	-3.199878000	-0.579987000	-2.709909000
1	2.444142000	4.447386000	-0.227482000
1	3.835181000	3.391514000	-0.579592000
1	2.760895000	3.949869000	-1.885228000
1	0.075973000	1.401669000	-0.767261000
6	-0.740521000	0.791172000	1.859002000
8	-1.312304000	1.228656000	2.899488000
8	0.585633000	0.609036000	1.789539000
1	1.876074000	-2.478938000	2.170414000
1	3.952619000	-1.726885000	0.621394000
1	3.072730000	-1.601849000	-1.948274000
1	0.481532000	-2.352290000	-1.990507000
1	-0.277873000	-2.892254000	0.570803000
1	-0.739136000	-0.222546000	-2.673579000
8	-4.820600000	-0.315600000	-0.767738000
6	-5.668865000	-0.125803000	0.415073000
1	-5.369952000	-0.809552000	1.212624000
1	-5.609168000	0.907858000	0.763442000
1	-6.675916000	-0.353765000	0.080710000

Int1_Cp; Gibbs free energy ... -1065.89872987 Eh

45	0.922662000	-0.509890000	-0.082410000
8	0.850583000	0.397263000	1.894102000
6	0.659111000	1.627010000	2.144327000

6	-1.070796000	-0.219615000	-0.259082000
6	0.810158000	2.185981000	3.517407000
8	0.310415000	2.534028000	1.218961000
6	-1.877242000	-1.287523000	0.175157000
6	-1.704126000	0.913564000	-0.793023000
6	3.152896000	-0.031746000	-0.641867000
6	2.873451000	-1.350161000	-1.048124000
6	1.713938000	-1.312161000	-1.944622000
6	1.363637000	0.077310000	-2.152154000
6	2.189899000	0.868100000	-1.284293000
6	-3.276907000	-1.256264000	0.031154000
6	-3.877668000	-0.136275000	-0.554449000
6	-3.096434000	0.963741000	-0.959214000
1	-3.865536000	-2.100962000	0.373554000
1	-3.576523000	1.836016000	-1.387612000
1	-4.951877000	-0.097375000	-0.687541000
1	-0.163210000	2.519950000	3.881430000
1	1.212180000	1.436168000	4.191680000
1	1.462093000	3.059321000	3.493681000
1	0.062858000	2.200588000	0.288606000
6	-1.153054000	-2.406292000	0.829995000
8	-1.718791000	-3.430125000	1.319699000
8	0.176021000	-2.229034000	0.890947000
1	3.376708000	-2.243388000	-0.715940000
1	3.907496000	0.272015000	0.066091000
1	2.171175000	1.942439000	-1.193927000
1	0.571846000	0.446714000	-2.782198000
1	1.278551000	-2.158206000	-2.450782000
8	-0.844188000	1.996283000	-1.093787000
6	-1.445866000	3.223471000	-1.627830000
1	-1.919656000	3.019077000	-2.589128000
1	-2.176186000	3.629417000	-0.923219000
1	-0.618103000	3.915784000	-1.754106000

Int'1_Cp; Gibbs free energy ... -1065.88657076 Eh

45	1.356274000	-0.360966000	0.116784000
8	1.033634000	1.691374000	0.857852000
6	0.789290000	2.686745000	0.117166000
6	-0.606098000	-0.322928000	-0.421838000
6	0.495376000	4.048930000	0.631405000
8	0.770343000	2.587638000	-1.235062000
6	-1.493889000	-0.482056000	0.662694000
6	-1.149760000	-0.129848000	-1.708711000
6	3.679489000	-0.425323000	-0.305090000
6	3.308042000	-1.627122000	0.321834000
6	2.244628000	-2.248559000	-0.474920000
6	2.056799000	-1.440765000	-1.662498000
6	2.875187000	-0.269471000	-1.521693000
6	-2.889121000	-0.433050000	0.497262000
6	-3.407039000	-0.230103000	-0.789033000
6	-2.538767000	-0.082678000	-1.890009000
1	-3.522358000	-0.556420000	1.369980000
1	-2.965087000	0.064368000	-2.875754000

1	-0.527723000	4.322015000	0.366662000
1	0.610997000	4.076239000	1.710196000
1	1.158654000	4.776089000	0.163112000
1	0.953317000	1.658621000	-1.536228000
6	-0.879939000	-0.722439000	1.990782000
8	-1.536760000	-0.865549000	3.066317000
8	0.459574000	-0.788999000	1.964945000
1	3.680165000	-2.000703000	1.261942000
1	4.392088000	0.293713000	0.065663000
1	2.982407000	0.522826000	-2.245793000
1	1.378850000	-1.654084000	-2.472259000
1	1.782241000	-3.201741000	-0.277544000
1	-0.508094000	-0.012805000	-2.577241000
8	-4.770511000	-0.163420000	-1.083925000
6	-5.697955000	-0.338810000	0.033172000
1	-5.572726000	-1.325854000	0.486994000
1	-5.545950000	0.436507000	0.789276000
1	-6.689582000	-0.247139000	-0.400358000

Int2_T_Cp: Gibbs free energy ... -1376.05441992 Eh

45	0.489890000	-1.079275000	-0.165103000
6	-1.319279000	-0.787484000	0.758668000
6	-1.242724000	-0.524713000	2.136195000
6	-2.585299000	-0.780768000	0.137279000
6	1.769157000	-1.826829000	-1.954688000
6	2.016613000	-2.693232000	-0.859048000
6	0.750600000	-3.299084000	-0.469978000
6	-0.258820000	-2.835003000	-1.383353000
6	0.347550000	-1.876115000	-2.266120000
6	-2.393742000	-0.256414000	2.904261000
6	-3.640329000	-0.251672000	2.275136000
6	-3.742331000	-0.515518000	0.895736000
1	-2.287980000	-0.056517000	3.965372000
1	-4.717774000	-0.504147000	0.422323000
1	-4.539720000	-0.039193000	2.840761000
6	0.114858000	-0.539281000	2.723988000
8	0.372271000	-0.318137000	3.945900000
8	1.089253000	-0.818567000	1.842335000
6	0.177858000	1.166678000	-0.531714000
6	1.400179000	0.902473000	-0.330993000
1	-1.303678000	-3.093146000	-1.366356000
1	0.610446000	-4.021550000	0.317576000
1	2.966831000	-2.854371000	-0.375922000
1	2.495668000	-1.195989000	-2.442537000
1	-0.150174000	-1.341901000	-3.059013000
8	-2.615248000	-1.038211000	-1.234436000
6	-3.904792000	-0.944742000	-1.912637000
1	-4.606355000	-1.687876000	-1.522490000
1	-4.329989000	0.058108000	-1.803023000
1	-3.690229000	-1.147093000	-2.959007000
6	-1.039958000	1.923989000	-0.617434000
6	-1.438813000	2.697765000	0.499791000
6	-1.837497000	1.926755000	-1.783207000

6	-2.606585000	3.466959000	0.442211000
6	-3.003879000	2.700208000	-1.833101000
6	-3.392888000	3.471146000	-0.723242000
1	-0.829578000	2.686879000	1.397216000
1	-1.543569000	1.319255000	-2.631709000
1	-2.903027000	4.056581000	1.301392000
1	-3.610829000	2.697267000	-2.730701000
1	-4.297638000	4.065692000	-0.763992000
6	2.807699000	1.190195000	-0.229755000
6	3.720308000	0.258049000	0.309833000
6	3.282950000	2.445867000	-0.683560000
6	5.081462000	0.572258000	0.394031000
6	4.645978000	2.751062000	-0.597153000
6	5.549860000	1.816893000	-0.060893000
1	3.343029000	-0.692335000	0.671762000
1	2.583179000	3.162027000	-1.098950000
1	5.775286000	-0.147559000	0.811224000
1	5.004331000	3.710377000	-0.951094000
1	6.604582000	2.057031000	-0.000476000

Int'2_T_Cp; Gibbs free energy ... -1376.05279225 Eh

45	0.763944000	-1.005219000	-0.630609000
6	-1.178430000	-0.952088000	0.012419000
6	-1.328872000	-1.047620000	1.412097000
6	-2.319978000	-0.766987000	-0.779711000
6	2.483473000	-1.339677000	-2.199052000
6	2.321710000	-2.535775000	-1.461482000
6	0.948918000	-2.999397000	-1.629619000
6	0.291519000	-2.092813000	-2.537516000
6	1.212153000	-1.032219000	-2.840626000
6	-2.585988000	-0.926580000	2.021244000
6	-3.714790000	-0.711918000	1.218570000
6	-3.588584000	-0.649669000	-0.183608000
1	-2.677977000	-0.989802000	3.100850000
1	-4.456144000	-0.492357000	-0.814347000
6	-0.092936000	-1.283871000	2.188770000
8	-0.041734000	-1.409359000	3.449216000
8	1.011496000	-1.375649000	1.428722000
6	0.439427000	1.277226000	-0.428665000
6	1.575130000	0.938822000	0.012450000
1	-0.722761000	-2.172430000	-2.892148000
1	0.535968000	-3.908977000	-1.225029000
1	3.064062000	-3.002350000	-0.832940000
1	3.371381000	-0.728938000	-2.240309000
1	1.016220000	-0.187539000	-3.481573000
6	-0.767700000	1.984431000	-0.742723000
6	-1.627090000	2.388525000	0.306671000
6	-1.128712000	2.260482000	-2.081026000
6	-2.820938000	3.058514000	0.018040000
6	-2.321555000	2.937961000	-2.360392000
6	-3.172805000	3.335475000	-1.314456000
1	-1.357334000	2.160097000	1.332092000
1	-0.477401000	1.941897000	-2.887254000

1	-3.475485000	3.357965000	0.828185000
1	-2.588029000	3.152309000	-3.388323000
1	-4.098397000	3.853255000	-1.535447000
6	2.873435000	1.169386000	0.591297000
6	3.797967000	0.124951000	0.806375000
6	3.228557000	2.494210000	0.948878000
6	5.054026000	0.398137000	1.360643000
6	4.486041000	2.758862000	1.502118000
6	5.403678000	1.713815000	1.708713000
1	3.514827000	-0.890425000	0.548003000
1	2.517433000	3.296581000	0.788799000
1	5.758461000	-0.409031000	1.521301000
1	4.750103000	3.775183000	1.769206000
1	6.376764000	1.920337000	2.137857000
1	-2.244433000	-0.673110000	-1.858019000
8	-4.929014000	-0.566828000	1.897191000
6	-6.105357000	-0.238414000	1.093729000
1	-5.944403000	0.690427000	0.536856000
1	-6.341618000	-1.048964000	0.398696000
1	-6.912585000	-0.110768000	1.809134000

Int2_H_Cp; Gibbs free energy ... -1071.32081084 Eh

45	-0.634039000	-0.555049000	-0.466695000
6	1.220250000	0.288368000	-0.477008000
6	1.326984000	1.488867000	-1.200238000
6	2.367166000	-0.208930000	0.175786000
6	-2.046864000	-2.367059000	-0.091341000
6	-2.076135000	-2.081920000	-1.478449000
6	-0.716757000	-2.210037000	-1.991715000
6	0.127481000	-2.634634000	-0.907806000
6	-0.671163000	-2.667234000	0.287071000
6	2.544554000	2.193881000	-1.291777000
6	3.671541000	1.684780000	-0.643221000
6	3.588772000	0.486169000	0.092011000
1	2.579977000	3.116636000	-1.861258000
1	4.472084000	0.108201000	0.594465000
1	4.619034000	2.207794000	-0.695927000
6	0.084392000	1.965062000	-1.848935000
8	-0.008384000	3.034414000	-2.526094000
8	-0.970403000	1.155848000	-1.662824000
6	-0.696545000	0.515402000	1.554680000
6	-1.795631000	0.715174000	0.973596000
6	-3.151798000	1.160247000	0.609462000
1	-3.122852000	1.582048000	-0.400037000
1	-3.816331000	0.289926000	0.567526000
6	0.329530000	0.531601000	2.615841000
1	1.233292000	1.029375000	2.247188000
1	0.623760000	-0.497015000	2.847962000
1	1.187375000	-2.817726000	-0.958473000
1	-0.413526000	-2.074170000	-3.017351000
1	-2.939578000	-1.788144000	-2.053300000
1	-2.884117000	-2.315923000	0.586686000
1	-0.325787000	-2.933207000	1.272840000

6	-3.699181000	2.196825000	1.607569000
1	-3.742792000	1.783470000	2.618183000
1	-3.069946000	3.089442000	1.627677000
1	-4.708586000	2.492378000	1.313942000
6	-0.189344000	1.242089000	3.877994000
1	-1.090274000	0.754537000	4.258658000
1	0.574034000	1.213936000	4.658436000
1	-0.429122000	2.287134000	3.666977000
8	2.208675000	-1.392740000	0.903995000
6	3.318968000	-1.807346000	1.757938000
1	4.200968000	-2.060835000	1.163155000
1	3.568560000	-1.016844000	2.473306000
1	2.961255000	-2.688376000	2.284564000

Int'2_H_Cp; Gibbs free energy ... -1071.31481578 Eh

45	1.052066000	-0.663352000	0.038155000
6	-0.971584000	-0.421128000	-0.065552000
6	-1.562072000	0.074064000	1.118937000
6	-1.801359000	-0.694131000	-1.163424000
6	3.130537000	-1.591396000	-0.568482000
6	2.627371000	-2.326175000	0.529307000
6	1.330515000	-2.882055000	0.157751000
6	1.077969000	-2.518196000	-1.214418000
6	2.150727000	-1.663898000	-1.645232000
6	-2.941272000	0.302936000	1.211651000
6	-3.757200000	0.022019000	0.106316000
6	-3.190220000	-0.480863000	-1.082063000
1	-3.367805000	0.686986000	2.132825000
1	-3.808811000	-0.707653000	-1.942625000
6	-0.647283000	0.316146000	2.256726000
8	-1.002665000	0.780534000	3.382344000
8	0.627282000	-0.017672000	2.001714000
6	0.981425000	1.402909000	-0.928739000
6	1.865412000	1.442659000	-0.034625000
6	2.917838000	1.851553000	0.910949000
1	2.613027000	1.561678000	1.921449000
1	3.836227000	1.296844000	0.689197000
6	0.138572000	1.815300000	-2.067282000
1	-0.911667000	1.830278000	-1.757539000
1	0.211736000	1.062305000	-2.860229000
1	0.216110000	-2.797652000	-1.797517000
1	0.718388000	-3.523804000	0.770117000
1	3.091153000	-2.425650000	1.497793000
1	4.047557000	-1.025021000	-0.593510000
1	2.249548000	-1.209370000	-2.618347000
6	3.187736000	3.365983000	0.847544000
1	3.508289000	3.665941000	-0.153148000
1	2.291644000	3.934626000	1.105915000
1	3.978104000	3.627010000	1.554389000
6	0.556386000	3.196729000	-2.599406000
1	1.602884000	3.195139000	-2.913997000
1	-0.061563000	3.467394000	-3.458069000
1	0.431822000	3.963184000	-1.830635000

1	-1.388363000	-1.057171000	-2.098886000
8	-5.122744000	0.271938000	0.276636000
6	-5.999291000	-0.001257000	-0.860363000
1	-5.714709000	0.604354000	-1.725480000
1	-5.971844000	-1.061722000	-1.127064000
1	-6.995757000	0.273110000	-0.525846000

TS2_T_Cp; Gibbs free energy ... -1376.03674349 Eh

45	0.440218000	-1.237495000	-0.496642000
6	-1.233333000	-0.744583000	0.665878000
6	-1.131660000	-1.184251000	2.008734000
6	-2.529815000	-0.526819000	0.130150000
6	1.491335000	-1.328521000	-2.535092000
6	1.721078000	-2.554423000	-1.845811000
6	0.428346000	-3.213299000	-1.647051000
6	-0.579697000	-2.379815000	-2.204458000
6	0.060034000	-1.175438000	-2.697547000
6	-2.265137000	-1.291912000	2.829340000
6	-3.529717000	-1.015487000	2.294603000
6	-3.667564000	-0.653258000	0.942363000
1	-2.141660000	-1.618115000	3.856456000
1	-4.654883000	-0.475272000	0.532606000
6	0.211303000	-1.616366000	2.462752000
8	0.512270000	-1.841791000	3.674863000
8	1.090437000	-1.795936000	1.467819000
6	-0.066014000	0.818700000	0.248126000
6	1.212867000	0.540636000	0.208300000
1	-1.641586000	-2.561450000	-2.197095000
1	0.280954000	-4.172791000	-1.178602000
1	2.677864000	-2.946802000	-1.539626000
1	2.238635000	-0.602908000	-2.815010000
1	-0.443181000	-0.344988000	-3.166736000
1	-4.414823000	-1.095302000	2.913799000
8	-2.575518000	-0.181638000	-1.213967000
6	-3.841777000	0.334605000	-1.737397000
1	-4.615984000	-0.436426000	-1.711095000
1	-4.161574000	1.208524000	-1.161078000
1	-3.629133000	0.615974000	-2.765397000
6	-0.922459000	1.966865000	-0.054191000
6	-0.634862000	2.727589000	-1.209714000
6	-1.966035000	2.373721000	0.801931000
6	-1.388034000	3.869795000	-1.507970000
6	-2.713186000	3.521445000	0.502770000
6	-2.431414000	4.267717000	-0.654609000
1	0.171424000	2.410275000	-1.863880000
1	-2.178581000	1.800125000	1.698301000
1	-1.163433000	4.445238000	-2.397995000
1	-3.510058000	3.831874000	1.168047000
1	-3.017132000	5.148680000	-0.888515000
6	2.551164000	1.029936000	0.374827000
6	3.670457000	0.262248000	-0.025488000
6	2.764649000	2.320470000	0.929526000
6	4.965809000	0.775430000	0.102830000

6	4.062640000	2.824893000	1.055176000
6	5.167628000	2.058496000	0.640449000
1	3.506466000	-0.732233000	-0.429787000
1	1.912535000	2.911927000	1.246518000
1	5.815316000	0.179072000	-0.207724000
1	4.214833000	3.811864000	1.475769000
1	6.170413000	2.455810000	0.741813000

TS'2_T_Cp; Gibbs free energy ... -1376.03040921 Eh

45	0.567690000	-1.148211000	-0.682982000
6	-1.258912000	-0.424381000	0.068529000
6	-1.562795000	-0.975248000	1.341853000
6	-2.325302000	0.019726000	-0.741004000
6	2.038395000	-1.314508000	-2.432951000
6	1.948869000	-2.586279000	-1.796296000
6	0.574363000	-3.069341000	-1.942845000
6	-0.164223000	-2.090733000	-2.659284000
6	0.714403000	-0.964224000	-2.907994000
6	-2.874665000	-1.006797000	1.820866000
6	-3.920844000	-0.547595000	1.003657000
6	-3.648113000	-0.053181000	-0.289538000
1	-3.083875000	-1.428549000	2.798145000
1	-4.449263000	0.280674000	-0.937718000
6	-0.456181000	-1.631421000	2.079864000
8	-0.515948000	-1.961614000	3.302979000
8	0.615517000	-1.893528000	1.322265000
6	0.229801000	0.936987000	0.064564000
6	1.412038000	0.439416000	0.328142000
1	-1.211754000	-2.136018000	-2.909423000
1	0.200379000	-4.011676000	-1.576470000
1	2.752968000	-3.117927000	-1.312987000
1	2.913387000	-0.685669000	-2.483205000
1	0.448226000	-0.059231000	-3.431654000
6	-0.329740000	2.210129000	-0.389704000
6	0.331799000	2.903868000	-1.428999000
6	-1.468680000	2.785091000	0.212192000
6	-0.148184000	4.145622000	-1.865145000
6	-1.937631000	4.032301000	-0.219515000
6	-1.284445000	4.711623000	-1.263388000
1	1.207592000	2.456779000	-1.889482000
1	-1.972101000	2.258226000	1.015867000
1	0.358533000	4.666346000	-2.668739000
1	-2.807599000	4.472476000	0.252789000
1	-1.657919000	5.669823000	-1.604397000
6	2.717277000	0.646053000	0.883501000
6	3.743368000	-0.313284000	0.711254000
6	3.000625000	1.834627000	1.607906000
6	5.021297000	-0.088666000	1.233601000
6	4.280419000	2.049148000	2.129897000
6	5.295635000	1.092178000	1.944677000
1	3.515737000	-1.229620000	0.174655000
1	2.219059000	2.573231000	1.749559000
1	5.797269000	-0.831737000	1.094713000

1	4.490147000	2.958656000	2.680420000
1	6.283304000	1.262187000	2.356184000
1	-2.124978000	0.438751000	-1.722178000
8	-5.198129000	-0.641709000	1.547308000
6	-6.324695000	-0.236910000	0.704591000
1	-6.258221000	0.824714000	0.453021000
1	-6.355184000	-0.835879000	-0.209221000
1	-7.209430000	-0.426850000	1.305067000

TS2_H_Cp; Gibbs free energy ... -1071.29767934 Eh

45	-0.846872000	-0.359409000	-0.302276000
6	1.148520000	0.293010000	-0.313718000
6	1.385955000	1.354114000	-1.220224000
6	2.246253000	-0.525847000	0.059580000
6	-2.441811000	-1.871618000	0.330276000
6	-2.616236000	-1.567231000	-1.051410000
6	-1.423244000	-2.019438000	-1.772685000
6	-0.521927000	-2.569565000	-0.823088000
6	-1.115429000	-2.427128000	0.495254000
6	2.680492000	1.656382000	-1.671535000
6	3.755089000	0.862381000	-1.253291000
6	3.539920000	-0.239009000	-0.403170000
1	2.820098000	2.482213000	-2.360621000
1	4.380455000	-0.859035000	-0.114396000
6	0.185531000	2.061261000	-1.727530000
8	0.231499000	3.159077000	-2.367145000
8	-0.965729000	1.423458000	-1.490309000
6	0.199429000	0.940750000	1.292080000
6	-1.090783000	1.047561000	1.202094000
6	-2.334836000	1.600305000	1.794325000
1	-2.733021000	0.859871000	2.499449000
1	-2.070121000	2.485410000	2.384634000
6	1.321768000	1.177217000	2.258099000
1	2.133126000	1.714956000	1.753766000
1	1.734795000	0.212764000	2.572636000
1	0.463846000	-2.957795000	-1.020055000
1	-1.270976000	-1.947327000	-2.837286000
1	-3.484899000	-1.113333000	-1.501154000
1	-3.142406000	-1.661706000	1.122512000
1	-0.668596000	-2.747883000	1.422307000
6	0.824768000	1.967635000	3.475109000
1	0.028437000	1.429872000	3.996778000
1	1.646889000	2.127445000	4.175950000
1	0.435218000	2.943814000	3.175009000
6	-3.423762000	1.956327000	0.773586000
1	-3.083030000	2.738349000	0.091768000
1	-3.687513000	1.080475000	0.172585000
1	-4.321652000	2.307195000	1.287467000
1	4.760376000	1.077347000	-1.594754000
8	1.943594000	-1.592080000	0.902304000
6	3.062646000	-2.385928000	1.411665000
1	3.582607000	-2.890593000	0.593211000
1	3.763223000	-1.752843000	1.964480000

1	2.613855000	-3.117531000	2.077577000
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TS'2_H_Cp; Gibbs free energy ... -1071.29054845 Eh

45	1.165314000	-0.702356000	0.034072000
6	-0.824987000	-0.032080000	-0.185041000
6	-1.436271000	0.211179000	1.076089000
6	-1.659682000	-0.373347000	-1.271735000
6	2.974079000	-1.559672000	-1.058750000
6	2.951088000	-2.098413000	0.260506000
6	1.732065000	-2.900789000	0.391407000
6	1.023642000	-2.848437000	-0.837286000
6	1.746905000	-1.955345000	-1.722578000
6	-2.824811000	0.196978000	1.223439000
6	-3.636085000	-0.117783000	0.120357000
6	-3.051054000	-0.428992000	-1.124895000
1	-1.223606000	-0.584490000	-2.242849000
1	-3.269750000	0.388640000	2.194125000
1	-3.663065000	-0.703781000	-1.975463000
6	-0.535773000	0.371313000	2.244343000
8	-0.911894000	0.823784000	3.369920000
8	0.716765000	-0.040851000	2.023006000
6	0.456081000	1.350472000	-0.691277000
6	1.605425000	1.314595000	-0.079605000
6	2.828228000	1.958181000	0.453025000
1	3.032968000	1.532094000	1.442025000
1	3.679125000	1.673007000	-0.177801000
6	-0.264525000	2.122696000	-1.758663000
1	-1.297319000	2.308246000	-1.443286000
1	-0.326495000	1.494677000	-2.654780000
1	0.075215000	-3.315466000	-1.047683000
1	1.436918000	-3.446134000	1.273654000
1	3.707701000	-1.973635000	1.017818000
1	3.730146000	-0.912303000	-1.472938000
1	1.468179000	-1.702494000	-2.733609000
8	-5.008219000	-0.117485000	0.358944000
6	-5.889917000	-0.431530000	-0.766327000
1	-5.753256000	0.291671000	-1.574684000
1	-5.702065000	-1.443105000	-1.135261000
1	-6.896768000	-0.358877000	-0.365940000
6	0.443951000	3.438488000	-2.093100000
1	1.473405000	3.260827000	-2.417096000
1	-0.086469000	3.950353000	-2.899174000
1	0.468095000	4.101902000	-1.225325000
6	2.738251000	3.488854000	0.562527000
1	2.639602000	3.952715000	-0.420831000
1	1.877957000	3.785615000	1.168480000
1	3.643566000	3.877232000	1.034650000

Int0_Cp*; Gibbs free energy ... -1262.33163222 Eh

45	-0.998817000	0.039006000	-0.178649000
8	-2.145149000	1.407620000	-1.538487000
6	-1.315138000	2.398908000	-1.343763000
6	2.311407000	0.422772000	-0.413424000

6	-1.442168000	3.680264000	-2.101040000
8	-0.356376000	2.210857000	-0.475093000
6	2.290981000	-0.762123000	-1.160777000
6	3.361503000	0.660625000	0.488347000
6	-2.112454000	-1.703817000	0.444983000
6	-0.724518000	-1.905552000	0.832072000
6	-0.346520000	-0.834010000	1.729571000
6	-1.525402000	0.017596000	1.941207000
6	-2.615752000	-0.530954000	1.170912000
6	3.334196000	-1.702362000	-1.022018000
6	4.369503000	-1.457800000	-0.114095000
6	4.395383000	-0.277603000	0.650789000
1	5.202472000	-0.107348000	1.352630000
1	-1.146703000	4.524020000	-1.478690000
1	-0.777089000	3.654599000	-2.967990000
1	-2.461345000	3.816610000	-2.458477000
6	1.178953000	-1.028830000	-2.131578000
8	1.345429000	-1.858561000	-3.082219000
8	0.042882000	-0.353684000	-1.988715000
1	3.311578000	-2.608472000	-1.615870000
6	-1.572695000	1.216791000	2.821204000
1	-1.762367000	0.913281000	3.856272000
1	-0.625235000	1.759578000	2.804017000
1	-2.369282000	1.900170000	2.521716000
6	0.144751000	-3.017159000	0.362003000
1	-0.052693000	-3.912561000	0.960582000
1	-0.058120000	-3.270158000	-0.681905000
1	1.204313000	-2.772474000	0.460987000
6	-2.903864000	-2.580659000	-0.459231000
1	-2.266752000	-3.047612000	-1.213231000
1	-3.382067000	-3.380411000	0.116534000
1	-3.691806000	-2.022797000	-0.969125000
1	1.526165000	1.163548000	-0.524304000
6	0.963464000	-0.663453000	2.412004000
1	1.261558000	0.387969000	2.454383000
1	0.888654000	-1.027523000	3.442774000
1	1.756345000	-1.223207000	1.911567000
6	-4.004351000	-0.004527000	1.100522000
1	-4.635247000	-0.538594000	1.818971000
1	-4.044272000	1.058298000	1.344513000
1	-4.438690000	-0.149411000	0.109503000
1	5.163189000	-2.184797000	0.010204000
8	3.273625000	1.860198000	1.195218000
6	4.317586000	2.139007000	2.180914000
1	4.040941000	3.089692000	2.627315000
1	4.345671000	1.357544000	2.946177000
1	5.295261000	2.219806000	1.697974000

Int'0_Cp*; Gibbs free energy ... -1262.33102960 Eh

45	-1.272891000	0.061729000	-0.109135000
8	-2.800038000	1.566698000	-0.805534000
6	-2.365850000	2.469960000	0.033397000
6	1.717025000	1.562323000	0.572558000

6	-2.903873000	3.863769000	0.024650000
8	-1.421706000	2.107274000	0.862435000
6	2.087284000	0.867407000	-0.591560000
6	2.612488000	1.625229000	1.653745000
6	-1.843855000	-1.950304000	-0.669457000
6	-0.439131000	-1.972103000	-0.303086000
6	-0.323943000	-1.526032000	1.071965000
6	-1.678700000	-1.269796000	1.578516000
6	-2.613960000	-1.541561000	0.513809000
6	3.342691000	0.232026000	-0.673723000
6	4.211156000	0.276322000	0.426763000
6	3.851660000	0.981447000	1.593328000
1	4.544177000	1.012326000	2.425738000
1	-2.775643000	4.330600000	0.999771000
1	-2.356512000	4.455464000	-0.713516000
1	-3.955831000	3.865575000	-0.257909000
6	1.188501000	0.836233000	-1.793174000
8	1.681534000	0.668749000	-2.953911000
8	-0.114158000	1.027128000	-1.606446000
1	3.605701000	-0.284455000	-1.589914000
6	-2.004768000	-0.819365000	2.957980000
1	-2.016467000	-1.680664000	3.634223000
1	-1.258348000	-0.115448000	3.333114000
1	-2.984969000	-0.342138000	3.004233000
6	0.685989000	-2.363056000	-1.193318000
1	0.838811000	-3.445809000	-1.137361000
1	0.480045000	-2.110567000	-2.235767000
1	1.620888000	-1.880802000	-0.894733000
6	-2.415745000	-2.344540000	-1.984615000
1	-1.692662000	-2.206735000	-2.790386000
1	-2.698344000	-3.402752000	-1.965546000
1	-3.312425000	-1.768013000	-2.221634000
1	0.749646000	2.049795000	0.626856000
1	2.338832000	2.172910000	2.547569000
8	5.460254000	-0.341918000	0.456744000
6	5.854214000	-1.105680000	-0.727350000
1	5.142221000	-1.914511000	-0.915057000
1	5.914426000	-0.456056000	-1.604857000
1	6.833648000	-1.512795000	-0.494721000
6	0.925953000	-1.463807000	1.875272000
1	0.866869000	-0.696698000	2.649822000
1	1.090526000	-2.428318000	2.368838000
1	1.798657000	-1.253441000	1.250322000
6	-4.095693000	-1.427926000	0.573796000
1	-4.536575000	-2.416765000	0.738189000
1	-4.415691000	-0.776459000	1.388427000
1	-4.500759000	-1.038771000	-0.362776000

TS0_Cp*; Gibbs free energy ... -1262.30611326 Eh

45	0.692842000	-0.041249000	0.175340000
8	1.198796000	1.728194000	1.357832000
6	0.307616000	2.400973000	2.000635000
6	-1.481966000	0.074835000	0.368892000

6	0.696161000	3.608066000	2.798085000
8	-0.966066000	2.077266000	1.961765000
6	-1.889952000	-1.061082000	1.119634000
6	-2.381878000	0.562644000	-0.611685000
6	1.173442000	-1.786264000	-1.032736000
6	2.431232000	-1.254163000	-0.486879000
6	2.597602000	0.081072000	-0.988503000
6	1.449814000	0.401674000	-1.842590000
6	0.613046000	-0.783124000	-1.916869000
6	-3.129361000	-1.681724000	0.914473000
6	-3.987523000	-1.175489000	-0.074740000
6	-3.629517000	-0.049417000	-0.835597000
1	-4.315938000	0.331694000	-1.582452000
1	0.127985000	3.644142000	3.726464000
1	1.763274000	3.602095000	3.006256000
1	0.453251000	4.505514000	2.224463000
1	-1.119131000	1.120379000	1.179067000
6	-0.925063000	-1.542033000	2.157139000
8	-1.252215000	-2.368138000	3.064846000
8	0.299382000	-1.017284000	2.063021000
1	-3.404501000	-2.543940000	1.512007000
6	1.255354000	1.662716000	-2.612671000
1	1.719250000	1.582773000	-3.602320000
1	0.192137000	1.872491000	-2.752680000
1	1.710129000	2.513346000	-2.099398000
6	3.354631000	-1.996914000	0.415496000
1	2.802394000	-2.658573000	1.086963000
1	4.033837000	-2.621432000	-0.175064000
1	3.961727000	-1.319454000	1.018776000
6	0.642467000	-3.157880000	-0.796717000
1	1.085112000	-3.866893000	-1.504597000
1	0.882825000	-3.502331000	0.212193000
1	-0.442335000	-3.192995000	-0.923429000
6	-0.576105000	-0.958415000	-2.793489000
1	-1.305778000	-1.646431000	-2.359896000
1	-1.065774000	-0.004752000	-2.998523000
1	-0.251800000	-1.379100000	-3.751797000
6	3.720934000	1.007497000	-0.681921000
1	3.391632000	2.048425000	-0.689011000
1	4.167530000	0.793520000	0.291079000
1	4.504206000	0.902200000	-1.440308000
1	-4.945397000	-1.648842000	-0.255559000
8	-1.947564000	1.695008000	-1.294612000
6	-2.857416000	2.300555000	-2.270865000
1	-2.330293000	3.174163000	-2.644012000
1	-3.060529000	1.603843000	-3.088945000
1	-3.793414000	2.598431000	-1.791750000

TS'0_Cp*; Gibbs free energy ... -1262.30091871 Eh

45	0.923414000	-0.024367000	0.155079000
8	1.960580000	1.902785000	0.139930000
6	1.339239000	2.995311000	-0.141091000
6	-1.048156000	0.631294000	-0.555670000

6	2.058044000	4.308790000	-0.117983000
8	0.064081000	3.001589000	-0.464084000
6	-1.941907000	0.516101000	0.546736000
6	-1.602149000	0.446328000	-1.849719000
6	0.625351000	-2.173893000	0.114428000
6	1.693683000	-1.898655000	1.081166000
6	2.777803000	-1.259555000	0.389111000
6	2.407332000	-1.159607000	-1.027686000
6	1.113369000	-1.773787000	-1.201311000
6	-3.308663000	0.257665000	0.388272000
6	-3.813505000	0.081057000	-0.911815000
6	-2.959007000	0.177127000	-2.031943000
1	-3.380818000	0.047112000	-3.021687000
1	3.109067000	4.164920000	0.118784000
1	1.960081000	4.796959000	-1.088677000
1	1.601825000	4.965315000	0.624727000
1	-0.362588000	1.830782000	-0.505671000
6	-1.355265000	0.708532000	1.907555000
8	-2.064932000	0.864862000	2.949641000
8	-0.020800000	0.723640000	1.935630000
1	-3.938561000	0.197675000	1.269585000
6	3.269557000	-0.603775000	-2.107807000
1	2.677136000	-0.304929000	-2.974893000
1	3.836768000	0.262428000	-1.759900000
1	3.991332000	-1.358344000	-2.440127000
6	1.624997000	-2.192733000	2.538275000
1	0.594722000	-2.167595000	2.899126000
1	2.021168000	-3.195262000	2.731924000
1	2.214480000	-1.482462000	3.121247000
6	-0.652646000	-2.887949000	0.396841000
1	-0.527423000	-3.969065000	0.272694000
1	-0.989011000	-2.707138000	1.420894000
1	-1.442980000	-2.561321000	-0.284311000
1	-0.966374000	0.540491000	-2.724834000
8	-5.145096000	-0.182780000	-1.199570000
6	-6.070352000	-0.307124000	-0.070296000
1	-5.791098000	-1.154987000	0.560057000
1	-6.080854000	0.610756000	0.522457000
1	-7.044996000	-0.474804000	-0.518339000
6	0.432194000	-2.031846000	-2.499807000
1	-0.649073000	-2.118327000	-2.378764000
1	0.638776000	-1.250345000	-3.234020000
1	0.798880000	-2.978000000	-2.913355000
6	4.065175000	-0.795587000	0.979414000
1	4.409001000	0.128801000	0.509478000
1	3.973911000	-0.621847000	2.053475000
1	4.844717000	-1.550356000	0.828642000

Int1_Cp*; Gibbs free energy ... -1262.32268845 Eh

45	0.537555000	-0.285262000	0.239537000
8	0.452996000	1.076731000	1.982057000
6	0.197548000	2.317801000	1.959459000
6	-1.488146000	-0.319738000	0.072743000

6	0.553304000	3.224612000	3.089633000
8	-0.382736000	2.939971000	0.920124000
6	-2.113597000	-1.444890000	0.649118000
6	-2.307506000	0.598708000	-0.603444000
6	2.706441000	0.226661000	-0.381118000
6	2.537845000	-1.178090000	-0.426146000
6	1.405119000	-1.469236000	-1.331826000
6	0.974357000	-0.212078000	-1.927554000
6	1.706553000	0.847044000	-1.276333000
6	-3.491400000	-1.688841000	0.487942000
6	-4.264287000	-0.788022000	-0.253208000
6	-3.679433000	0.375398000	-0.792189000
1	-4.293629000	1.082652000	-1.337951000
1	-0.282494000	3.881411000	3.327961000
1	0.840015000	2.644052000	3.961702000
1	1.393365000	3.856168000	2.790208000
1	-0.726751000	2.358997000	0.150536000
6	-1.238956000	-2.308746000	1.488387000
8	-1.652208000	-3.347651000	2.094920000
8	0.022820000	-1.874957000	1.587367000
1	-3.931434000	-2.570165000	0.943680000
1	-5.322225000	-0.965909000	-0.404085000
8	-1.653652000	1.777503000	-1.037585000
6	-2.430408000	2.766936000	-1.788262000
1	-2.783548000	2.329753000	-2.724618000
1	-3.275481000	3.122515000	-1.193861000
1	-1.738029000	3.581474000	-1.987818000
6	-0.004846000	-0.074337000	-3.044112000
1	0.490818000	-0.299257000	-3.994983000
1	-0.840120000	-0.771255000	-2.935972000
1	-0.405876000	0.938180000	-3.101905000
6	3.291764000	-2.219447000	0.329945000
1	3.943251000	-2.784995000	-0.344897000
1	3.913682000	-1.781325000	1.112389000
1	2.609243000	-2.936089000	0.796062000
6	3.684578000	0.998239000	0.440751000
1	4.148297000	0.374821000	1.207092000
1	4.479419000	1.404306000	-0.194339000
1	3.206061000	1.848505000	0.937257000
6	1.650992000	2.300154000	-1.612810000
1	1.884474000	2.922807000	-0.745161000
1	2.386134000	2.534660000	-2.391720000
1	0.664178000	2.584571000	-1.986160000
6	0.945215000	-2.833213000	-1.723617000
1	1.601146000	-3.251248000	-2.495705000
1	0.961763000	-3.517246000	-0.871410000
1	-0.071492000	-2.808514000	-2.123410000

Int'1_Cp*; Gibbs free energy ... -1262.30941671 Eh

45	-0.841691000	-0.145719000	-0.209561000
8	-0.777385000	2.025039000	-0.834118000
6	-0.259260000	3.037427000	-0.292048000
6	1.136509000	-0.165093000	0.332573000

6	-0.633796000	4.440809000	-0.620428000
8	0.701201000	2.941965000	0.663931000
6	2.029499000	-0.385576000	-0.745460000
6	1.706110000	0.022628000	1.614933000
6	-3.138635000	-0.095091000	0.064759000
6	-2.784983000	-1.313843000	-0.558615000
6	-1.797872000	-1.999573000	0.305298000
6	-1.659887000	-1.220535000	1.531141000
6	-2.396975000	0.003695000	1.341969000
6	3.424380000	-0.417002000	-0.574002000
6	3.954925000	-0.223247000	0.709731000
6	3.095930000	-0.002043000	1.803670000
1	3.526585000	0.148200000	2.787232000
1	0.198261000	4.936667000	-1.123628000
1	-1.506732000	4.453351000	-1.266286000
1	-0.836305000	4.994571000	0.296711000
1	0.962602000	1.998407000	0.843722000
6	1.419911000	-0.571187000	-2.090233000
8	2.100440000	-0.762817000	-3.147921000
8	0.086107000	-0.513797000	-2.096486000
1	4.051565000	-0.590811000	-1.442726000
6	-0.935026000	-1.650583000	2.759750000
1	-1.582207000	-2.302076000	3.357087000
1	-0.030042000	-2.213554000	2.520323000
1	-0.657992000	-0.800129000	3.386200000
6	-3.244141000	-1.832462000	-1.879508000
1	-4.026611000	-2.586595000	-1.742693000
1	-3.649835000	-1.038241000	-2.509118000
1	-2.423657000	-2.311927000	-2.419915000
6	-4.052792000	0.963703000	-0.452717000
1	-4.298316000	0.807108000	-1.504533000
1	-4.987796000	0.969493000	0.117967000
1	-3.606822000	1.957560000	-0.347837000
1	1.074226000	0.204388000	2.480288000
8	5.320543000	-0.226582000	1.004645000
6	6.239793000	-0.441052000	-0.112065000
1	6.084946000	-1.427715000	-0.557374000
1	6.110032000	0.332017000	-0.874603000
1	7.234547000	-0.375593000	0.319351000
6	-1.247735000	-3.365461000	0.065989000
1	-1.106377000	-3.555621000	-1.000525000
1	-0.287121000	-3.503175000	0.568379000
1	-1.938872000	-4.125029000	0.449194000
6	-2.529234000	1.120041000	2.323849000
1	-1.670636000	1.155491000	2.999251000
1	-2.607930000	2.086529000	1.817746000
1	-3.431714000	0.994747000	2.933027000

Int2_T_Cp*; Gibbs free energy ... -1572.47923353 Eh

45	0.377337000	-0.641487000	-0.166145000
6	-1.471970000	-0.905325000	0.675196000
6	-1.467376000	-1.415259000	1.986519000
6	-2.718902000	-0.664738000	0.058519000

6	0.455498000	-0.635345000	-2.421815000
6	1.850750000	-0.594278000	-1.961758000
6	2.098796000	-1.760919000	-1.185993000
6	0.857275000	-2.552655000	-1.156174000
6	-0.116849000	-1.893679000	-2.000951000
6	-2.662530000	-1.713095000	2.673790000
6	-3.884857000	-1.500936000	2.031205000
6	-3.918976000	-0.977321000	0.724427000
1	-2.607517000	-2.101552000	3.685634000
1	-4.877701000	-0.806613000	0.247431000
6	-0.135542000	-1.593189000	2.613670000
8	0.039753000	-2.032062000	3.794541000
8	0.890755000	-1.237203000	1.831815000
6	-0.094437000	1.601129000	0.314601000
6	1.130243000	1.344015000	0.486416000
6	3.373638000	-2.162408000	-0.524294000
1	3.852434000	-2.975905000	-1.080769000
1	4.078061000	-1.329543000	-0.470409000
1	3.196061000	-2.525740000	0.492317000
6	-1.417204000	-2.487846000	-2.427872000
1	-2.012251000	-1.776765000	-2.999731000
1	-1.220233000	-3.364192000	-3.055802000
1	-2.016145000	-2.824868000	-1.576409000
6	-0.167295000	0.360543000	-3.339406000
1	0.138940000	1.379707000	-3.087167000
1	0.139934000	0.171508000	-4.374712000
1	-1.255904000	0.308325000	-3.289198000
6	-1.326855000	2.335758000	0.285809000
6	-2.299459000	2.181757000	1.301669000
6	-1.553644000	3.275922000	-0.749135000
6	-3.470075000	2.950090000	1.278748000
6	-2.726632000	4.040008000	-0.764032000
6	-3.690336000	3.879398000	0.247574000
1	-2.130944000	1.462469000	2.095971000
1	-0.806602000	3.402137000	-1.525366000
1	-4.209245000	2.821082000	2.060824000
1	-2.886676000	4.761485000	-1.556530000
1	-4.596319000	4.473466000	0.234496000
6	2.515487000	1.635612000	0.748726000
6	3.039354000	2.885403000	0.334754000
6	3.368192000	0.700166000	1.375354000
6	4.390917000	3.184598000	0.543097000
6	4.717587000	1.009793000	1.582691000
6	5.235618000	2.248150000	1.164527000
1	2.385262000	3.599868000	-0.153909000
1	2.952216000	-0.250086000	1.692891000
1	4.785294000	4.139158000	0.215055000
1	5.366874000	0.286239000	2.061825000
1	6.282292000	2.480319000	1.321348000
1	-4.817415000	-1.729041000	2.534052000
8	-2.680068000	-0.081335000	-1.208882000
6	-3.950758000	0.121370000	-1.896160000
1	-3.692154000	0.577081000	-2.849853000

1	-4.457757000	-0.835377000	-2.061782000
1	-4.603944000	0.791687000	-1.328206000
6	2.821433000	0.480899000	-2.313234000
1	3.676551000	0.498249000	-1.632703000
1	3.202466000	0.321766000	-3.328241000
1	2.351173000	1.468717000	-2.295197000
6	0.711869000	-3.895624000	-0.522285000
1	1.069518000	-4.677784000	-1.201844000
1	1.299994000	-3.962308000	0.396092000
1	-0.331048000	-4.113854000	-0.280905000

Int'2_T_Cp*; Gibbs free energy ... -1572.47465822 Eh

45	-0.565715000	-0.614751000	0.228496000
6	1.441611000	-0.640763000	-0.188627000
6	1.761465000	-0.872154000	-1.546356000
6	2.495955000	-0.432833000	0.713043000
6	-1.272693000	-0.815605000	2.352259000
6	-2.485698000	-0.978736000	1.537068000
6	-2.289232000	-2.088064000	0.676201000
6	-0.950313000	-2.646465000	0.944777000
6	-0.381091000	-1.912433000	2.059664000
6	3.090870000	-0.895524000	-1.994605000
6	4.127702000	-0.682282000	-1.076239000
6	3.834129000	-0.457288000	0.283535000
1	3.308296000	-1.067496000	-3.044198000
1	4.624373000	-0.284022000	1.005400000
6	0.622310000	-1.047412000	-2.478810000
8	0.749507000	-1.277203000	-3.723030000
8	-0.576140000	-0.931662000	-1.895937000
6	-0.212912000	1.732393000	0.124339000
6	-1.346010000	1.433039000	-0.334287000
6	-3.237438000	-2.633186000	-0.337608000
1	-2.733985000	-2.817740000	-1.291466000
1	-3.647611000	-3.589875000	0.004115000
1	-4.071156000	-1.950948000	-0.517154000
6	0.849529000	-2.281766000	2.814743000
1	1.275011000	-1.427201000	3.344966000
1	0.599783000	-3.041971000	3.563295000
1	1.618783000	-2.701318000	2.162633000
6	-1.101673000	0.207761000	3.424515000
1	-1.500436000	1.176920000	3.110560000
1	-1.641287000	-0.091278000	4.330207000
1	-0.049416000	0.340816000	3.687559000
1	2.293296000	-0.216238000	1.758207000
8	5.425530000	-0.698575000	-1.602852000
6	6.517959000	-0.383986000	-0.685927000
1	6.377403000	0.605835000	-0.239955000
1	6.594579000	-1.135937000	0.104932000
1	7.416722000	-0.393508000	-1.296225000
6	1.028601000	2.376225000	0.438978000
6	1.984418000	2.591310000	-0.583622000
6	1.332585000	2.772107000	1.761336000
6	3.211601000	3.192294000	-0.285473000

6	2.564691000	3.370776000	2.052184000
6	3.510070000	3.579573000	1.032799000
1	1.755590000	2.278210000	-1.596757000
1	0.603455000	2.609553000	2.546790000
1	3.939034000	3.346873000	-1.074001000
1	2.788821000	3.668109000	3.069726000
1	4.465276000	4.037482000	1.260632000
6	-2.673984000	1.616687000	-0.859701000
6	-3.416798000	2.765599000	-0.494377000
6	-3.258966000	0.657390000	-1.716403000
6	-4.717371000	2.944727000	-0.982417000
6	-4.556853000	0.847647000	-2.203430000
6	-5.292337000	1.989262000	-1.838429000
1	-2.975932000	3.496012000	0.174772000
1	-2.676658000	-0.217083000	-1.988023000
1	-5.282259000	3.823474000	-0.694589000
1	-4.995285000	0.108494000	-2.863848000
1	-6.298316000	2.131737000	-2.214771000
6	-0.399789000	-3.883931000	0.317739000
1	-0.861100000	-4.775670000	0.757405000
1	-0.603647000	-3.905121000	-0.756368000
1	0.680261000	-3.957690000	0.462260000
6	-3.709308000	-0.137331000	1.670577000
1	-4.306007000	-0.132689000	0.754530000
1	-4.339924000	-0.520382000	2.480968000
1	-3.457260000	0.897904000	1.916009000

Int2_H_Cp*; Gibbs free energy ... -1267.74005190 Eh

45	0.452821000	-0.293550000	0.031263000
6	-1.542869000	-0.213140000	0.463143000
6	-1.899253000	-0.679722000	1.744650000
6	-2.579791000	0.243835000	-0.380557000
6	2.318407000	-0.406779000	-1.330344000
6	2.201074000	-1.623246000	-0.604082000
6	0.897352000	-2.224568000	-0.941302000
6	0.269279000	-1.401192000	-1.950417000
6	1.089757000	-0.224386000	-2.120540000
6	-3.240149000	-0.717492000	2.182889000
6	-4.247842000	-0.274766000	1.323877000
6	-3.922896000	0.209193000	0.040864000
1	-3.457979000	-1.086960000	3.179979000
1	-4.716331000	0.557154000	-0.611403000
1	-5.286142000	-0.293120000	1.634528000
6	-0.781669000	-1.118461000	2.614611000
8	-0.936514000	-1.564604000	3.797082000
8	0.426829000	-1.000262000	2.054684000
6	0.324660000	1.993957000	0.335524000
6	1.273506000	1.548904000	1.031247000
6	2.421074000	1.422328000	1.947862000
1	2.119196000	0.822187000	2.811884000
1	3.224778000	0.863641000	1.453003000
6	-0.604216000	2.970774000	-0.266351000
1	-1.615660000	2.793497000	0.117635000

1	-0.664706000	2.807883000	-1.346379000
6	2.940195000	2.800505000	2.395250000
1	3.268890000	3.388130000	1.533507000
1	2.157661000	3.361859000	2.911691000
1	3.786396000	2.679925000	3.075078000
6	-0.158150000	4.411872000	0.036344000
1	0.827130000	4.609140000	-0.395247000
1	-0.869603000	5.122941000	-0.389602000
1	-0.098113000	4.585477000	1.114180000
8	-2.185882000	0.729431000	-1.629729000
6	-3.222213000	1.263633000	-2.503385000
1	-3.950170000	0.489192000	-2.767434000
1	-3.737803000	2.105443000	-2.028495000
1	-2.698945000	1.601115000	-3.395664000
6	0.406247000	-3.549895000	-0.459994000
1	-0.680391000	-3.624164000	-0.549331000
1	0.847149000	-4.361825000	-1.050209000
1	0.677194000	-3.720951000	0.584908000
6	0.849559000	0.895569000	-3.075625000
1	1.285611000	1.828576000	-2.706666000
1	1.305206000	0.680488000	-4.049357000
1	-0.220753000	1.053723000	-3.223856000
6	3.461066000	0.554396000	-1.328864000
1	4.239723000	0.254662000	-0.624375000
1	3.911213000	0.612269000	-2.325559000
1	3.134464000	1.567676000	-1.065583000
6	-0.956519000	-1.771991000	-2.718524000
1	-1.306855000	-0.941833000	-3.331055000
1	-0.728631000	-2.621411000	-3.372685000
1	-1.775991000	-2.076030000	-2.061139000
6	3.171807000	-2.213978000	0.363319000
1	2.679107000	-2.449250000	1.312380000
1	3.588881000	-3.147910000	-0.028194000
1	3.998575000	-1.531965000	0.571096000

Int'2_H_Cp*; Gibbs free energy ... -1267.73851876 Eh

45	0.675843000	-0.272995000	0.097227000
6	-1.350522000	-0.080474000	-0.086601000
6	-2.060856000	-0.134389000	1.137382000
6	-2.087722000	0.087173000	-1.269374000
6	2.808925000	-0.701325000	-0.704909000
6	2.478521000	-1.704318000	0.244655000
6	1.259879000	-2.388477000	-0.223684000
6	0.906899000	-1.841922000	-1.513945000
6	1.798678000	-0.734027000	-1.774920000
6	-3.459048000	-0.035135000	1.182778000
6	-4.174349000	0.121634000	-0.012280000
6	-3.491716000	0.184477000	-1.243493000
1	-3.978332000	-0.083434000	2.134944000
1	-4.031457000	0.311662000	-2.175199000
6	-1.252438000	-0.310423000	2.368765000
8	-1.747902000	-0.374052000	3.539374000
8	0.062285000	-0.400252000	2.145758000

6	0.595704000	1.989167000	-0.250729000
6	1.309670000	1.785470000	0.763896000
6	2.168168000	1.938236000	1.952048000
1	1.592192000	1.658096000	2.839602000
1	3.003256000	1.229513000	1.894302000
6	-0.096884000	2.700279000	-1.342238000
1	-1.147585000	2.845791000	-1.066787000
1	-0.103516000	2.083035000	-2.246671000
6	2.707853000	3.373641000	2.080629000
1	3.304905000	3.642889000	1.204754000
1	1.890080000	4.092861000	2.170414000
1	3.339901000	3.454923000	2.967555000
6	0.572875000	4.054687000	-1.633514000
1	1.612221000	3.912380000	-1.943286000
1	0.041752000	4.573170000	-2.434691000
1	0.567766000	4.691467000	-0.745195000
6	0.624093000	-3.561148000	0.446530000
1	-0.410450000	-3.694617000	0.121669000
1	1.171667000	-4.480557000	0.209332000
1	0.630056000	-3.447187000	1.533687000
6	1.831108000	0.099364000	-3.013204000
1	2.228474000	1.098139000	-2.812347000
1	2.474604000	-0.363248000	-3.770425000
1	0.833664000	0.208369000	-3.448155000
6	3.948476000	0.262858000	-0.659892000
1	4.493614000	0.201909000	0.284119000
1	4.654431000	0.061500000	-1.472559000
1	3.598597000	1.294807000	-0.784400000
1	-1.582777000	0.154926000	-2.229813000
8	-5.567159000	0.206748000	0.115810000
6	-6.340691000	0.364804000	-1.113105000
1	-6.079802000	1.297919000	-1.621078000
1	-6.174406000	-0.479569000	-1.788500000
1	-7.380243000	0.389964000	-0.798237000
6	-0.165298000	-2.353556000	-2.415666000
1	-1.041625000	-2.683407000	-1.852062000
1	-0.486695000	-1.595901000	-3.133430000
1	0.205852000	-3.212531000	-2.985124000
6	3.195223000	-2.035733000	1.512263000
1	3.959362000	-1.292447000	1.746854000
1	2.501038000	-2.088864000	2.356640000
1	3.683989000	-3.012776000	1.432171000

TS2_T_Cp*; Gibbs free energy ... -1572.45589213 Eh

45	0.675052000	-0.789094000	-0.017593000
6	-1.258525000	-0.648939000	0.807799000
6	-1.263129000	-0.801484000	2.216479000
6	-2.460142000	-0.938838000	0.107870000
6	2.084577000	-1.102839000	-1.785887000
6	2.541506000	-1.861382000	-0.661462000
6	1.494759000	-2.851780000	-0.330941000
6	0.420660000	-2.699523000	-1.260775000
6	0.743571000	-1.569448000	-2.125173000

6	2.817088000	-0.032262000	-2.527229000
6	-2.428679000	-1.175257000	2.909433000
6	-3.599474000	-1.452184000	2.194755000
6	-3.614895000	-1.347957000	0.790824000
6	1.606606000	-3.885269000	0.739589000
6	-0.801262000	-3.555847000	-1.324502000
1	-0.559324000	-4.530763000	-1.761309000
1	-2.387177000	-1.269075000	3.989487000
1	-4.523390000	-1.576732000	0.245848000
1	0.623321000	-4.223105000	1.075803000
1	-1.580499000	-3.094402000	-1.933074000
1	2.171211000	0.828587000	-2.725515000
1	2.150196000	-4.761525000	0.367872000
1	-1.216341000	-3.737133000	-0.328094000
1	3.691103000	0.317850000	-1.974417000
1	2.153773000	-3.505744000	1.605510000
1	3.161404000	-0.412710000	-3.495199000
6	0.034308000	-0.629678000	2.918330000
8	0.132684000	-0.520163000	4.183153000
8	1.098620000	-0.630408000	2.114316000
6	-0.559964000	1.115403000	0.153635000
6	0.736550000	1.268021000	0.231572000
6	1.786998000	2.242014000	0.387319000
6	1.465537000	3.623381000	0.456208000
6	3.141517000	1.854396000	0.488815000
6	2.477440000	4.577090000	0.610106000
6	4.150583000	2.812619000	0.640411000
6	3.823576000	4.178419000	0.698774000
1	0.427591000	3.933249000	0.392709000
1	3.381497000	0.795676000	0.464263000
1	2.220018000	5.628771000	0.658841000
1	5.184865000	2.498032000	0.717131000
1	4.603029000	4.921184000	0.819600000
6	-1.729513000	1.885534000	-0.272303000
6	-2.875502000	1.988916000	0.544673000
6	-1.677096000	2.612402000	-1.483268000
6	-3.950363000	2.798441000	0.156319000
6	-2.758040000	3.415460000	-1.871612000
6	-3.899202000	3.507660000	-1.055548000
1	-2.909609000	1.447096000	1.484618000
1	-0.792174000	2.540587000	-2.108866000
1	-4.823032000	2.874196000	0.794300000
1	-2.711905000	3.965286000	-2.804325000
1	-4.735686000	4.126554000	-1.358050000
1	-4.499567000	-1.755799000	2.715534000
8	-2.403216000	-0.766286000	-1.269554000
6	-3.661707000	-0.821100000	-2.009463000
1	-3.403150000	-0.569909000	-3.035788000
1	-4.095358000	-1.824758000	-1.968068000
1	-4.373015000	-0.090586000	-1.610318000
6	3.875780000	-1.805048000	0.005651000
1	3.780226000	-1.766295000	1.094935000
1	4.454753000	-2.703283000	-0.235995000

1	4.457203000	-0.939445000	-0.318719000
6	-0.034064000	-1.108220000	-3.310774000
1	0.419969000	-1.499659000	-4.228972000
1	-1.067620000	-1.449983000	-3.266532000
1	-0.038594000	-0.017195000	-3.389817000

TS'2_T_Cp*; Gibbs free energy ... -1572.45023754 Eh

45	-0.552985000	-0.915040000	0.147725000
6	1.391141000	-0.206045000	-0.295902000
6	1.752173000	-0.467062000	-1.646132000
6	2.427193000	-0.041453000	0.646438000
6	-2.155630000	-1.474776000	1.675521000
6	-2.114067000	-2.469657000	0.647955000
6	-0.775322000	-3.097104000	0.677026000
6	-0.018782000	-2.493808000	1.725577000
6	-0.832696000	-1.423269000	2.295066000
6	-3.316493000	-0.622690000	2.074603000
6	3.093951000	-0.502929000	-2.040818000
6	4.106631000	-0.331727000	-1.082799000
6	3.773126000	-0.123905000	0.271766000
6	-0.355905000	-4.222162000	-0.209077000
6	1.356843000	-2.868928000	2.162604000
1	1.310679000	-3.560695000	3.010684000
1	3.346220000	-0.701473000	-3.077254000
1	4.542061000	-0.002430000	1.025191000
1	0.731594000	-4.292436000	-0.285649000
1	1.929181000	-1.995564000	2.485479000
1	-3.034531000	0.432117000	2.148610000
1	-0.727011000	-5.175732000	0.183142000
1	1.912019000	-3.360109000	1.359586000
1	-4.137135000	-0.700466000	1.358664000
1	-0.764724000	-4.103436000	-1.215623000
1	-3.692038000	-0.931471000	3.055958000
6	0.663250000	-0.803406000	-2.601357000
8	0.827490000	-0.834915000	-3.862991000
8	-0.496910000	-1.103730000	-2.018936000
6	0.022858000	1.258548000	-0.025018000
6	-1.189038000	0.969789000	-0.424493000
6	-2.425349000	1.504774000	-0.929654000
6	-2.563365000	2.902915000	-1.138749000
6	-3.519704000	0.661233000	-1.227960000
6	-3.767445000	3.428682000	-1.619725000
6	-4.722500000	1.193075000	-1.705740000
6	-4.852627000	2.578907000	-1.902367000
1	-1.728191000	3.559983000	-0.919444000
1	-3.402273000	-0.409006000	-1.087305000
1	-3.862614000	4.497494000	-1.772022000
1	-5.552860000	0.533764000	-1.930216000
1	-5.783603000	2.989888000	-2.274506000
6	0.711659000	2.367996000	0.634574000
6	1.927165000	2.885489000	0.137054000
6	0.099592000	2.989882000	1.746941000
6	2.518850000	4.002021000	0.739968000

6	0.701360000	4.100216000	2.354570000
6	1.912199000	4.608505000	1.854026000
1	2.391897000	2.415967000	-0.723827000
1	-0.839719000	2.597278000	2.124525000
1	3.447778000	4.396873000	0.345990000
1	0.227801000	4.567528000	3.209848000
1	2.377439000	5.465974000	2.325654000
1	2.185026000	0.178391000	1.682473000
8	5.414339000	-0.395601000	-1.562140000
6	6.493955000	-0.221570000	-0.589739000
1	6.418733000	0.754724000	-0.102880000
1	6.466494000	-1.014488000	0.162605000
1	7.411232000	-0.281294000	-1.167872000
6	-0.461059000	-0.570800000	3.462830000
1	-0.662576000	-1.104549000	4.398889000
1	0.601291000	-0.312411000	3.455894000
1	-1.040344000	0.354768000	3.479458000
6	-3.229939000	-2.932378000	-0.230441000
1	-2.939129000	-2.930619000	-1.285674000
1	-3.509852000	-3.960359000	0.024632000
1	-4.118792000	-2.307052000	-0.120634000

TS2_H_Cp*; Gibbs free energy ... -1267.71487956 Eh

45	0.629834000	0.007338000	0.109580000
6	-1.471841000	0.143731000	0.339276000
6	-1.841956000	0.884290000	1.488672000
6	-2.414210000	-0.782860000	-0.179346000
6	2.543422000	-0.940001000	-0.679820000
6	2.647072000	-0.725984000	0.732603000
6	1.618187000	-1.552298000	1.398162000
6	0.890162000	-2.249779000	0.388605000
6	1.405923000	-1.821639000	-0.912793000
6	3.446497000	-0.392977000	-1.736033000
6	-3.108310000	0.736179000	2.083296000
6	-4.015692000	-0.188636000	1.554683000
6	-3.667176000	-0.958925000	0.427618000
6	1.444683000	-1.669754000	2.875836000
6	-0.200094000	-3.244597000	0.614605000
1	0.224596000	-4.238431000	0.794368000
1	-3.349774000	1.329890000	2.958767000
1	-4.376115000	-1.677587000	0.033295000
1	0.453280000	-2.051260000	3.131905000
1	-0.856683000	-3.307568000	-0.254400000
1	-4.990130000	-0.324279000	2.008543000
1	2.916795000	-0.244046000	-2.680536000
1	2.185939000	-2.358535000	3.297106000
1	-0.809343000	-2.982092000	1.484661000
1	3.890287000	0.559443000	-1.434148000
1	1.578130000	-0.704512000	3.371294000
1	4.266296000	-1.093826000	-1.928521000
6	-0.807026000	1.774101000	2.078399000
8	-1.073754000	2.647431000	2.968903000
8	0.425838000	1.569183000	1.620447000

6	-0.817404000	1.323855000	-1.162227000
6	0.436536000	1.646136000	-1.165819000
6	1.475842000	2.542465000	-1.733055000
1	2.073550000	1.971548000	-2.453931000
1	0.985083000	3.345098000	-2.297043000
6	-2.095614000	1.573726000	-1.905054000
1	-2.867515000	1.904496000	-1.199207000
1	-2.454574000	0.636459000	-2.341082000
8	-2.014668000	-1.471280000	-1.326301000
6	-2.998779000	-2.338849000	-1.971567000
1	-2.505564000	-2.714252000	-2.864796000
1	-3.273216000	-3.171974000	-1.317344000
1	-3.892931000	-1.770694000	-2.245951000
6	-1.885814000	2.624022000	-3.003563000
1	-2.828245000	2.809385000	-3.524104000
1	-1.534712000	3.570995000	-2.585180000
1	-1.149636000	2.281565000	-3.736089000
6	2.408381000	3.138526000	-0.669547000
1	2.876146000	2.337409000	-0.087867000
1	3.194504000	3.734669000	-1.139509000
1	1.854085000	3.773349000	0.025575000
6	3.670289000	0.085433000	1.455090000
1	4.242963000	0.714138000	0.769678000
1	3.208829000	0.729364000	2.209357000
1	4.375353000	-0.572028000	1.976443000
6	0.987598000	-2.355849000	-2.240660000
1	-0.062873000	-2.650429000	-2.227783000
1	1.125490000	-1.610164000	-3.028720000
1	1.587460000	-3.233945000	-2.507598000

TS'2_H_Cp*; Gibbs free energy ... -1267.71387920 Eh

45	0.831563000	-0.121784000	0.095134000
6	-1.220784000	0.143462000	-0.355635000
6	-2.017865000	0.234486000	0.813032000
6	-1.848894000	-0.287784000	-1.550378000
6	2.963267000	-0.668478000	-0.482865000
6	2.619157000	-1.324075000	0.741440000
6	1.500463000	-2.250704000	0.466309000
6	1.170599000	-2.150055000	-0.916869000
6	2.009054000	-1.101125000	-1.499647000
6	4.087747000	0.288151000	-0.707987000
6	-3.398080000	-0.029441000	0.786732000
6	-3.992146000	-0.443756000	-0.413308000
6	-3.208523000	-0.594078000	-1.578354000
6	0.891511000	-3.177574000	1.465487000
6	0.149840000	-2.959202000	-1.645118000
1	0.589698000	-3.901037000	-1.991299000
1	-3.957691000	0.062919000	1.712014000
1	-3.683185000	-0.936712000	-2.490568000
1	-0.139464000	-3.427537000	1.201544000
1	-0.226952000	-2.433119000	-2.525372000
1	3.829364000	1.037838000	-1.460654000
1	1.458424000	-4.114049000	1.518469000

1	-0.703229000	-3.207065000	-1.007584000
1	4.370520000	0.808037000	0.210945000
1	0.891268000	-2.738435000	2.466294000
1	4.972340000	-0.247064000	-1.070623000
6	-1.327843000	0.526502000	2.095575000
8	-1.950305000	0.858928000	3.157885000
8	-0.006645000	0.376503000	2.051036000
6	-0.147948000	1.784254000	-0.702690000
6	0.929855000	1.955403000	0.001745000
6	1.962981000	2.907134000	0.481616000
1	2.833065000	2.841133000	-0.183640000
1	1.571970000	3.926869000	0.381612000
6	-0.940731000	2.474267000	-1.772810000
1	-2.002570000	2.483674000	-1.499702000
1	-0.871192000	1.894804000	-2.701089000
6	-0.424421000	3.899536000	-2.002424000
1	-1.006726000	4.389386000	-2.786100000
1	-0.504672000	4.498478000	-1.091373000
1	0.625603000	3.890561000	-2.308701000
6	2.420435000	2.657322000	1.925560000
1	2.778765000	1.628280000	2.037259000
1	3.231702000	3.339302000	2.192542000
1	1.597016000	2.798121000	2.629210000
6	3.312981000	-1.206045000	2.057762000
1	3.989762000	-0.348937000	2.079371000
1	2.596222000	-1.096903000	2.877047000
1	3.903347000	-2.106625000	2.261458000
6	2.022362000	-0.679820000	-2.931675000
1	1.033431000	-0.779592000	-3.386956000
1	2.340217000	0.361852000	-3.033397000
1	2.717036000	-1.297306000	-3.512503000
1	-1.270361000	-0.369288000	-2.465673000
8	-5.347448000	-0.745386000	-0.555498000
6	-6.190727000	-0.574075000	0.627222000
1	-7.192650000	-0.847362000	0.309032000
1	-5.860832000	-1.231503000	1.436296000
1	-6.172573000	0.465992000	0.965146000

Int0_CpE; Gibbs free energy ... -1639.32560566 Eh

45	0.729929000	-0.708590000	-0.006058000
8	2.094962000	-1.751351000	1.344213000
6	1.655265000	-1.115978000	2.406818000
6	-2.333517000	-0.082412000	1.114182000
6	2.177594000	-1.427317000	3.765339000
8	0.741154000	-0.208319000	2.194340000
6	-2.750286000	-1.282186000	0.518676000
6	-3.237482000	0.986645000	1.234498000
6	1.901257000	-0.660713000	-1.868587000
6	0.490900000	-0.700901000	-2.202979000
6	-0.129053000	0.492668000	-1.633827000
6	0.892911000	1.274744000	-0.935546000
6	2.141926000	0.543742000	-1.074518000
6	-4.074631000	-1.414033000	0.052153000

6	-4.963540000	-0.342476000	0.175381000
6	-4.558841000	0.865702000	0.767781000
1	-5.264431000	1.682012000	0.863363000
1	1.768583000	-0.737909000	4.499897000
1	1.907627000	-2.449574000	4.037194000
1	3.266853000	-1.366340000	3.767104000
6	-1.835997000	-2.461186000	0.416454000
8	-2.309363000	-3.629755000	0.268271000
8	-0.516784000	-2.289082000	0.527264000
1	-4.385768000	-2.349525000	-0.396478000
1	-5.979522000	-0.437181000	-0.188334000
8	-2.726794000	2.131234000	1.843541000
6	-3.640665000	3.257871000	2.033332000
1	-4.005053000	3.629291000	1.071386000
1	-4.487123000	2.966648000	2.660963000
1	-3.051957000	4.023488000	2.530049000
6	0.681097000	2.556087000	-0.213974000
1	0.524694000	3.352487000	-0.947006000
1	-0.223816000	2.513055000	0.395263000
1	1.535607000	2.803614000	0.409994000
6	-0.174939000	-1.762250000	-3.003446000
1	-0.319974000	-1.404897000	-4.027960000
1	0.431002000	-2.667440000	-3.041024000
1	-1.160330000	-2.004947000	-2.607011000
6	2.910081000	-1.687400000	-2.230457000
1	2.444947000	-2.656631000	-2.411424000
1	3.424319000	-1.379672000	-3.146563000
1	3.669172000	-1.795144000	-1.455122000
6	-1.519250000	0.897759000	-1.911563000
8	-2.378315000	0.178637000	-2.462776000
8	-1.745668000	2.205207000	-1.567188000
6	3.474275000	0.912483000	-0.555619000
8	4.545031000	0.626933000	-1.130139000
8	3.408897000	1.585621000	0.633147000
6	-3.069202000	2.754908000	-1.928422000
1	-3.209434000	2.681366000	-3.006478000
1	-3.853796000	2.201328000	-1.409743000
1	-3.035691000	3.789558000	-1.603423000
6	4.703284000	2.001597000	1.222370000
1	4.432165000	2.570308000	2.104605000
1	5.282236000	1.116407000	1.482090000
1	5.250016000	2.614062000	0.506620000
1	-1.338556000	0.025010000	1.533344000

Int'0_CpE; Gibbs free energy ... -1639.32722574 Eh

45	0.979053000	0.481383000	0.254380000
8	2.443184000	2.086835000	0.011302000
6	2.203249000	2.215082000	-1.274117000
6	-1.887134000	0.763484000	-1.416156000
6	2.885090000	3.256161000	-2.090755000
8	1.327523000	1.388799000	-1.780092000
6	-2.419348000	1.288234000	-0.224139000
6	-2.706817000	-0.006478000	-2.257576000

6	1.838180000	-0.670814000	1.918295000
6	0.403530000	-0.872657000	1.914404000
6	0.047227000	-1.482729000	0.638067000
6	1.263152000	-1.661438000	-0.161748000
6	2.359332000	-1.141714000	0.633818000
6	-3.762358000	1.047955000	0.125059000
6	-4.560394000	0.258434000	-0.714673000
6	-4.036579000	-0.265188000	-1.913446000
1	-4.676446000	-0.865590000	-2.548958000
1	2.998869000	2.915957000	-3.118735000
1	2.277906000	4.164435000	-2.098257000
1	3.856703000	3.499051000	-1.664090000
6	-1.605487000	2.166130000	0.671921000
8	-2.166831000	2.988619000	1.458609000
8	-0.273228000	2.108215000	0.600827000
1	-4.144225000	1.470714000	1.047081000
6	1.354374000	-2.264620000	-1.516148000
1	1.166268000	-3.338969000	-1.437315000
1	0.582606000	-1.864799000	-2.175802000
1	2.334783000	-2.099895000	-1.955197000
6	-0.516322000	-0.532488000	3.031916000
1	-0.723364000	-1.434720000	3.616786000
1	-0.074426000	0.208600000	3.698667000
1	-1.475219000	-0.166069000	2.666329000
6	2.635763000	-0.072781000	3.018507000
1	2.025636000	0.575834000	3.647289000
1	3.036928000	-0.874506000	3.646972000
1	3.485883000	0.492489000	2.635290000
6	-1.294003000	-2.014533000	0.336242000
8	-2.301509000	-1.859874000	1.057670000
8	-1.295112000	-2.781695000	-0.799328000
6	3.790848000	-1.082977000	0.275327000
8	4.718566000	-1.205256000	1.100793000
8	3.986230000	-0.855255000	-1.058841000
6	-2.565150000	-3.469322000	-1.116573000
1	-2.749662000	-4.237237000	-0.365984000
1	-3.384041000	-2.749402000	-1.127666000
1	-2.408237000	-3.905050000	-2.097562000
6	5.393485000	-0.769566000	-1.513670000
1	5.325375000	-0.547627000	-2.572849000
1	5.901468000	0.028066000	-0.972972000
1	5.890029000	-1.723241000	-1.339531000
1	-0.864755000	0.986753000	-1.702273000
1	-2.308576000	-0.404090000	-3.183685000
8	-5.889274000	-0.063247000	-0.450599000
6	-6.469735000	0.455784000	0.788537000
1	-5.928468000	0.071816000	1.657493000
1	-6.452055000	1.548902000	0.794752000
1	-7.495341000	0.098866000	0.796398000

TS0_CpE; Gibbs free energy ... -1639.31095764 Eh

45	-0.460411000	0.276221000	0.028713000
8	-1.110900000	0.722496000	2.032200000

6	-0.480020000	1.555086000	2.799258000
6	1.375980000	1.405508000	0.025001000
6	-0.985464000	1.804987000	4.187462000
8	0.600357000	2.177045000	2.409120000
6	1.218930000	2.452298000	-0.929822000
6	2.664700000	0.824509000	0.156402000
6	0.275616000	-1.206194000	-1.477743000
6	-1.005875000	-0.690106000	-1.900458000
6	-1.994441000	-1.052602000	-0.881441000
6	-1.326933000	-1.786303000	0.175598000
6	0.083942000	-1.859602000	-0.185736000
6	2.291862000	2.938613000	-1.677512000
6	3.559373000	2.351039000	-1.502940000
6	3.757796000	1.306965000	-0.588941000
1	4.742791000	0.870850000	-0.476626000
1	-1.960890000	1.347466000	4.330094000
1	-0.279503000	1.384947000	4.906482000
1	-1.043545000	2.877573000	4.372456000
1	0.938216000	1.752857000	1.209722000
6	-0.166689000	2.987551000	-1.060778000
8	-0.453471000	4.072255000	-1.640846000
8	-1.104748000	2.216349000	-0.481581000
1	2.136991000	3.740531000	-2.389879000
6	-1.952124000	-2.366264000	1.394777000
1	-1.244175000	-2.991738000	1.934751000
1	-2.298165000	-1.574008000	2.063252000
1	-2.832335000	-2.949027000	1.117439000
6	-1.255915000	0.056068000	-3.163045000
1	-0.332879000	0.492178000	-3.549832000
1	-1.651761000	-0.628318000	-3.920173000
1	-1.997500000	0.842314000	-3.021348000
6	1.532389000	-1.109057000	-2.272098000
1	1.528078000	-1.880428000	-3.049169000
1	1.614103000	-0.138320000	-2.768282000
1	2.413313000	-1.272849000	-1.653968000
6	-3.416041000	-0.698461000	-0.952752000
8	-4.001312000	-0.289451000	-1.980497000
8	-4.051225000	-0.850908000	0.256455000
6	1.079033000	-2.616183000	0.592399000
8	1.035637000	-2.817879000	1.824644000
8	2.051536000	-3.148016000	-0.219282000
6	-5.486942000	-0.500508000	0.286175000
1	-6.031231000	-1.115372000	-0.429722000
1	-5.798410000	-0.710041000	1.303842000
1	-5.609462000	0.554766000	0.044387000
6	3.023633000	-4.057057000	0.426554000
1	2.515197000	-4.980356000	0.701899000
1	3.781637000	-4.233096000	-0.329115000
1	3.448347000	-3.587695000	1.312901000
8	2.753848000	-0.203980000	1.074839000
6	4.084313000	-0.748489000	1.371322000
1	4.496694000	-1.242417000	0.487163000
1	4.754728000	0.043728000	1.710821000

1	3.920697000	-1.471051000	2.166020000
1	4.401039000	2.699702000	-2.088768000

TS'0_CpE; Gibbs free energy ... -1639.30624790 Eh

45	0.923414000	-0.024367000	0.155079000
8	1.960580000	1.902785000	0.139930000
6	1.339239000	2.995311000	-0.141091000
6	-1.048156000	0.631294000	-0.555670000
6	2.058044000	4.308790000	-0.117983000
8	0.064081000	3.001589000	-0.464084000
6	-1.941907000	0.516101000	0.546736000
6	-1.602149000	0.446328000	-1.849719000
6	0.625351000	-2.173893000	0.114428000
6	1.693683000	-1.898655000	1.081166000
6	2.777803000	-1.259555000	0.389111000
6	2.407332000	-1.159607000	-1.027686000
6	1.113369000	-1.773787000	-1.201311000
6	-3.308663000	0.257665000	0.388272000
6	-3.813505000	0.081057000	-0.911815000
6	-2.959007000	0.177127000	-2.031943000
1	-3.380818000	0.047112000	-3.021687000
1	3.109067000	4.164920000	0.118784000
1	1.960081000	4.796959000	-1.088677000
1	1.601825000	4.965315000	0.624727000
1	-0.362588000	1.830782000	-0.505671000
6	-1.355265000	0.708532000	1.907555000
8	-2.064932000	0.864862000	2.949641000
8	-0.020800000	0.723640000	1.935630000
1	-3.938561000	0.197675000	1.269585000
6	3.269557000	-0.603775000	-2.107807000
1	2.677136000	-0.304929000	-2.974893000
1	3.836768000	0.262428000	-1.759900000
1	3.991332000	-1.358344000	-2.440127000
6	1.624997000	-2.192733000	2.538275000
1	0.594722000	-2.167595000	2.899126000
1	2.021168000	-3.195262000	2.731924000
1	2.214480000	-1.482462000	3.121247000
6	-0.652646000	-2.887949000	0.396841000
1	-0.527423000	-3.969065000	0.272694000
1	-0.989011000	-2.707138000	1.420894000
1	-1.442980000	-2.561321000	-0.284311000
1	-0.966374000	0.540491000	-2.724834000
8	-5.145096000	-0.182780000	-1.199570000
6	-6.070352000	-0.307124000	-0.070296000
1	-5.791098000	-1.154987000	0.560057000
1	-6.080854000	0.610756000	0.522457000
1	-7.044996000	-0.474804000	-0.518339000
6	0.432194000	-2.031846000	-2.499807000
1	-0.649073000	-2.118327000	-2.378764000
1	0.638776000	-1.250345000	-3.234020000
1	0.798880000	-2.978000000	-2.913355000
6	4.065175000	-0.795587000	0.979414000
1	4.409001000	0.128801000	0.509478000

1	3.973911000	-0.621847000	2.053475000
1	4.844717000	-1.550356000	0.828642000

Int1_CpE; Gibbs free energy ... -1639.32544167 Eh

45	-0.113519000	-0.478024000	0.571723000
8	1.040893000	0.032001000	2.321804000
6	2.113365000	0.714361000	2.381023000
6	-0.770475000	1.428457000	0.323439000
6	3.005979000	0.654252000	3.573534000
8	2.554782000	1.506550000	1.401013000
6	-2.070007000	1.661165000	0.808615000
6	-0.123438000	2.475123000	-0.346676000
6	1.068410000	-2.433572000	0.005374000
6	-0.310060000	-2.716629000	-0.080010000
6	-0.912311000	-1.718132000	-0.987086000
6	0.145013000	-0.908084000	-1.586918000
6	1.358879000	-1.291314000	-0.893546000
6	-2.738201000	2.876496000	0.573110000
6	-2.090065000	3.880526000	-0.155128000
6	-0.770396000	3.692592000	-0.608449000
1	-0.266556000	4.488769000	-1.143964000
1	3.326119000	1.654894000	3.859962000
1	2.501966000	0.161855000	4.399728000
1	3.900309000	0.083381000	3.310334000
1	1.971429000	1.642277000	0.565558000
6	-2.656517000	0.564611000	1.612609000
8	-3.802510000	0.594466000	2.147895000
8	-1.832773000	-0.492056000	1.769202000
1	-3.741515000	3.015197000	0.962150000
1	-2.589700000	4.819247000	-0.360033000
8	1.227246000	2.226687000	-0.691850000
6	1.948855000	3.263325000	-1.440213000
1	1.472924000	3.414176000	-2.410827000
1	1.970718000	4.195681000	-0.872330000
1	2.955694000	2.876099000	-1.568358000
6	-0.003655000	0.056752000	-2.712602000
1	0.197899000	-0.465489000	-3.654018000
1	-1.014535000	0.459155000	-2.749197000
1	0.720278000	0.863385000	-2.624659000
6	-1.063880000	-3.757225000	0.676960000
1	-1.299229000	-4.604866000	0.026939000
1	-0.485629000	-4.123962000	1.525945000
1	-2.013696000	-3.364868000	1.045857000
6	2.065654000	-3.139469000	0.860764000
1	1.586463000	-3.912558000	1.462243000
1	2.832719000	-3.609770000	0.239014000
1	2.585473000	-2.445819000	1.525083000
6	-2.351682000	-1.687691000	-1.309113000
8	-3.110158000	-2.679165000	-1.263442000
8	-2.786091000	-0.426051000	-1.625643000
6	2.721526000	-0.791652000	-1.114851000
8	3.691275000	-1.010650000	-0.351968000
8	2.850052000	-0.063752000	-2.274203000

6	-4.231745000	-0.272134000	-1.891326000
1	-4.513019000	-0.861053000	-2.763662000
1	-4.799342000	-0.596015000	-1.018688000
1	-4.364234000	0.789888000	-2.071521000
6	4.204379000	0.464043000	-2.544876000
1	4.088831000	1.087275000	-3.425839000
1	4.549172000	1.044748000	-1.688257000
1	4.888409000	-0.363046000	-2.732154000

Int'1_CpE; Gibbs free energy ... -1639.31404041 Eh

45	-0.636063000	0.161729000	0.547728000
8	-0.306175000	-1.478055000	1.935794000
6	-0.037642000	-2.689942000	1.685008000
6	1.230876000	-0.250244000	-0.146351000
6	0.408550000	-3.645624000	2.733970000
8	-0.113425000	-3.224076000	0.450667000
6	2.262014000	0.299891000	0.641097000
6	1.579259000	-1.022614000	-1.270470000
6	-3.031585000	0.302972000	0.414395000
6	-2.518273000	1.603240000	0.569306000
6	-1.511287000	1.813463000	-0.498233000
6	-1.510527000	0.658886000	-1.396211000
6	-2.363449000	-0.313812000	-0.746458000
6	3.619762000	0.098847000	0.332033000
6	3.945368000	-0.671587000	-0.792708000
6	2.926970000	-1.231649000	-1.591327000
1	3.205619000	-1.826008000	-2.453903000
1	1.449792000	-3.916498000	2.547400000
1	0.323467000	-3.191815000	3.716320000
1	-0.181603000	-4.560232000	2.686958000
1	-0.458853000	-2.616033000	-0.265878000
6	1.844723000	1.101773000	1.815866000
8	2.643521000	1.656383000	2.627320000
8	0.511164000	1.198800000	1.960119000
1	4.372377000	0.544789000	0.974076000
6	-0.909178000	0.544274000	-2.755145000
1	-1.498448000	1.150038000	-3.451067000
1	0.110091000	0.924493000	-2.777303000
1	-0.920924000	-0.489058000	-3.102196000
6	-2.852811000	2.570897000	1.652408000
1	-3.443075000	3.399592000	1.250821000
1	-3.427627000	2.089725000	2.445120000
1	-1.950465000	3.008498000	2.083605000
6	-4.021864000	-0.399392000	1.279553000
1	-4.126644000	0.088479000	2.249320000
1	-5.003382000	-0.409558000	0.795305000
1	-3.736590000	-1.441643000	1.445536000
6	-0.750640000	3.063572000	-0.667421000
8	-0.971561000	4.124557000	-0.045333000
8	0.271893000	2.930763000	-1.574620000
6	-2.725303000	-1.627475000	-1.294248000
8	-3.876929000	-2.083381000	-1.396979000
8	-1.597999000	-2.343631000	-1.683671000

6	1.152956000	4.105624000	-1.743216000
1	0.564606000	4.970735000	-2.046513000
1	1.663539000	4.309590000	-0.801796000
1	1.855576000	3.813403000	-2.516366000
6	-1.839670000	-3.640421000	-2.366232000
1	-0.850146000	-4.061154000	-2.514846000
1	-2.451458000	-4.276369000	-1.727950000
1	-2.338914000	-3.453874000	-3.315078000
1	0.815671000	-1.469427000	-1.901703000
8	5.251240000	-0.943845000	-1.205014000
6	6.331404000	-0.387917000	-0.390153000
1	6.284271000	0.704588000	-0.379982000
1	6.277249000	-0.769167000	0.633485000
1	7.250174000	-0.719177000	-0.865134000

Int2_T_CpE; Gibbs free energy ... -1949.48525046 Eh

45	0.066551000	-0.444257000	-0.030375000
6	-1.829335000	-0.123179000	0.618705000
6	-2.129948000	-0.686498000	1.867780000
6	-2.845845000	0.520578000	-0.112829000
6	0.592097000	-0.503393000	-2.263403000
6	1.714599000	-1.131562000	-1.545228000
6	1.243177000	-2.281807000	-0.849612000
6	-0.203231000	-2.355656000	-1.098705000
6	-0.567844000	-1.334476000	-2.072365000
6	-3.439133000	-0.655673000	2.388453000
6	-4.449893000	-0.050349000	1.636572000
6	-4.160543000	0.541530000	0.391630000
1	-3.633648000	-1.100815000	3.358524000
1	-4.954856000	1.026937000	-0.164299000
6	-0.988418000	-1.275153000	2.604019000
8	-1.071513000	-1.827071000	3.740081000
8	0.189536000	-1.162247000	1.960192000
6	0.257733000	1.858287000	0.410457000
6	1.293345000	1.204904000	0.724868000
6	-1.079299000	-3.365601000	-0.487460000
8	-0.701236000	-4.266829000	0.294443000
8	-2.399196000	-3.186160000	-0.825968000
6	-3.366621000	-4.085373000	-0.163973000
1	-3.178421000	-5.115603000	-0.464383000
1	-3.274204000	-3.987967000	0.918369000
1	-4.336918000	-3.742448000	-0.508324000
6	3.116306000	-0.693149000	-1.564490000
8	4.104024000	-1.428323000	-1.337476000
8	3.243147000	0.636526000	-1.884622000
6	2.014960000	-3.192923000	0.039379000
1	1.997322000	-4.208560000	-0.366158000
1	3.049997000	-2.869055000	0.131912000
1	1.546362000	-3.245308000	1.026538000
6	-1.837524000	-1.262414000	-2.849492000
1	-1.868941000	-0.374550000	-3.479187000
1	-1.893673000	-2.148461000	-3.491454000
1	-2.717435000	-1.276278000	-2.209667000

6	0.672437000	0.671191000	-3.179240000
1	1.183974000	1.506307000	-2.700760000
1	1.246464000	0.414244000	-4.075514000
1	-0.322535000	0.995452000	-3.487344000
6	4.624658000	1.158091000	-1.935571000
1	5.176990000	0.653290000	-2.727733000
1	4.512102000	2.217055000	-2.143826000
1	5.111683000	0.996366000	-0.972882000
6	-0.688477000	2.925702000	0.279787000
6	-1.709680000	3.098841000	1.244034000
6	-0.571237000	3.852247000	-0.783245000
6	-2.595685000	4.177133000	1.140903000
6	-1.457603000	4.930985000	-0.873830000
6	-2.473109000	5.096355000	0.084779000
1	-1.799803000	2.388027000	2.058371000
1	0.209896000	3.717573000	-1.522968000
1	-3.374027000	4.303422000	1.883963000
1	-1.357370000	5.640951000	-1.685928000
1	-3.158933000	5.931705000	0.010016000
6	2.632156000	1.061227000	1.238987000
6	3.462409000	2.208170000	1.291860000
6	3.128804000	-0.176906000	1.696871000
6	4.761251000	2.108279000	1.802399000
6	4.430682000	-0.268254000	2.203338000
6	5.250997000	0.871205000	2.258918000
1	3.083578000	3.157140000	0.928469000
1	2.476691000	-1.043361000	1.677422000
1	5.391144000	2.989115000	1.836692000
1	4.803298000	-1.222643000	2.556244000
1	6.257729000	0.796591000	2.652055000
1	-5.466775000	-0.019980000	2.008960000
8	-2.460229000	1.127671000	-1.301730000
6	-3.472990000	1.872887000	-2.040977000
1	-2.948212000	2.303651000	-2.890753000
1	-4.270596000	1.208774000	-2.389423000
1	-3.894340000	2.669747000	-1.419210000

Int'2_T_CpE; Gibbs free energy ... -1949.48307778 Eh

45	0.311899000	-0.366295000	-0.010120000
6	-1.661979000	-0.048917000	0.419125000
6	-1.982625000	-0.141030000	1.789953000
6	-2.681856000	0.201583000	-0.504182000
6	1.393140000	-0.806382000	-1.987827000
6	2.153110000	-1.494204000	-0.950659000
6	1.294794000	-2.450756000	-0.308211000
6	-0.012522000	-2.357018000	-0.950852000
6	0.065525000	-1.377774000	-2.031110000
6	-3.302601000	0.007117000	2.234836000
6	-4.319488000	0.246273000	1.298294000
6	-4.012661000	0.342581000	-0.073462000
1	-3.531150000	-0.058556000	3.293619000
1	-4.785574000	0.536739000	-0.807977000
6	-0.857942000	-0.388603000	2.719213000

8	-0.970213000	-0.493652000	3.975862000
8	0.330996000	-0.497152000	2.102914000
6	0.283023000	1.960229000	-0.201499000
6	1.334997000	1.560309000	0.370641000
6	-1.187202000	-3.141901000	-0.532129000
8	-1.342553000	-3.661280000	0.595931000
8	-2.135830000	-3.231764000	-1.519761000
6	-3.387800000	-3.926031000	-1.148829000
1	-3.165726000	-4.953152000	-0.862029000
1	-3.864738000	-3.399859000	-0.320817000
1	-3.999619000	-3.890505000	-2.043709000
6	3.568726000	-1.327184000	-0.623175000
8	4.207903000	-2.016049000	0.206364000
8	4.157316000	-0.318952000	-1.353045000
6	1.675155000	-3.359899000	0.807099000
1	0.838926000	-3.986665000	1.106386000
1	2.520409000	-3.980146000	0.499096000
1	2.016202000	-2.785443000	1.672992000
6	-0.933368000	-1.074676000	-3.097203000
1	-0.938405000	-0.009544000	-3.345563000
1	-0.662745000	-1.621793000	-4.006906000
1	-1.937315000	-1.381833000	-2.817366000
6	1.896105000	0.226896000	-2.937109000
1	2.365924000	1.062593000	-2.415037000
1	2.664719000	-0.208603000	-3.581822000
1	1.091875000	0.603524000	-3.569610000
6	5.588772000	-0.081892000	-1.084541000
1	6.169090000	-0.953118000	-1.387867000
1	5.843501000	0.789086000	-1.680214000
1	5.736243000	0.111572000	-0.020671000
1	-2.465488000	0.325697000	-1.559226000
8	-5.606987000	0.381306000	1.821247000
6	-6.681044000	0.698599000	0.881574000
1	-6.494131000	1.658590000	0.391216000
1	-6.786807000	-0.087403000	0.128621000
1	-7.581058000	0.754996000	1.487009000
6	-0.811653000	2.732427000	-0.707585000
6	-1.756413000	3.282711000	0.191910000
6	-0.977253000	2.929393000	-2.097561000
6	-2.838061000	4.023099000	-0.294822000
6	-2.064692000	3.669149000	-2.576147000
6	-2.998747000	4.215603000	-1.678316000
1	-1.635811000	3.113689000	1.256260000
1	-0.256913000	2.504347000	-2.787783000
1	-3.557464000	4.439792000	0.399727000
1	-2.185343000	3.816656000	-3.642311000
1	-3.842162000	4.784184000	-2.050957000
6	2.656614000	1.686418000	0.930724000
6	3.442680000	2.803869000	0.554022000
6	3.182702000	0.739987000	1.836418000
6	4.721655000	2.974880000	1.096028000
6	4.463514000	0.920709000	2.373072000
6	5.234616000	2.038953000	2.011397000

1	3.043357000	3.521939000	-0.153275000
1	2.574728000	-0.113417000	2.118619000
1	5.315258000	3.833932000	0.807281000
1	4.859102000	0.192685000	3.071152000
1	6.223661000	2.175730000	2.431702000

Int2_H_CpE; Gibbs free energy ... -1644.75024444 Eh

45	-0.342906000	0.096589000	-0.087507000
6	1.277529000	1.104911000	-0.786010000
6	1.021932000	1.977237000	-1.859016000
6	2.597087000	0.997760000	-0.304557000
6	-1.367952000	-1.565296000	1.197552000
6	-1.727210000	-1.736297000	-0.179324000
6	-0.504980000	-1.965777000	-0.963941000
6	0.592718000	-1.979561000	-0.020143000
6	0.083124000	-1.687819000	1.298251000
6	2.047566000	2.742872000	-2.448816000
6	3.347534000	2.634710000	-1.949814000
6	3.627957000	1.762415000	-0.880863000
1	1.805956000	3.396683000	-3.280337000
1	4.641739000	1.686835000	-0.504388000
1	4.152521000	3.215190000	-2.384151000
6	-0.375403000	2.016459000	-2.342764000
8	-0.793123000	2.744676000	-3.292199000
8	-1.195854000	1.180063000	-1.684233000
6	-0.191035000	1.698581000	1.553703000
6	-1.366344000	1.702574000	1.103359000
6	-2.791658000	1.986737000	0.864487000
1	-2.899470000	2.440992000	-0.125435000
1	-3.349331000	1.043095000	0.831406000
6	0.977319000	2.045105000	2.384217000
1	1.688944000	2.623128000	1.783035000
1	1.503410000	1.136157000	2.689089000
6	-3.368861000	2.907924000	1.954242000
1	-3.311855000	2.430495000	2.936335000
1	-2.820203000	3.851672000	2.000177000
1	-4.416300000	3.126063000	1.736410000
6	0.544621000	2.850846000	3.622529000
1	-0.112601000	2.253733000	4.260704000
1	1.423287000	3.135989000	4.204592000
1	0.009141000	3.758827000	3.334327000
8	2.803967000	0.100907000	0.745421000
6	4.111981000	0.114537000	1.396715000
1	4.903459000	-0.172272000	0.697890000
1	4.322274000	1.105337000	1.811040000
1	4.038989000	-0.620285000	2.196100000
6	1.982314000	-2.308998000	-0.380038000
8	2.513019000	-2.129625000	-1.497446000
8	2.628971000	-2.936473000	0.657539000
6	4.007455000	-3.386106000	0.374169000
1	3.984170000	-4.164724000	-0.387948000
1	4.607650000	-2.545030000	0.027868000
1	4.375593000	-3.770507000	1.319662000

6	-3.059883000	-1.680384000	-0.791683000
8	-3.341672000	-2.106820000	-1.933964000
8	-3.996916000	-1.084959000	0.022470000
6	-0.433672000	-2.268087000	-2.422617000
1	0.590313000	-2.181076000	-2.782068000
1	-0.791984000	-3.285331000	-2.609530000
1	-1.078562000	-1.598640000	-2.993592000
6	0.824258000	-1.634389000	2.588921000
1	0.288851000	-1.016579000	3.314644000
1	0.923456000	-2.640511000	3.009412000
1	1.826888000	-1.233486000	2.446924000
6	-2.234216000	-1.314627000	2.386111000
1	-3.288331000	-1.308595000	2.123315000
1	-2.054074000	-2.082735000	3.144092000
1	-1.989721000	-0.348784000	2.846947000
6	-5.363579000	-0.970699000	-0.526785000
1	-5.768869000	-1.963598000	-0.718044000
1	-5.925324000	-0.458559000	0.247754000
1	-5.341507000	-0.388517000	-1.447585000

Int'2_H_CpE; Gibbs free energy ... -1644.74333695 Eh

45	0.471011000	-0.057147000	-0.052856000
6	-1.521588000	-0.452658000	-0.173920000
6	-1.903873000	-1.179925000	-1.323185000
6	-2.509169000	-0.021105000	0.718172000
6	2.076543000	1.133072000	1.129991000
6	2.343315000	1.321099000	-0.272669000
6	1.179105000	1.960382000	-0.884429000
6	0.215876000	2.186971000	0.170118000
6	0.746342000	1.654571000	1.413568000
6	-3.248508000	-1.484388000	-1.572184000
6	-4.229776000	-1.048129000	-0.669673000
6	-3.864434000	-0.310139000	0.474139000
1	-3.523814000	-2.045963000	-2.458853000
1	-4.612411000	0.043729000	1.174144000
6	-0.821207000	-1.558699000	-2.259960000
8	-0.989451000	-2.232331000	-3.319962000
8	0.385670000	-1.100963000	-1.892925000
6	0.330923000	-1.784696000	1.424261000
6	1.265439000	-2.042358000	0.621252000
6	2.403512000	-2.662804000	-0.076739000
1	2.058918000	-3.046875000	-1.041484000
1	3.158970000	-1.898716000	-0.293665000
6	-0.595187000	-1.908178000	2.565211000
1	-1.561820000	-2.276499000	2.205716000
1	-0.785428000	-0.922813000	3.003882000
6	3.027128000	-3.788728000	0.768327000
1	3.405912000	-3.398202000	1.717013000
1	2.292133000	-4.567033000	0.986130000
1	3.858872000	-4.240297000	0.223916000
6	-0.020904000	-2.859433000	3.630539000
1	0.923346000	-2.476346000	4.026549000
1	-0.727960000	-2.960238000	4.456279000

1	0.161473000	-3.850610000	3.207925000
6	-1.098993000	2.821801000	-0.016730000
8	-1.653114000	3.069590000	-1.110421000
8	-1.685020000	3.121634000	1.189308000
6	-3.032780000	3.725202000	1.122240000
1	-2.963138000	4.717049000	0.676964000
1	-3.687910000	3.090863000	0.524812000
1	-3.362801000	3.776918000	2.154436000
6	3.538023000	0.955370000	-1.037413000
8	3.769275000	1.295779000	-2.220259000
8	4.414083000	0.164116000	-0.323001000
6	1.050290000	2.354246000	-2.316000000
1	0.021086000	2.606914000	-2.559905000
1	1.685853000	3.223467000	-2.513456000
1	1.404511000	1.558846000	-2.972512000
6	0.188211000	1.749890000	2.794362000
1	0.690279000	1.047164000	3.462939000
1	0.341214000	2.759472000	3.189052000
1	-0.885561000	1.564557000	2.824317000
6	2.948188000	0.555340000	2.193777000
1	3.862521000	0.134608000	1.786705000
1	3.203506000	1.337820000	2.916161000
1	2.417226000	-0.226510000	2.747245000
6	5.628969000	-0.273069000	-1.039711000
1	6.209862000	0.595492000	-1.347595000
1	6.172293000	-0.872985000	-0.316645000
1	5.348029000	-0.865228000	-1.910715000
1	-2.251693000	0.542351000	1.610756000
8	-5.546784000	-1.386914000	-0.988622000
6	-6.590378000	-0.945959000	-0.064437000
1	-6.435994000	-1.376770000	0.928876000
1	-6.611350000	0.145308000	0.004813000
1	-7.521779000	-1.311331000	-0.487246000

TS2_T_CpE; Gibbs free energy ... -1949.46297632 Eh

45	0.459745000	-0.509209000	0.400158000
6	-1.420490000	-0.227347000	1.296849000
6	-1.314723000	-0.103232000	2.703874000
6	-2.637488000	-0.711288000	0.754175000
6	1.629207000	-1.159435000	-1.444334000
6	2.299606000	-1.609340000	-0.253875000
6	1.426123000	-2.572522000	0.457307000
6	0.228723000	-2.714619000	-0.298546000
6	0.312661000	-1.789598000	-1.427239000
6	2.151423000	-0.238810000	-2.496102000
6	-2.398082000	-0.404712000	3.544642000
6	-3.591797000	-0.877073000	2.984006000
6	-3.711946000	-1.043068000	1.592067000
6	1.761965000	-3.307181000	1.710619000
6	-0.919181000	-3.603142000	0.050154000
1	-0.794757000	-4.582998000	-0.421255000
1	-2.280304000	-0.293243000	4.616780000
1	-4.636533000	-1.424208000	1.174797000

1	0.872698000	-3.775855000	2.135802000
1	-1.863628000	-3.189856000	-0.304575000
1	1.338233000	0.147409000	-3.109758000
1	2.496363000	-4.093006000	1.505496000
1	-0.984107000	-3.756370000	1.130659000
1	2.702815000	0.593613000	-2.054390000
1	2.204257000	-2.644336000	2.454208000
1	2.854234000	-0.778337000	-3.137766000
6	0.018198000	0.265960000	3.238049000
8	0.226539000	0.644694000	4.428678000
8	1.013701000	0.132633000	2.349102000
6	-0.883306000	1.406502000	0.276225000
6	0.400124000	1.530880000	0.094515000
6	-0.659178000	-1.645301000	-2.525746000
6	3.650194000	-1.255295000	0.195602000
6	-2.238104000	-2.844526000	-3.923688000
1	-1.633110000	-2.849197000	-4.829903000
1	-2.802454000	-3.765645000	-3.823429000
1	-2.892280000	-1.973730000	-3.921485000
6	5.763213000	-0.251165000	-0.420184000
1	6.155149000	0.245596000	-1.301721000
1	5.718125000	0.428564000	0.431007000
1	6.355604000	-1.129032000	-0.164062000
8	-0.820555000	-0.624480000	-3.228465000
8	4.107029000	-1.460547000	1.343404000
8	-1.342581000	-2.817434000	-2.747698000
8	4.397082000	-0.666962000	-0.799514000
6	1.495525000	2.406380000	-0.251135000
6	1.304734000	3.456262000	-1.181699000
6	2.777674000	2.203980000	0.309340000
6	2.378298000	4.280445000	-1.541081000
6	3.842914000	3.038780000	-0.046949000
6	3.649173000	4.074923000	-0.976788000
1	0.326176000	3.608941000	-1.623820000
1	2.912705000	1.405144000	1.034132000
1	2.226466000	5.073953000	-2.262924000
1	4.820018000	2.885059000	0.395296000
1	4.479490000	4.710819000	-1.259447000
6	-2.144871000	2.058835000	-0.067073000
6	-3.131335000	2.315004000	0.909350000
6	-2.347063000	2.503696000	-1.393057000
6	-4.291869000	3.018831000	0.569159000
6	-3.514151000	3.201867000	-1.729725000
6	-4.487939000	3.461653000	-0.751136000
1	-2.975841000	1.973109000	1.928062000
1	-1.597917000	2.287332000	-2.147897000
1	-5.040318000	3.217864000	1.326550000
1	-3.664784000	3.536542000	-2.748945000
1	-5.388586000	4.003251000	-1.014094000
1	-4.431364000	-1.130698000	3.619271000
8	-2.682131000	-0.795989000	-0.629713000
6	-3.993016000	-0.979490000	-1.253455000
1	-3.836240000	-0.767233000	-2.308663000

1	-4.342208000	-2.007071000	-1.117895000
1	-4.718514000	-0.274590000	-0.836924000

TS'2_T_CpE; Gibbs free energy ... -1949.46043088 Eh

45	-0.449526000	-0.593428000	-0.239030000
6	1.561477000	-0.172552000	-0.679110000
6	1.812888000	-0.305354000	-2.071181000
6	2.627708000	-0.373268000	0.221369000
6	-1.804203000	-1.000813000	1.526402000
6	-2.310956000	-1.730100000	0.394192000
6	-1.298593000	-2.722736000	-0.024005000
6	-0.193619000	-2.638387000	0.869840000
6	-0.461138000	-1.522609000	1.774723000
6	-2.486763000	0.074180000	2.303980000
6	3.094677000	-0.587863000	-2.546486000
6	4.143255000	-0.790126000	-1.631272000
6	3.906510000	-0.696737000	-0.242565000
6	-1.441774000	-3.680974000	-1.156982000
6	1.037256000	-3.481331000	0.829305000
1	0.980858000	-4.273044000	1.581841000
1	3.269075000	-0.689444000	-3.612118000
1	4.703904000	-0.855945000	0.472750000
1	-0.502436000	-4.198312000	-1.355635000
1	1.929712000	-2.893161000	1.052373000
1	-1.759354000	0.689446000	2.833142000
1	-2.205853000	-4.429689000	-0.925494000
1	1.163893000	-3.947192000	-0.149870000
1	-3.094466000	0.702225000	1.651006000
1	-1.765582000	-3.171308000	-2.065276000
1	-3.165721000	-0.374270000	3.035530000
6	0.641101000	-0.253477000	-2.981811000
8	0.724894000	-0.121428000	-4.237875000
8	-0.534334000	-0.398326000	-2.353989000
6	0.567365000	1.520133000	-0.178959000
6	-0.715702000	1.448116000	-0.384283000
6	0.408536000	-1.048292000	2.865202000
6	-3.640773000	-1.626356000	-0.208864000
6	2.180837000	-1.651749000	4.397452000
1	1.613603000	-1.345069000	5.275411000
1	2.759766000	-2.547136000	4.596207000
1	2.816929000	-0.834017000	4.057742000
6	-5.898277000	-0.789271000	0.070524000
1	-6.364176000	-0.057342000	0.722655000
1	-5.868928000	-0.441664000	-0.961864000
1	-6.410963000	-1.749311000	0.126091000
8	0.410501000	0.107689000	3.344989000
8	-3.978293000	-2.112199000	-1.313810000
8	1.247216000	-2.037424000	3.316627000
8	-4.525274000	-0.938836000	0.593621000
6	-1.954231000	2.162102000	-0.583008000
6	-2.126692000	3.462851000	-0.048923000
6	-3.018558000	1.560357000	-1.292144000
6	-3.343093000	4.134623000	-0.219962000

6	-4.228101000	2.241117000	-1.465611000
6	-4.397674000	3.527108000	-0.924245000
1	-1.316015000	3.930862000	0.499058000
1	-2.867958000	0.572915000	-1.719319000
1	-3.470811000	5.125571000	0.199020000
1	-5.035246000	1.771561000	-2.015534000
1	-5.339054000	4.048409000	-1.049689000
6	1.578684000	2.413741000	0.372714000
6	2.780983000	2.684734000	-0.317212000
6	1.306265000	3.085450000	1.586842000
6	3.687456000	3.620376000	0.191453000
6	2.224106000	4.013854000	2.096770000
6	3.413997000	4.284034000	1.401587000
1	2.986735000	2.172418000	-1.251807000
1	0.387178000	2.866227000	2.120872000
1	4.600236000	3.834821000	-0.350786000
1	2.012852000	4.520065000	3.030815000
1	4.122296000	5.001552000	1.797928000
1	2.476144000	-0.241411000	1.289033000
8	5.379279000	-1.088765000	-2.187209000
6	6.488883000	-1.357352000	-1.268873000
1	6.706218000	-0.477467000	-0.658202000
1	6.255827000	-2.210713000	-0.627121000
1	7.335978000	-1.589561000	-1.907077000

TS2_H_CpE; Gibbs free energy ... -1644.72237388 Eh

45	0.394525000	-0.158885000	-0.221723000
6	-1.429077000	-1.205449000	-0.373168000
6	-1.300069000	-2.367081000	-1.180711000
6	-2.702794000	-0.577642000	-0.327214000
6	1.424862000	1.767233000	0.430746000
6	2.114893000	1.189589000	-0.693976000
6	1.203690000	1.200641000	-1.867922000
6	-0.031421000	1.776542000	-1.462003000
6	0.070263000	2.050463000	-0.032689000
6	1.933724000	2.095209000	1.794241000
6	-2.403629000	-2.940414000	-1.827249000
6	-3.657781000	-2.324648000	-1.725870000
6	-3.805526000	-1.133560000	-0.994845000
6	1.541872000	0.736997000	-3.244589000
6	-1.232716000	1.990313000	-2.322033000
1	-1.269683000	3.025307000	-2.674514000
1	-2.258584000	-3.834744000	-2.423135000
1	-4.773180000	-0.648112000	-0.954257000
1	0.654846000	0.719312000	-3.879713000
1	-2.151576000	1.811201000	-1.760561000
1	-4.517818000	-2.749771000	-2.228198000
1	1.147627000	1.969074000	2.538505000
1	2.276733000	1.409555000	-3.697890000
1	-1.219996000	1.333706000	-3.194941000
1	2.803208000	1.499228000	2.057544000
1	1.991132000	-0.256453000	-3.231749000
1	2.238529000	3.147913000	1.815065000

6	0.074916000	-2.879843000	-1.387959000
8	0.343762000	-4.021899000	-1.868069000
8	1.034724000	-2.002119000	-1.062546000
6	-0.698102000	-1.461400000	1.387582000
6	0.592705000	-1.325051000	1.484332000
6	1.896119000	-1.619386000	2.122849000
1	2.569950000	-1.998890000	1.343823000
1	2.338715000	-0.677933000	2.468932000
6	-1.914149000	-1.756127000	2.220220000
1	-2.499114000	-2.537648000	1.720314000
1	-2.544080000	-0.861548000	2.243210000
6	-0.931553000	2.732155000	0.806130000
6	3.481979000	0.664959000	-0.754133000
6	-2.691849000	4.423297000	0.763205000
1	-2.247363000	5.411879000	0.865240000
1	-3.578766000	4.458263000	0.137037000
1	-2.911151000	4.004704000	1.744882000
6	5.556620000	0.297472000	0.436281000
1	5.932833000	0.529469000	1.427086000
1	5.517573000	-0.779265000	0.270718000
1	6.159915000	0.771522000	-0.337333000
8	-1.032341000	2.634672000	2.047722000
8	3.986190000	0.084617000	-1.743874000
8	-1.726379000	3.561681000	0.048429000
8	4.189135000	0.855653000	0.414060000
8	-2.772796000	0.590911000	0.423850000
6	-4.095853000	1.177725000	0.640915000
1	-3.946347000	1.956186000	1.384456000
1	-4.478888000	1.606982000	-0.289491000
1	-4.792947000	0.428800000	1.026667000
6	-1.552921000	-2.176691000	3.646922000
1	-2.467174000	-2.372158000	4.212046000
1	-0.947699000	-3.085638000	3.653351000
1	-0.994370000	-1.388752000	4.159718000
6	1.833092000	-2.624534000	3.283305000
1	1.387670000	-3.568837000	2.959828000
1	2.844048000	-2.826582000	3.644331000
1	1.243742000	-2.233288000	4.114765000

TS'2_H_CpE; Gibbs free energy ... -1644.72294611 Eh

45	0.501209000	-0.088085000	-0.268329000
6	-1.505455000	-0.614545000	0.085189000
6	-1.956174000	-1.552586000	-0.887718000
6	-2.459612000	0.252293000	0.662400000
6	1.923374000	1.500068000	0.496430000
6	2.443521000	0.997776000	-0.750526000
6	1.474926000	1.302311000	-1.817096000
6	0.384818000	2.035873000	-1.250407000
6	0.622043000	2.093593000	0.183346000
6	2.578491000	1.488684000	1.837181000
6	-3.308140000	-1.665342000	-1.210874000
6	-4.241581000	-0.802271000	-0.609276000
6	-3.812912000	0.173437000	0.314102000

6	1.640433000	0.961180000	-3.258395000
6	-0.804861000	2.551941000	-1.990319000
1	-0.730236000	3.632789000	-2.139832000
1	-3.632874000	-2.388929000	-1.950951000
1	-4.517241000	0.860890000	0.766910000
1	0.740665000	1.194088000	-3.828432000
1	-1.726190000	2.373300000	-1.430888000
1	1.863186000	1.732111000	2.620761000
1	2.472937000	1.532576000	-3.681028000
1	-0.894725000	2.077346000	-2.969287000
1	3.034750000	0.520399000	2.045663000
1	1.886695000	-0.092640000	-3.392665000
1	3.388288000	2.224467000	1.854691000
6	-0.920752000	-2.321077000	-1.622545000
8	-1.161956000	-3.353712000	-2.316002000
8	0.309205000	-1.799321000	-1.520333000
6	-0.354016000	-1.389071000	1.446761000
6	0.865156000	-1.637610000	1.068315000
6	2.144509000	-2.380471000	1.095801000
1	2.361717000	-2.711040000	0.071753000
1	2.951874000	-1.685587000	1.362027000
6	-1.219215000	-1.450187000	2.671801000
1	-2.202359000	-1.849785000	2.399788000
1	-1.389785000	-0.427883000	3.027504000
6	-0.251720000	2.725509000	1.186344000
6	3.698653000	0.285490000	-0.969945000
6	-2.029461000	4.335832000	1.528704000
1	-1.493987000	4.837290000	2.333885000
1	-2.553159000	5.047300000	0.899444000
1	-2.713853000	3.592308000	1.938631000
6	5.774866000	-0.457306000	0.029902000
1	6.250253000	-0.348427000	0.999307000
1	5.549156000	-1.502508000	-0.184681000
1	6.395173000	-0.039335000	-0.762513000
8	-0.283270000	2.450179000	2.407780000
8	4.028711000	-0.302435000	-2.027961000
8	-1.066818000	3.673363000	0.622184000
8	4.518434000	0.309836000	0.140794000
6	-0.574391000	-2.285749000	3.780933000
1	-1.226244000	-2.302459000	4.657007000
1	-0.411513000	-3.315661000	3.454521000
1	0.390019000	-1.865179000	4.079122000
6	2.159199000	-3.588854000	2.045690000
1	1.345097000	-4.279600000	1.812973000
1	3.106614000	-4.121743000	1.939455000
1	2.057063000	-3.274798000	3.086291000
1	-2.158228000	0.975746000	1.414028000
8	-5.563559000	-0.977239000	-1.000453000
6	-6.567132000	-0.087985000	-0.411303000
1	-7.513226000	-0.405587000	-0.838943000
1	-6.588512000	-0.199875000	0.675941000
1	-6.360868000	0.952474000	-0.674700000

Int0_CpPh3; Gibbs free energy ... -1758.68599697 Eh

45	-0.276136000	-0.482983000	0.533250000
8	-1.054175000	-1.566298000	2.309604000
6	0.144731000	-1.876660000	2.733226000
6	2.531631000	1.225853000	1.048325000
6	0.356578000	-2.550829000	4.046744000
8	1.143031000	-1.540992000	1.958745000
6	1.647260000	2.308597000	0.932660000
6	3.789662000	1.284486000	0.426450000
6	-1.774133000	-0.907190000	-1.034999000
6	-1.330405000	0.488292000	-1.123769000
6	0.095070000	0.459941000	-1.401016000
6	0.541312000	-0.911757000	-1.498685000
6	-0.604888000	-1.750793000	-1.204125000
6	2.009103000	3.441358000	0.174950000
6	3.247144000	3.467777000	-0.477134000
6	4.151608000	2.399134000	-0.352811000
1	1.319180000	4.274197000	0.100546000
1	5.113996000	2.447530000	-0.847729000
1	0.498769000	-1.791574000	4.819873000
1	-0.512173000	-3.149358000	4.315433000
1	1.249324000	-3.173610000	4.018735000
6	0.336769000	2.287174000	1.660565000
8	-0.203359000	3.370582000	2.045283000
8	-0.210719000	1.101176000	1.932206000
1	-0.623449000	-2.829116000	-1.220467000
1	0.720607000	1.333653000	-1.511322000
1	2.263877000	0.352091000	1.633789000
6	-2.093528000	1.728514000	-0.936680000
6	-3.114934000	1.835435000	0.033827000
6	-1.758755000	2.860504000	-1.711353000
6	-3.794784000	3.044581000	0.210853000
6	-2.443880000	4.068941000	-1.532986000
6	-3.463933000	4.164660000	-0.573216000
1	-3.355031000	0.981742000	0.660012000
1	-0.974470000	2.786633000	-2.457483000
1	-4.568687000	3.121862000	0.964610000
1	-2.180811000	4.929626000	-2.135578000
1	-3.987815000	5.102043000	-0.430327000
6	-3.132600000	-1.412229000	-0.833824000
6	-3.349282000	-2.594133000	-0.090800000
6	-4.230872000	-0.768705000	-1.445848000
6	-4.642134000	-3.107552000	0.054751000
6	-5.521113000	-1.293278000	-1.307357000
6	-5.731619000	-2.459253000	-0.552793000
1	-2.509952000	-3.088167000	0.387634000
1	-4.069826000	0.123335000	-2.040790000
1	-4.802495000	-4.006645000	0.636879000
1	-6.354559000	-0.798065000	-1.790010000
1	-6.731088000	-2.861596000	-0.440776000
6	1.905102000	-1.344979000	-1.771391000
6	2.825505000	-0.446068000	-2.357098000
6	2.319909000	-2.662839000	-1.472351000

6	4.127211000	-0.861420000	-2.649786000
6	3.628183000	-3.069243000	-1.752784000
6	4.534381000	-2.171275000	-2.344485000
1	2.518119000	0.565949000	-2.598108000
1	1.625045000	-3.357933000	-1.013595000
1	4.823338000	-0.167514000	-3.105878000
1	3.940942000	-4.077986000	-1.513822000
1	5.547417000	-2.487182000	-2.563041000
1	3.524095000	4.326095000	-1.077612000
8	4.617780000	0.185235000	0.649221000
6	5.980675000	0.254607000	0.122857000
1	6.454250000	-0.672198000	0.434914000
1	5.973801000	0.320895000	-0.969001000
1	6.511207000	1.112514000	0.545548000

Int'0_CpPh3; Gibbs free energy ... -1758.68522237 Eh

45	-0.586507000	-0.765568000	0.568832000
8	-1.937805000	-1.502879000	2.154624000
6	-1.029257000	-2.296674000	2.664796000
6	2.611133000	-0.255150000	1.262392000
6	-1.279209000	-3.049495000	3.928128000
8	0.106123000	-2.374791000	2.023043000
6	2.180533000	1.081991000	1.333318000
6	3.814843000	-0.556301000	0.605029000
6	-1.900156000	-0.297625000	-1.143812000
6	-0.794079000	0.661360000	-1.086750000
6	0.433937000	-0.097107000	-1.245804000
6	0.112791000	-1.500232000	-1.420978000
6	-1.323100000	-1.623122000	-1.291676000
6	2.942916000	2.112224000	0.752926000
6	4.125729000	1.789843000	0.069587000
6	4.568740000	0.454211000	-0.000825000
1	2.589729000	3.133672000	0.839820000
1	5.491457000	0.232166000	-0.523112000
1	-0.999405000	-2.426744000	4.781452000
1	-2.335853000	-3.295433000	4.022493000
1	-0.677250000	-3.956097000	3.957249000
6	0.930543000	1.446290000	2.073551000
8	0.834967000	2.570406000	2.658657000
8	-0.046913000	0.544627000	2.138494000
1	-1.895345000	-2.532374000	-1.388691000
1	1.427780000	0.326371000	-1.234166000
1	2.018454000	-1.038314000	1.725489000
1	4.162454000	-1.581516000	0.558815000
8	4.937107000	2.726888000	-0.567040000
6	4.526435000	4.129718000	-0.493418000
1	3.549188000	4.271967000	-0.963736000
1	4.489648000	4.465184000	0.546633000
1	5.289455000	4.678813000	-1.037084000
6	-0.837124000	2.107802000	-0.836839000
6	-1.796146000	2.672635000	0.034418000
6	0.127676000	2.946627000	-1.434095000
6	-1.800083000	4.047676000	0.284996000

6	0.118548000	4.325330000	-1.182789000
6	-0.844521000	4.879688000	-0.324755000
1	-2.513569000	2.029465000	0.533866000
1	0.870364000	2.522388000	-2.102397000
1	-2.531302000	4.466924000	0.965086000
1	0.860006000	4.961579000	-1.650812000
1	-0.846195000	5.944542000	-0.125572000
6	-3.339468000	-0.032411000	-1.102097000
6	-4.206967000	-0.935955000	-0.449474000
6	-3.880724000	1.083723000	-1.776903000
6	-5.588014000	-0.713854000	-0.453483000
6	-5.264048000	1.295182000	-1.787506000
6	-6.120274000	0.401960000	-1.121907000
1	-3.791045000	-1.789450000	0.076364000
1	-3.223086000	1.768882000	-2.300354000
1	-6.245999000	-1.403835000	0.060105000
1	-5.672846000	2.149046000	-2.313488000
1	-7.190080000	0.572200000	-1.126404000
6	1.068095000	-2.585821000	-1.603428000
6	2.404145000	-2.303444000	-1.966183000
6	0.670907000	-3.931632000	-1.426750000
6	3.322500000	-3.343028000	-2.143039000
6	1.592278000	-4.967663000	-1.601579000
6	2.921275000	-4.676588000	-1.958898000
1	2.718658000	-1.277417000	-2.121194000
1	-0.349951000	-4.161216000	-1.141301000
1	4.344674000	-3.115635000	-2.419877000
1	1.281745000	-5.994993000	-1.457979000
1	3.636116000	-5.479103000	-2.093373000

TS0_CpPh3; Gibbs free energy ... -1758.66127773 Eh

45	0.267169000	-0.349264000	0.485644000
8	1.664360000	-1.164445000	1.932136000
6	2.344516000	-0.411267000	2.733815000
6	0.534157000	1.759912000	0.930555000
6	3.322400000	-1.032534000	3.684944000
8	2.214286000	0.890431000	2.742891000
6	-0.659350000	2.225258000	1.552914000
6	1.247351000	2.679647000	0.114110000
6	-0.971751000	-0.292666000	-1.351313000
6	-1.099298000	-1.643187000	-0.772551000
6	0.204819000	-2.228320000	-0.747465000
6	1.172683000	-1.293888000	-1.315982000
6	0.432861000	-0.109558000	-1.673111000
6	-1.098520000	3.545306000	1.422579000
6	-0.357387000	4.431179000	0.621344000
6	0.810679000	4.012001000	-0.032725000
1	1.361908000	4.713379000	-0.647033000
1	4.313010000	-0.606615000	3.519412000
1	3.034324000	-0.798494000	4.711092000
1	3.356946000	-2.110620000	3.551545000
1	1.370369000	1.240061000	1.805899000
6	-1.402908000	1.215431000	2.365552000

8	-2.334775000	1.523903000	3.167603000
8	-0.996960000	-0.046101000	2.183437000
1	-2.004020000	3.862805000	1.926965000
8	2.401035000	2.183308000	-0.469448000
6	3.217974000	3.104506000	-1.268130000
1	2.661278000	3.434326000	-2.148841000
1	3.524117000	3.965601000	-0.669982000
1	4.087350000	2.525579000	-1.566186000
1	-0.691488000	5.453998000	0.495736000
1	0.434400000	-3.196047000	-0.327040000
6	2.606580000	-1.524275000	-1.485042000
6	3.416939000	-0.570463000	-2.140535000
6	3.207733000	-2.703265000	-0.989909000
6	4.789886000	-0.789170000	-2.293172000
6	4.581433000	-2.920582000	-1.144877000
6	5.378821000	-1.964980000	-1.796492000
1	2.974126000	0.342021000	-2.524137000
1	2.605643000	-3.445236000	-0.477025000
1	5.398422000	-0.047685000	-2.797348000
1	5.026894000	-3.829646000	-0.759283000
1	6.442242000	-2.133021000	-1.916466000
6	-2.297630000	-2.272756000	-0.204491000
6	-2.455202000	-3.672982000	-0.290856000
6	-3.283780000	-1.508336000	0.458012000
6	-3.584201000	-4.294071000	0.257931000
6	-4.406946000	-2.132578000	1.009660000
6	-4.563509000	-3.526298000	0.908738000
1	-1.703226000	-4.265367000	-0.801382000
1	-3.155558000	-0.435880000	0.557276000
1	-3.699202000	-5.368191000	0.177662000
1	-5.154212000	-1.538910000	1.522165000
1	-5.435311000	-4.006700000	1.336555000
6	-2.044950000	0.622669000	-1.766126000
6	-3.263927000	0.120726000	-2.273762000
6	-1.840732000	2.018199000	-1.743516000
6	-4.258324000	0.997722000	-2.725385000
6	-2.835842000	2.893319000	-2.192394000
6	-4.051806000	2.386360000	-2.681986000
1	-3.425385000	-0.950333000	-2.326603000
1	-0.902555000	2.414129000	-1.365465000
1	-5.187775000	0.599222000	-3.114255000
1	-2.664580000	3.963207000	-2.158249000
1	-4.822862000	3.062754000	-3.030946000
1	0.846770000	0.782796000	-2.119823000

TS'0_CpPh3; Gibbs free energy ... -1758.65655991 Eh

45	-0.697060000	0.026527000	0.420183000
8	-2.236889000	-0.361767000	1.899383000
6	-2.233146000	-1.428259000	2.630289000
6	0.426462000	-1.815232000	0.617751000
6	-3.331376000	-1.648104000	3.625865000
8	-1.306623000	-2.345100000	2.512707000
6	1.674695000	-1.480718000	1.218300000

6	0.419029000	-2.889583000	-0.314852000
6	0.257995000	0.993337000	-1.329594000
6	-0.508049000	2.038733000	-0.622954000
6	-1.879638000	1.644498000	-0.624187000
6	-2.026976000	0.375848000	-1.333434000
6	-0.704254000	-0.002841000	-1.763491000
6	2.846799000	-2.192904000	0.957657000
6	2.797097000	-3.252988000	0.031905000
6	1.581728000	-3.603924000	-0.599766000
1	1.577641000	-4.433118000	-1.296581000
1	-4.041521000	-2.371894000	3.219383000
1	-2.927232000	-2.060630000	4.549337000
1	-3.855818000	-0.716938000	3.825891000
1	-0.506982000	-2.021424000	1.547952000
6	1.666911000	-0.319717000	2.159525000
8	2.632502000	-0.052169000	2.936339000
8	0.547947000	0.410943000	2.119649000
1	3.763510000	-1.900615000	1.458140000
1	-2.669684000	2.182223000	-0.121603000
6	-3.275525000	-0.351988000	-1.564228000
6	-3.276349000	-1.579070000	-2.266445000
6	-4.501157000	0.151135000	-1.072405000
6	-4.468682000	-2.280700000	-2.470360000
6	-5.692642000	-0.553891000	-1.276583000
6	-5.682580000	-1.772103000	-1.975712000
1	-2.347330000	-1.983470000	-2.653526000
1	-4.526248000	1.089068000	-0.528921000
1	-4.454827000	-3.216549000	-3.015673000
1	-6.624718000	-0.156504000	-0.893433000
1	-6.606339000	-2.314925000	-2.135657000
6	0.002207000	3.234041000	0.059726000
6	-0.777493000	4.411505000	0.062093000
6	1.240701000	3.227475000	0.738616000
6	-0.322517000	5.561658000	0.718595000
6	1.687933000	4.375805000	1.400590000
6	0.910026000	5.547408000	1.390993000
1	-1.724717000	4.427703000	-0.466616000
1	1.833980000	2.319783000	0.763415000
1	-0.925529000	6.461391000	0.707243000
1	2.633497000	4.355961000	1.928902000
1	1.258812000	6.435482000	1.904278000
6	1.667651000	1.017716000	-1.745527000
6	2.304647000	2.229761000	-2.091840000
6	2.384508000	-0.190396000	-1.884311000
6	3.631432000	2.229488000	-2.540871000
6	3.710939000	-0.188727000	-2.328478000
6	4.342591000	1.023392000	-2.654207000
1	1.759690000	3.164849000	-2.025895000
1	1.898892000	-1.129292000	-1.633373000
1	4.106792000	3.166348000	-2.805644000
1	4.248248000	-1.126669000	-2.417658000
1	5.371412000	1.027752000	-2.993873000
1	-0.449368000	-0.875046000	-2.346724000

1	-0.512108000	-3.179543000	-0.791344000
8	3.893870000	-4.011596000	-0.329806000
6	5.186441000	-3.673838000	0.277840000
1	5.892030000	-4.382748000	-0.143340000
1	5.471810000	-2.651246000	0.018454000
1	5.137140000	-3.785680000	1.363361000

Int1_CpPh3; Gibbs free energy ... -1758.67398638 Eh

45	-0.256311000	-0.324577000	0.420785000
8	0.811533000	0.424814000	2.189505000
6	1.360030000	1.558355000	2.334445000
6	-1.827459000	0.925985000	0.733807000
6	2.323932000	1.839574000	3.437178000
8	1.150208000	2.599971000	1.513404000
6	-2.924971000	0.315539000	1.375381000
6	-1.985546000	2.250828000	0.299425000
6	1.471575000	-1.440854000	-0.722107000
6	0.258859000	-2.161220000	-0.823758000
6	-0.774340000	-1.314184000	-1.431763000
6	-0.121368000	-0.060997000	-1.765180000
6	1.245268000	-0.106260000	-1.329011000
6	-4.158912000	0.975669000	1.521434000
6	-4.302733000	2.273881000	1.020700000
6	-3.209974000	2.926957000	0.419568000
1	-3.324037000	3.943218000	0.060866000
1	1.911709000	2.597813000	4.105012000
1	2.531141000	0.932616000	3.997872000
1	3.250219000	2.239115000	3.021488000
1	0.431460000	2.505447000	0.796029000
6	-2.674186000	-1.030933000	1.945621000
8	-3.538936000	-1.713955000	2.573098000
8	-1.414742000	-1.465456000	1.775601000
1	0.089037000	-3.142574000	-0.404234000
1	-0.570036000	0.768505000	-2.290186000
6	2.657587000	-1.922919000	0.002987000
6	3.457602000	-1.040918000	0.764532000
6	2.976227000	-3.298372000	0.000998000
6	4.543606000	-1.521524000	1.503209000
6	4.066800000	-3.777914000	0.738478000
6	4.853791000	-2.892877000	1.493651000
1	3.222863000	0.018828000	0.775927000
1	2.376298000	-3.983882000	-0.588608000
1	5.139404000	-0.832278000	2.090434000
1	4.303629000	-4.835167000	0.722424000
1	5.696006000	-3.263492000	2.065672000
6	2.254310000	0.899903000	-1.693363000
6	3.589402000	0.526348000	-1.970698000
6	1.874800000	2.245738000	-1.892057000
6	4.519560000	1.480941000	-2.401751000
6	2.805439000	3.198298000	-2.317859000
6	4.136328000	2.820931000	-2.569097000
1	3.895034000	-0.508865000	-1.873615000
1	0.846470000	2.531396000	-1.699376000

1	5.537545000	1.177644000	-2.615431000
1	2.496404000	4.227830000	-2.457020000
1	4.858414000	3.556320000	-2.903354000
6	-2.165480000	-1.681461000	-1.713189000
6	-3.022559000	-0.780204000	-2.384274000
6	-2.690944000	-2.912518000	-1.263784000
6	-4.366943000	-1.102142000	-2.598838000
6	-4.038214000	-3.231026000	-1.474865000
6	-4.882661000	-2.327690000	-2.141397000
1	-2.640162000	0.172651000	-2.735420000
1	-2.052151000	-3.613256000	-0.736973000
1	-5.011888000	-0.401344000	-3.115393000
1	-4.428084000	-4.176279000	-1.116529000
1	-5.925009000	-2.573747000	-2.305000000
1	-4.974719000	0.466104000	2.023597000
1	-5.248292000	2.794902000	1.107332000
8	-0.819461000	2.865058000	-0.219030000
6	-0.899071000	4.286737000	-0.583035000
1	-1.597286000	4.421091000	-1.410100000
1	-1.206967000	4.882398000	0.279162000
1	0.108602000	4.562388000	-0.887201000

Int'1_CpPh3; Gibbs free energy ... -1758.66563023 Eh

45	-0.048901000	0.284511000	0.392915000
8	-1.034698000	-1.208273000	1.731918000
6	-0.962394000	-2.467525000	1.764568000
6	1.733234000	-0.700471000	0.265131000
6	-1.949004000	-3.334371000	2.464518000
8	0.028399000	-3.157230000	1.147456000
6	2.634505000	-0.390768000	1.318286000
6	2.201352000	-1.520272000	-0.778685000
6	-2.021925000	1.334455000	-0.399364000
6	-0.987883000	2.287314000	-0.285785000
6	0.172060000	1.863510000	-1.080321000
6	-0.219769000	0.630855000	-1.746186000
6	-1.528801000	0.255778000	-1.292248000
6	3.940471000	-0.887849000	1.339857000
6	4.384687000	-1.705005000	0.286557000
6	3.517731000	-2.024139000	-0.774524000
1	3.845132000	-2.648882000	-1.597051000
1	-1.448022000	-3.912926000	3.241885000
1	-2.736275000	-2.729215000	2.904536000
1	-2.377048000	-4.044047000	1.754190000
1	0.685442000	-2.557104000	0.698764000
6	2.121280000	0.502909000	2.388264000
8	2.781976000	0.828497000	3.420201000
8	0.876701000	0.947990000	2.168603000
1	-1.009942000	3.148665000	0.366146000
1	0.357607000	0.083766000	-2.475651000
1	1.562323000	-1.774797000	-1.619523000
6	-3.292529000	1.369710000	0.337775000
6	-3.884220000	0.190035000	0.843716000
6	-3.928891000	2.607168000	0.580414000

6	-5.079302000	0.248333000	1.569515000
6	-5.127315000	2.662062000	1.304216000
6	-5.708301000	1.483595000	1.801393000
1	-3.395719000	-0.766013000	0.688176000
1	-3.492186000	3.520192000	0.188770000
1	-5.511910000	-0.666243000	1.958248000
1	-5.605744000	3.619146000	1.475069000
1	-6.633590000	1.526122000	2.363471000
6	-2.287996000	-0.901022000	-1.791868000
6	-3.631715000	-0.752158000	-2.196647000
6	-1.668493000	-2.161369000	-1.925332000
6	-4.338903000	-1.844608000	-2.715209000
6	-2.377997000	-3.253778000	-2.437598000
6	-3.717390000	-3.099026000	-2.833429000
1	-4.114171000	0.215697000	-2.111052000
1	-0.635129000	-2.282058000	-1.609155000
1	-5.368736000	-1.717288000	-3.026672000
1	-1.892792000	-4.218254000	-2.527238000
1	-4.268862000	-3.943901000	-3.228086000
6	1.434650000	2.587621000	-1.251873000
6	2.494946000	2.002116000	-1.981132000
6	1.636035000	3.853526000	-0.658688000
6	3.722348000	2.659133000	-2.107150000
6	2.865284000	4.512679000	-0.790073000
6	3.914375000	3.918579000	-1.510686000
1	2.362191000	1.024936000	-2.433880000
1	0.835560000	4.324669000	-0.098762000
1	4.527407000	2.191497000	-2.661389000
1	3.004191000	5.484446000	-0.331567000
1	4.866745000	4.426078000	-1.606669000
1	4.605650000	-0.637572000	2.159916000
8	5.703125000	-2.150781000	0.380365000
6	6.201332000	-2.994181000	-0.706249000
1	5.616123000	-3.915059000	-0.777345000
1	6.167373000	-2.457155000	-1.658167000
1	7.229676000	-3.223664000	-0.442983000

Int2_T_CpPh3; Gibbs free energy ... -2068.84134237 Eh

45	0.019162000	0.267339000	0.161444000
6	0.945861000	-1.356281000	0.993484000
6	1.554691000	-1.119096000	2.237886000
6	1.084901000	-2.632263000	0.407348000
6	1.463498000	0.312012000	-1.592135000
6	0.177507000	-0.188468000	-2.020454000
6	-0.803722000	0.871706000	-1.905165000
6	-0.127643000	2.019736000	-1.362887000
6	1.265327000	1.703237000	-1.191023000
6	2.296270000	-2.115896000	2.903842000
6	2.434871000	-3.370213000	2.303463000
6	1.835255000	-3.631430000	1.056602000
1	1.952429000	-4.610840000	0.606377000
6	1.373421000	0.238049000	2.801924000
8	1.850693000	0.621774000	3.913479000

8	0.648352000	1.059347000	2.026883000
1	0.005189000	-1.186740000	-2.386397000
1	-0.559397000	2.991114000	-1.173279000
6	2.698114000	-0.490076000	-1.579668000
6	3.671244000	-0.335097000	-0.567848000
6	2.888164000	-1.485622000	-2.559688000
6	4.815742000	-1.139921000	-0.552075000
6	4.031564000	-2.297432000	-2.539485000
6	5.001771000	-2.125395000	-1.538716000
1	3.515851000	0.397936000	0.218640000
1	2.139055000	-1.627376000	-3.332213000
1	5.551451000	-1.010824000	0.233114000
1	4.163041000	-3.059487000	-3.298698000
1	5.885746000	-2.751857000	-1.523370000
6	2.264283000	2.678465000	-0.735954000
6	3.535857000	2.759772000	-1.344479000
6	1.928510000	3.600279000	0.278700000
6	4.453688000	3.734192000	-0.932290000
6	2.851034000	4.565849000	0.696535000
6	4.117903000	4.634527000	0.092775000
1	3.795614000	2.070473000	-2.140721000
1	0.954777000	3.528205000	0.753953000
1	5.424541000	3.794354000	-1.409449000
1	2.587977000	5.256155000	1.488957000
1	4.833981000	5.380074000	0.417462000
6	-2.216542000	0.774366000	-2.272574000
6	-3.053234000	1.911943000	-2.236170000
6	-2.765207000	-0.461044000	-2.685423000
6	-4.397897000	1.818023000	-2.611630000
6	-4.111282000	-0.554828000	-3.054402000
6	-4.933030000	0.585949000	-3.022758000
1	-2.654943000	2.868274000	-1.912346000
1	-2.141227000	-1.349582000	-2.706669000
1	-5.026242000	2.700319000	-2.581420000
1	-4.517901000	-1.509198000	-3.367592000
1	-5.974564000	0.515817000	-3.312747000
1	2.745101000	-1.889737000	3.865629000
6	-1.859268000	-0.764640000	1.001732000
6	-1.984182000	0.492446000	1.065787000
6	-2.164850000	-2.164717000	1.089534000
6	-1.600690000	-2.988462000	2.091189000
6	-3.080423000	-2.726942000	0.166367000
6	-1.946230000	-4.343498000	2.163335000
6	-3.415230000	-4.083419000	0.242344000
6	-2.849398000	-4.897073000	1.238945000
1	-0.896848000	-2.562915000	2.798362000
1	-3.522241000	-2.092470000	-0.595231000
1	-1.507311000	-4.966498000	2.933903000
1	-4.117072000	-4.502733000	-0.468606000
1	-3.109393000	-5.947427000	1.294372000
6	-2.630947000	1.760428000	1.274075000
6	-4.029961000	1.856415000	1.075687000
6	-1.901833000	2.913447000	1.641486000

6	-4.677067000	3.088101000	1.233598000
6	-2.556379000	4.139959000	1.795889000
6	-3.944249000	4.233855000	1.588838000
1	-4.590452000	0.973900000	0.784774000
1	-0.833345000	2.819208000	1.806041000
1	-5.746587000	3.155657000	1.072935000
1	-1.987674000	5.019322000	2.074154000
1	-4.446340000	5.187167000	1.703180000
1	3.000188000	-4.154480000	2.792849000
8	0.438641000	-2.842155000	-0.810836000
6	0.542230000	-4.168100000	-1.411580000
1	1.581978000	-4.404609000	-1.658890000
1	0.138869000	-4.932160000	-0.739516000
1	-0.055882000	-4.118588000	-2.319031000

Int'2_T_CpPh3; Gibbs free energy ... -2068.83387785 Eh

45	0.303519000	0.219198000	-0.063000000
6	-1.463927000	-0.678513000	-0.557798000
6	-1.959364000	-0.337110000	-1.832773000
6	-2.230733000	-1.514062000	0.266180000
6	-0.639571000	1.316352000	1.699554000
6	0.169323000	0.209115000	2.157747000
6	1.561323000	0.484083000	1.844079000
6	1.601198000	1.741105000	1.150751000
6	0.267020000	2.272923000	1.070097000
6	-3.192703000	-0.824079000	-2.290566000
6	-3.949615000	-1.658102000	-1.455817000
6	-3.475465000	-2.000078000	-0.172923000
1	-4.058392000	-2.635512000	0.484070000
6	-1.129462000	0.583570000	-2.641293000
8	-1.426923000	0.986905000	-3.806607000
8	-0.008160000	0.982658000	-2.021341000
1	-0.200430000	-0.653029000	2.694060000
1	2.489691000	2.252677000	0.811624000
6	-2.100896000	1.390616000	1.865543000
6	-2.938564000	1.898381000	0.848235000
6	-2.689500000	0.879838000	3.040086000
6	-4.327448000	1.904323000	1.009007000
6	-4.083241000	0.883763000	3.199981000
6	-4.907218000	1.395784000	2.186039000
1	-2.501087000	2.260727000	-0.078272000
1	-2.056064000	0.485340000	3.828012000
1	-4.957998000	2.285963000	0.214464000
1	-4.518775000	0.488943000	4.110343000
1	-5.984193000	1.394301000	2.305441000
6	-0.045417000	3.586373000	0.493707000
6	-1.011989000	4.435535000	1.075992000
6	0.688165000	4.049395000	-0.620949000
6	-1.244654000	5.710561000	0.544345000
6	0.448319000	5.319484000	-1.155795000
6	-0.520767000	6.154721000	-0.575256000
1	-1.565990000	4.105056000	1.947633000
1	1.429449000	3.397956000	-1.073959000

1	-1.983309000	6.356737000	1.003238000
1	1.010643000	5.654119000	-2.019049000
1	-0.705814000	7.139485000	-0.987358000
6	2.704447000	-0.365791000	2.177602000
6	3.963915000	-0.149999000	1.574754000
6	2.566000000	-1.413729000	3.114046000
6	5.053803000	-0.965262000	1.898235000
6	3.657666000	-2.227920000	3.437480000
6	4.905450000	-2.007563000	2.829514000
1	4.085286000	0.644216000	0.843748000
1	1.608786000	-1.581389000	3.597018000
1	6.012691000	-0.794771000	1.422585000
1	3.538100000	-3.023756000	4.162538000
1	5.752012000	-2.635028000	3.081222000
1	-3.555876000	-0.549097000	-3.275710000
8	-5.167387000	-2.106664000	-1.979274000
6	-5.981362000	-2.964477000	-1.120426000
1	-5.434097000	-3.871379000	-0.847220000
1	-6.282975000	-2.429007000	-0.215417000
1	-6.854989000	-3.220755000	-1.712787000
1	-1.879984000	-1.799605000	1.253321000
6	1.125404000	-1.810671000	-0.699409000
6	1.899092000	-0.900552000	-1.115496000
6	0.497970000	-3.079982000	-0.460364000
6	-0.114011000	-3.783973000	-1.523981000
6	0.466307000	-3.625292000	0.842354000
6	-0.739094000	-5.013285000	-1.281736000
6	-0.154825000	-4.857610000	1.075312000
6	-0.762953000	-5.553163000	0.015614000
1	-0.098333000	-3.360872000	-2.522365000
1	0.927151000	-3.075402000	1.657637000
1	-1.211451000	-5.544767000	-2.099138000
1	-0.171402000	-5.270368000	2.076802000
1	-1.247839000	-6.504776000	0.197363000
6	3.091398000	-0.311854000	-1.665075000
6	4.267785000	-1.096721000	-1.748119000
6	3.125433000	1.034384000	-2.088395000
6	5.454144000	-0.530984000	-2.228979000
6	4.315610000	1.592106000	-2.568938000
6	5.485227000	0.814700000	-2.635739000
1	4.245072000	-2.129417000	-1.417866000
1	2.208450000	1.612284000	-2.043035000
1	6.353068000	-1.134038000	-2.276304000
1	4.332256000	2.628255000	-2.886091000
1	6.408254000	1.248356000	-3.001705000

Int2_H_CpPh3; Gibbs free energy ... -1764.10221445 Eh

45	-0.243705000	0.190414000	0.336045000
6	0.368645000	-1.670299000	0.931605000
6	1.138217000	-1.681519000	2.112778000
6	0.169368000	-2.901085000	0.265363000
6	1.055371000	0.351957000	-1.491028000
6	-0.252811000	-0.134997000	-1.868934000

6	-1.232615000	0.889977000	-1.588628000
6	-0.517511000	2.038016000	-1.070046000
6	0.876790000	1.737778000	-1.035958000
6	1.694023000	-2.866600000	2.636653000
6	1.486143000	-4.069412000	1.959935000
6	0.727725000	-4.090218000	0.774157000
1	0.576484000	-5.032098000	0.258866000
6	1.364834000	-0.369567000	2.759772000
8	2.019117000	-0.203315000	3.835508000
8	0.824176000	0.664492000	2.099805000
1	-0.454672000	-1.125300000	-2.242445000
1	-0.947435000	2.995423000	-0.817469000
6	2.291498000	-0.447069000	-1.559190000
6	3.294660000	-0.313262000	-0.573066000
6	2.457186000	-1.418866000	-2.567964000
6	4.440626000	-1.114400000	-0.606859000
6	3.602950000	-2.229025000	-2.596047000
6	4.600836000	-2.077794000	-1.619355000
1	3.161453000	0.405104000	0.230614000
1	1.691181000	-1.542052000	-3.327181000
1	5.197757000	-0.998800000	0.159766000
1	3.716370000	-2.972821000	-3.375969000
1	5.485356000	-2.703236000	-1.640606000
6	1.921390000	2.701970000	-0.669699000
6	3.122060000	2.750063000	-1.412175000
6	1.711143000	3.650262000	0.355525000
6	4.092301000	3.718550000	-1.131332000
6	2.686336000	4.614544000	0.638848000
6	3.879419000	4.652497000	-0.103289000
1	3.283690000	2.037976000	-2.214073000
1	0.794420000	3.612733000	0.937228000
1	5.004549000	3.748610000	-1.714794000
1	2.519048000	5.333001000	1.432272000
1	4.631174000	5.402299000	0.112560000
6	-2.679546000	0.782893000	-1.785847000
6	-3.553250000	1.738147000	-1.219224000
6	-3.228672000	-0.287515000	-2.525981000
6	-4.937373000	1.628212000	-1.392534000
6	-4.614077000	-0.397197000	-2.697639000
6	-5.473798000	0.560335000	-2.132655000
1	-3.149585000	2.556468000	-0.631352000
1	-2.571081000	-1.027151000	-2.971725000
1	-5.596548000	2.366079000	-0.951031000
1	-5.021624000	-1.222172000	-3.269544000
1	-6.545738000	0.474347000	-2.264632000
1	2.281266000	-2.816873000	3.547787000
1	1.903131000	-4.995578000	2.337383000
8	-0.594406000	-2.874907000	-0.905159000
6	-0.810170000	-4.134181000	-1.609690000
1	0.140413000	-4.567125000	-1.937482000
1	-1.345002000	-4.850174000	-0.978161000
1	-1.416208000	-3.873204000	-2.474281000
6	-1.973709000	0.656516000	1.709672000

6	-2.214555000	-0.485358000	1.237186000
6	-2.912262000	-1.740165000	0.901599000
1	-2.895175000	-1.876560000	-0.185664000
1	-2.355576000	-2.587094000	1.319004000
6	-2.042835000	1.900370000	2.495180000
1	-2.012901000	2.764758000	1.822022000
1	-1.150329000	1.965574000	3.125587000
6	-4.360892000	-1.737561000	1.418147000
1	-4.391937000	-1.622605000	2.504599000
1	-4.931156000	-0.918556000	0.970395000
1	-4.850001000	-2.678473000	1.156288000
6	-3.318286000	1.942991000	3.357426000
1	-3.360458000	1.081595000	4.028572000
1	-3.330566000	2.853024000	3.960634000
1	-4.213826000	1.931720000	2.729873000

Int'2_H_CpPh3; Gibbs free energy ... -1764.09981517 Eh

45	-0.464123000	0.108606000	0.279136000
6	0.813825000	-1.470764000	0.390330000
6	1.672031000	-1.456599000	1.513933000
6	0.975769000	-2.487349000	-0.563043000
6	0.521341000	1.113552000	-1.476103000
6	-0.544923000	0.250164000	-1.933812000
6	-1.805689000	0.760867000	-1.440960000
6	-1.516860000	1.968561000	-0.696371000
6	-0.111343000	2.205455000	-0.722764000
6	2.666312000	-2.429829000	1.688596000
6	2.824066000	-3.430307000	0.718521000
6	1.979755000	-3.462048000	-0.409632000
1	2.091090000	-4.229300000	-1.166774000
6	1.487424000	-0.342681000	2.471488000
8	2.154817000	-0.192536000	3.540635000
8	0.538881000	0.530747000	2.100477000
1	-0.411007000	-0.631746000	-2.542758000
1	-2.244397000	2.622685000	-0.239847000
6	1.947033000	0.896199000	-1.775197000
6	2.943917000	1.117705000	-0.799186000
6	2.327607000	0.392203000	-3.036154000
6	4.287618000	0.848708000	-1.081765000
6	3.674630000	0.119062000	-3.317029000
6	4.659115000	0.346130000	-2.341950000
1	2.655797000	1.476567000	0.185427000
1	1.570354000	0.222049000	-3.794608000
1	5.039774000	1.012027000	-0.318982000
1	3.953750000	-0.267565000	-4.290173000
1	5.698848000	0.130518000	-2.557903000
6	0.540168000	3.364817000	-0.100446000
6	1.609286000	4.027215000	-0.742389000
6	0.055419000	3.872432000	1.125606000
6	2.183013000	5.167677000	-0.166485000
6	0.632630000	5.010332000	1.700848000
6	1.699134000	5.661783000	1.056972000
1	1.978514000	3.658164000	-1.692972000

1	-0.753923000	3.354206000	1.632200000
1	2.997771000	5.672114000	-0.671877000
1	0.258399000	5.385241000	2.645878000
1	2.146334000	6.542602000	1.502079000
6	-3.127792000	0.170693000	-1.659463000
6	-4.235615000	0.588727000	-0.887988000
6	-3.314704000	-0.839663000	-2.628715000
6	-5.495771000	0.011658000	-1.081080000
6	-4.576379000	-1.415985000	-2.821699000
6	-5.671265000	-0.993119000	-2.049098000
1	-4.103985000	1.352674000	-0.128304000
1	-2.476606000	-1.166550000	-3.235193000
1	-6.335896000	0.336068000	-0.478711000
1	-4.707328000	-2.186739000	-3.571561000
1	-6.646968000	-1.440441000	-2.196602000
1	3.311055000	-2.398715000	2.561232000
6	-2.126281000	-0.372213000	1.730939000
6	-1.968545000	-1.409675000	1.036538000
6	-2.172666000	-2.743355000	0.443186000
1	-2.161383000	-2.651945000	-0.650510000
1	-1.326704000	-3.388518000	0.703170000
6	-2.578156000	0.622505000	2.717823000
1	-2.919089000	1.523388000	2.193944000
1	-1.721806000	0.925877000	3.328809000
6	-3.495511000	-3.375562000	0.907246000
1	-3.507278000	-3.503688000	1.992565000
1	-4.347401000	-2.749157000	0.628027000
1	-3.623060000	-4.356154000	0.443591000
6	-3.710777000	0.072130000	3.603002000
1	-3.382734000	-0.809660000	4.158138000
1	-4.024143000	0.834593000	4.319313000
1	-4.577654000	-0.206981000	2.997313000
8	3.850506000	-4.352089000	0.952422000
6	4.034552000	-5.407434000	-0.041818000
1	3.147065000	-6.044429000	-0.097444000
1	4.244204000	-4.980870000	-1.026964000
1	4.887729000	-5.984285000	0.303322000
1	0.332179000	-2.539339000	-1.435724000

TS2_T_CpPh3; Gibbs free energy ... -2068.82015220 Eh

45	-0.354061000	0.103534000	-0.009025000
6	0.554143000	-1.439042000	-1.108052000
6	-0.082254000	-1.668853000	-2.354935000
6	1.266244000	-2.520097000	-0.519851000
6	-0.010497000	0.451959000	2.192646000
6	-1.014204000	1.406651000	1.781693000
6	-2.156368000	0.697664000	1.289441000
6	-1.900762000	-0.747045000	1.451909000
6	-0.585034000	-0.871593000	1.993587000
6	0.047569000	-2.892460000	-3.030830000
6	0.772744000	-3.933943000	-2.439133000
6	1.369545000	-3.754989000	-1.177676000
1	-0.444569000	-3.014979000	-3.989734000

1	1.905520000	-4.575895000	-0.716171000
6	-0.968742000	-0.593660000	-2.861247000
8	-1.422350000	-0.555148000	-4.047294000
8	-1.289126000	0.323877000	-1.943035000
6	1.316649000	0.755884000	2.732122000
6	2.134406000	-0.272597000	3.248492000
6	1.813265000	2.079511000	2.726490000
6	3.413929000	0.011342000	3.739557000
6	3.092079000	2.362549000	3.219743000
6	3.899952000	1.329555000	3.726614000
1	1.768780000	-1.293208000	3.260751000
1	1.202565000	2.885402000	2.331996000
1	4.030504000	-0.791366000	4.127415000
1	3.457792000	3.382310000	3.206993000
1	4.891178000	1.548055000	4.105560000
6	-2.813812000	-1.874210000	1.203451000
6	-4.175399000	-1.803354000	1.568514000
6	-2.321377000	-3.069329000	0.634212000
6	-5.025009000	-2.896799000	1.353303000
6	-3.170666000	-4.161675000	0.422369000
6	-4.528008000	-4.078211000	0.777848000
1	-4.563376000	-0.895810000	2.019105000
1	-1.275503000	-3.125722000	0.340058000
1	-6.068844000	-2.830513000	1.636994000
1	-2.778528000	-5.069331000	-0.022163000
1	-5.188855000	-4.920106000	0.608381000
6	-3.343690000	1.328766000	0.697314000
6	-3.802863000	2.574026000	1.180628000
6	-4.023219000	0.718869000	-0.380366000
6	-4.926897000	3.185227000	0.608959000
6	-5.141299000	1.333787000	-0.952739000
6	-5.600941000	2.566782000	-0.457528000
1	-3.288985000	3.052237000	2.008153000
1	-3.650619000	-0.216863000	-0.782699000
1	-5.276982000	4.135492000	0.994043000
1	-5.649275000	0.857502000	-1.782734000
1	-6.468346000	3.041608000	-0.900473000
1	-0.911481000	2.481360000	1.795391000
1	-0.097704000	-1.805940000	2.225544000
6	1.670864000	0.200145000	-1.031865000
6	0.990757000	1.318169000	-0.990167000
6	3.065261000	-0.237158000	-0.960202000
6	3.590752000	-1.150555000	-1.898367000
6	3.914302000	0.313927000	0.025133000
6	4.945817000	-1.501973000	-1.855762000
6	5.266410000	-0.050529000	0.071578000
6	5.785889000	-0.958059000	-0.868392000
1	2.937922000	-1.565414000	-2.659863000
1	3.503587000	1.013382000	0.749359000
1	5.345160000	-2.196069000	-2.585678000
1	5.910411000	0.369518000	0.835915000
1	6.832441000	-1.236980000	-0.833931000
6	0.966427000	2.723061000	-1.293371000

6	2.081416000	3.333340000	-1.926209000
6	-0.153628000	3.521584000	-0.961880000
6	2.071085000	4.705724000	-2.196327000
6	-0.155646000	4.893770000	-1.233650000
6	0.957404000	5.492355000	-1.848560000
1	2.941153000	2.729334000	-2.195485000
1	-1.016064000	3.044574000	-0.503400000
1	2.927186000	5.164800000	-2.676650000
1	-1.020032000	5.492624000	-0.972207000
1	0.956520000	6.554689000	-2.061390000
1	0.868378000	-4.889840000	-2.939401000
8	1.844647000	-2.265465000	0.716690000
6	2.855629000	-3.209531000	1.195793000
1	2.394772000	-4.156264000	1.488212000
1	3.612476000	-3.380880000	0.424110000
1	3.308615000	-2.728273000	2.060129000

TS'2_T_CpPh3; Gibbs free energy ... -2068.81347656 Eh

45	0.276483000	-0.200553000	0.144111000
6	-0.960385000	1.393579000	-0.444471000
6	-0.411839000	2.106142000	-1.538106000
6	-1.815020000	2.086671000	0.448438000
6	0.083521000	-1.047862000	2.232985000
6	1.148989000	-1.788153000	1.592709000
6	2.189680000	-0.885792000	1.218012000
6	1.807166000	0.463823000	1.695557000
6	0.527613000	0.336318000	2.313660000
6	-0.744748000	3.448862000	-1.781010000
6	-1.591017000	4.111994000	-0.881112000
6	-2.110037000	3.432037000	0.244434000
1	-0.297995000	3.945108000	-2.636080000
1	-2.745851000	3.973778000	0.934414000
6	0.626011000	1.420499000	-2.345886000
8	1.027496000	1.836639000	-3.476808000
8	1.136578000	0.335191000	-1.757408000
6	-1.173686000	-1.597537000	2.747294000
6	-2.132156000	-0.758243000	3.359069000
6	-1.461443000	-2.975535000	2.621623000
6	-3.341210000	-1.281818000	3.831680000
6	-2.671024000	-3.497436000	3.096197000
6	-3.616997000	-2.653275000	3.702789000
1	-1.931160000	0.302244000	3.468981000
1	-0.741088000	-3.641548000	2.158437000
1	-4.065439000	-0.622362000	4.294840000
1	-2.874847000	-4.556547000	2.994098000
1	-4.553445000	-3.056675000	4.069212000
6	2.576540000	1.715851000	1.621269000
6	3.959972000	1.751101000	1.896202000
6	1.912947000	2.920974000	1.302118000
6	4.661200000	2.963602000	1.839977000
6	2.614835000	4.130331000	1.244141000
6	3.994690000	4.155816000	1.510390000
1	4.482118000	0.836437000	2.156695000

1	0.848457000	2.895970000	1.079753000
1	5.723053000	2.977872000	2.055918000
1	2.089399000	5.042560000	0.984361000
1	4.543469000	5.088861000	1.462912000
6	3.387156000	-1.268789000	0.457027000
6	3.954516000	-2.551380000	0.631925000
6	3.958350000	-0.392986000	-0.492964000
6	5.070576000	-2.943460000	-0.119747000
6	5.071839000	-0.788046000	-1.242960000
6	5.633931000	-2.063302000	-1.058957000
1	3.529544000	-3.233054000	1.361509000
1	3.506808000	0.577182000	-0.664274000
1	5.499293000	-3.927512000	0.027696000
1	5.493435000	-0.107581000	-1.973050000
1	6.496245000	-2.366491000	-1.640702000
1	1.135392000	-2.843410000	1.362759000
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TS2_H_CpPh3; Gibbs free energy ... -1764.07618999 Eh

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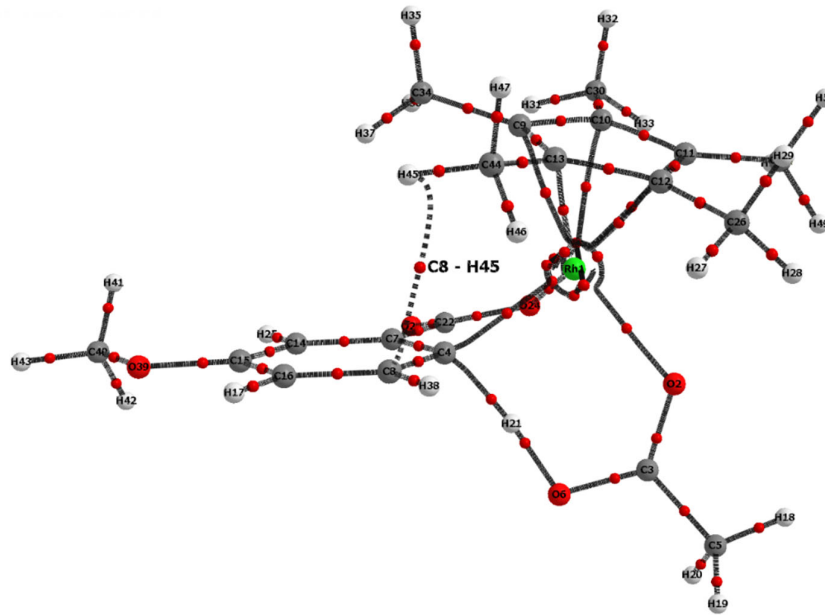
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TS'2_H_CpPh3; Gibbs free energy ... -1764.06959367 Eh

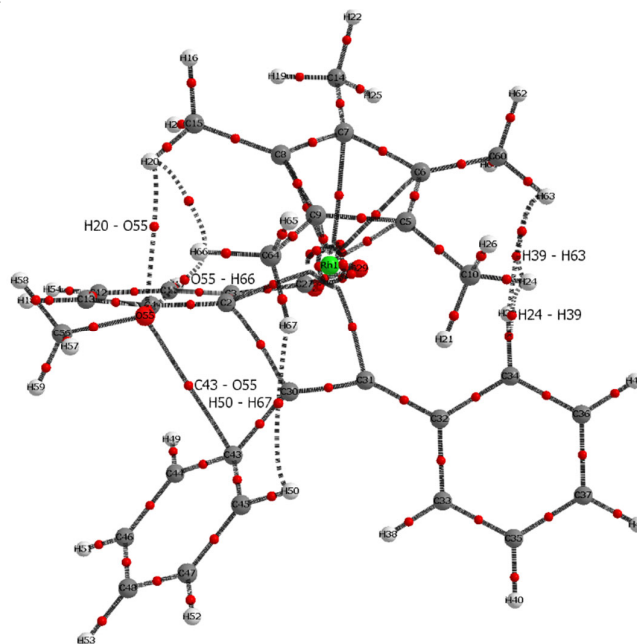
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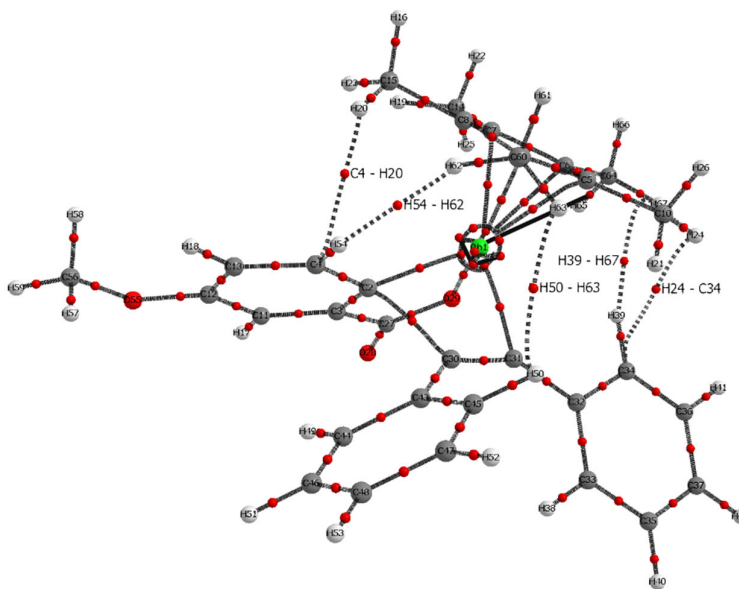
Transition state	BCP	$q(r)$	$\nabla^2 q(r)$	$H(r)$
TS'0_Cp*	C8-H45	0.006939	0.028227	0.001633

Figure S7. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS'0_Cp***.



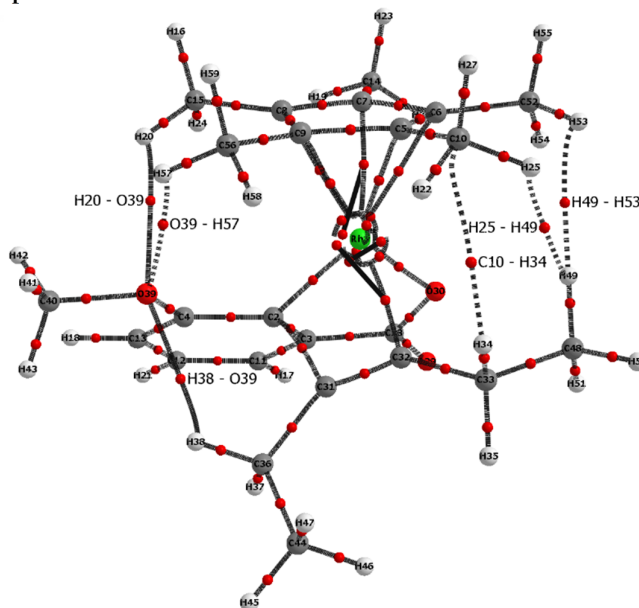
Transition state	BCP	$q(r)$	$\nabla^2 q(r)$	$H(r)$
TS1_T_Cp*	H20-O55	0.008827	0.037122	0.001937
	O55-H66	0.009232	0.042551	0.002365
	C43-O55	0.011001	0.045354	0.001850
	H50-H67	0.001244	0.004750	0.000355
	H24-H39	0.005043	0.021054	0.001531
	H39-H63	0.007741	0.034178	0.002156

Figure S8. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS1_T_Cp***.



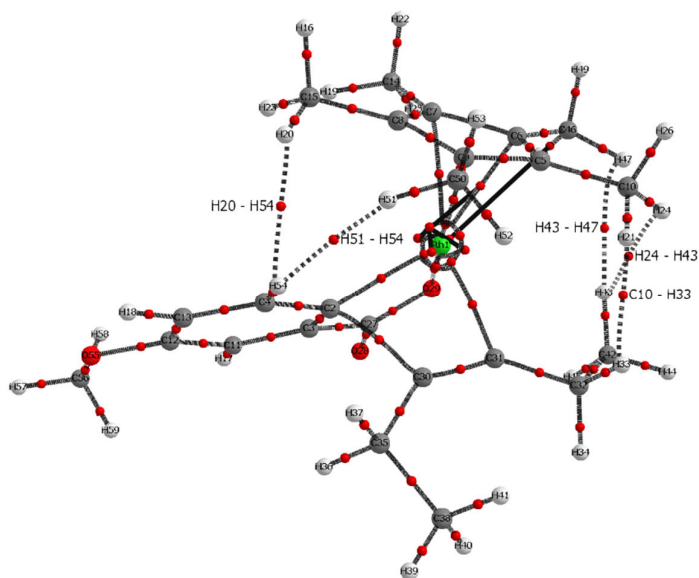
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'1_T_Cp*	C4-H20	0.007507	0.029983	0.001857
	H54-H62	0.003609	0.015923	0.001248
	H50-H63	0.002523	0.010905	0.000883
	H39-H67	0.007371	0.032628	0.002030
	H24-C34	0.004784	0.019581	0.001397

Figure S9. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS'1_T_Cp*.



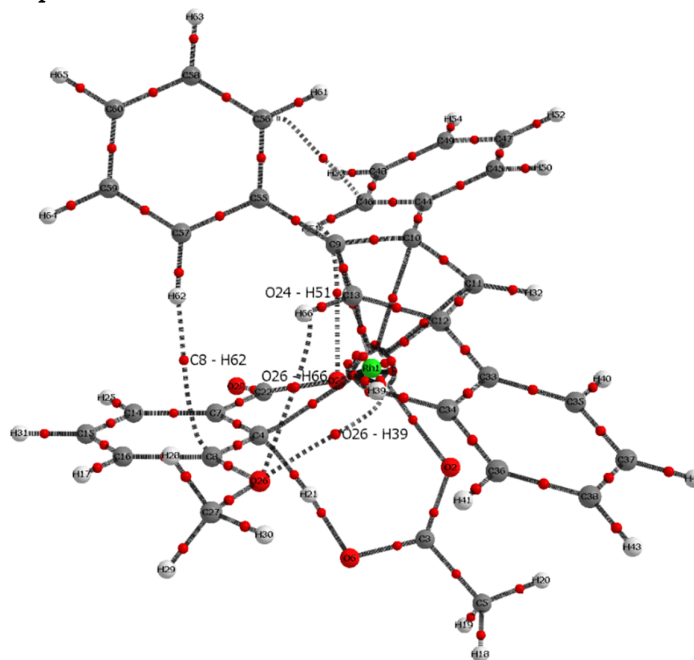
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_H_Cp*	H20-O39	0.011231	0.047304	0.002195
	O39-H57	0.009630	0.042898	0.002254
	H38-O39	0.012681	0.056070	0.002542
	C10-H34	0.006047	0.026452	0.001762
	H25-H49	0.004357	0.019183	0.001445
	H49-H53	0.006121	0.025983	0.001789

Figure S10. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS1_H_Cp*.



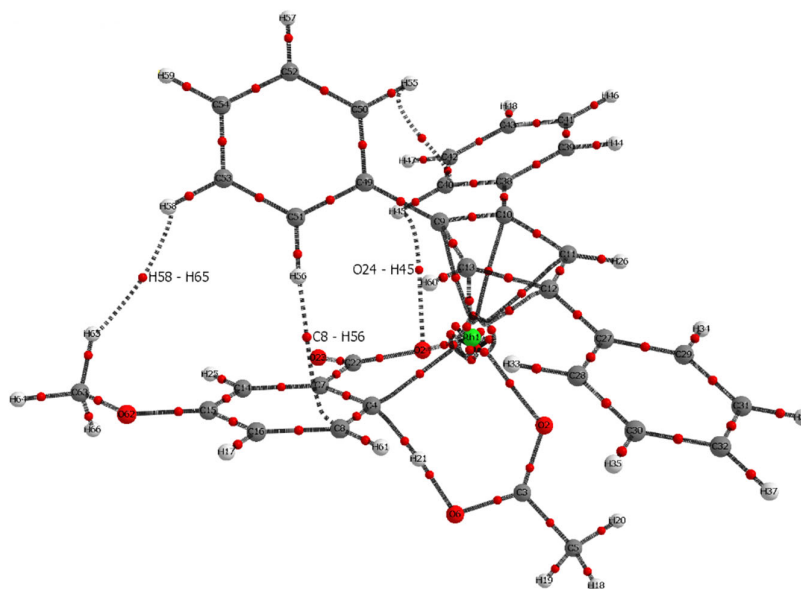
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'1_H_Cp*	H20-H54	0.006785	0.029246	0.002013
	H51-H54	0.003051	0.013174	0.001033
	H43-H47	0.005645	0.023982	0.001690
	H24-H43	0.003473	0.014989	0.001144
	C10-H33	0.005341	0.023619	0.001636

Figure S11. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS'1_H_Cp***.



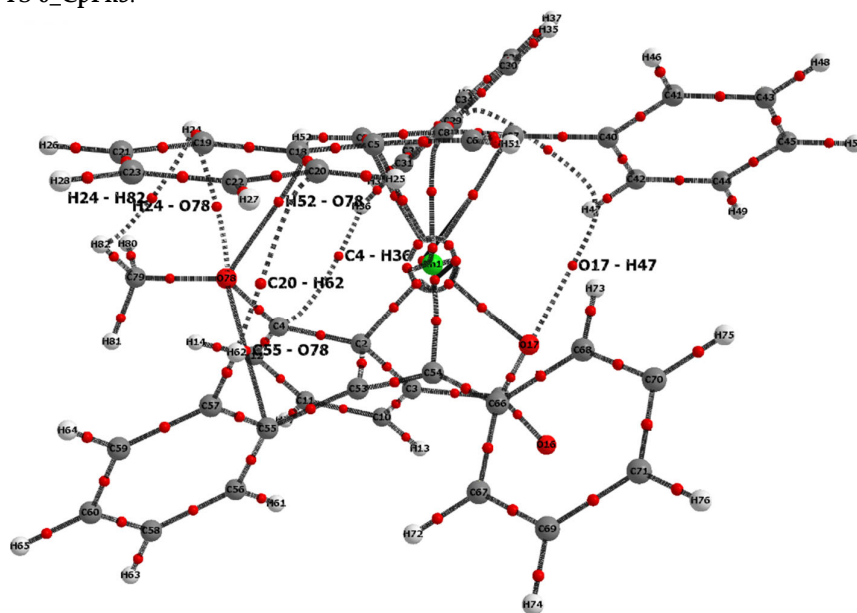
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS0_CpPh3	O26-H39	0.004922	0.021351	0.001313
	O26-H66	0.007092	0.031068	0.001750
	C8-H62	0.008363	0.033072	0.001894
	O24-H51	0.006970	0.028554	0.001550

Figure S12. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS0_CpPh3**.



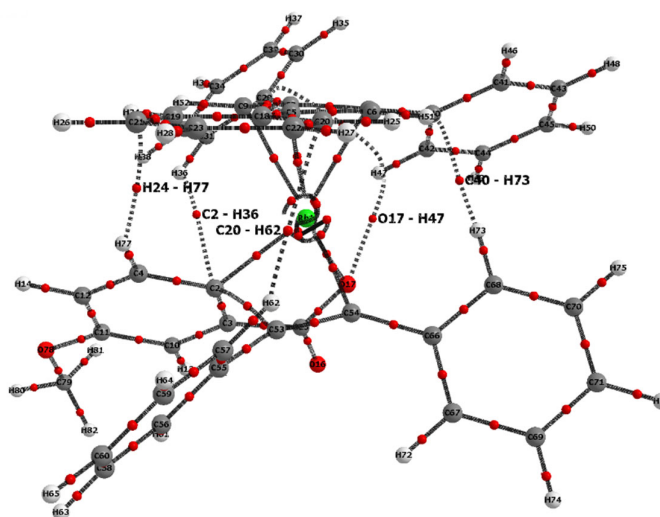
Transition state	BCP	$q(r)$	$\nabla^2 q(r)$	$H(r)$
TS'0_CpPh3	H58-H65	0.000887	0.003478	0.000245
	C8-H56	0.008206	0.032427	0.001879
	O24-H45	0.007440	0.030992	0.001712

Figure S13. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS'0_CpPh3**.



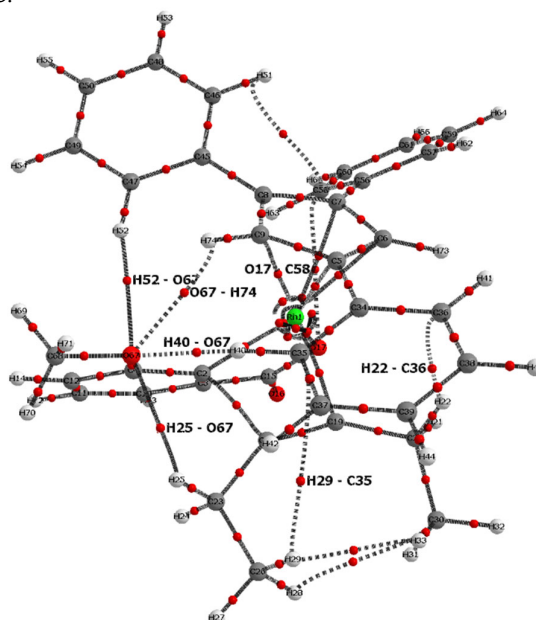
Transition state	BCP	$q(r)$	$\nabla^2 q(r)$	$H(r)$
TS1_T_CpPh3	H24-H82	0.004666	0.023221	0.001758
	H24-O78	0.006065	0.027049	0.001638
	H52-O78	0.010019	0.044881	0.002443
	C20-H62	0.005893	0.023170	0.001552
	C55-O78	0.011279	0.045225	0.001774
	O17-H47	0.007289	0.031270	0.001786
	C4-H36	0.006244	0.024173	0.001549

Figure S14. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS1_T_CpPh3**.



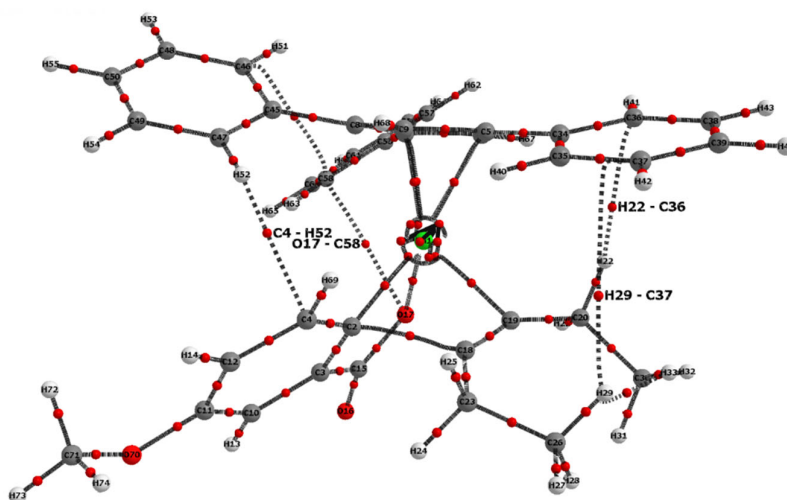
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'1_T_CpPh3	H24-H77	0.003201	0.014040	0.001118
	C2-H36	0.006370	0.024513	0.001516
	C20-H62	0.005384	0.020862	0.001440
	O17-H47	0.007762	0.034018	0.001975
	C40-H73	0.005205	0.020246	0.001344

Figure S15. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS'1_T_CpPh3.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_H_CpPh3	H52-O67	0.010045	0.042164	0.001926
	O67-H74	0.009588	0.042864	0.002351
	H40-O67	0.005403	0.022824	0.001346
	H25-O67	0.013987	0.061229	0.002605
	H29-C35	0.001084	0.003371	0.000224
	H22-C36	0.004925	0.018255	0.001272
	O17-C58	0.006725	0.026234	0.001248

Figure S16. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS1_H_CpPh3.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'1_H_CpPh3	C4-H52	0.008057	0.029722	0.001567
	O17-C58	0.005220	0.020289	0.000998
	H22-C36	0.005463	0.019914	0.001305
	H29-C37	0.001167	0.003679	0.000250

Figure S17. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS'1_H_CpPh3.

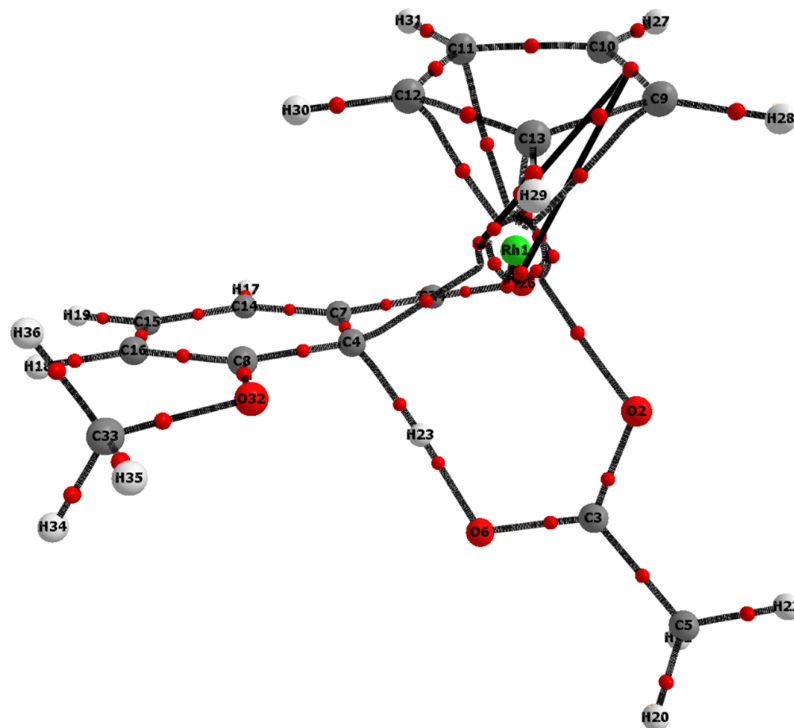


Figure S18. Theoretical molecular graph for TS0_Cp. No bond critical points between the methoxy group and the Cp ligand were found.

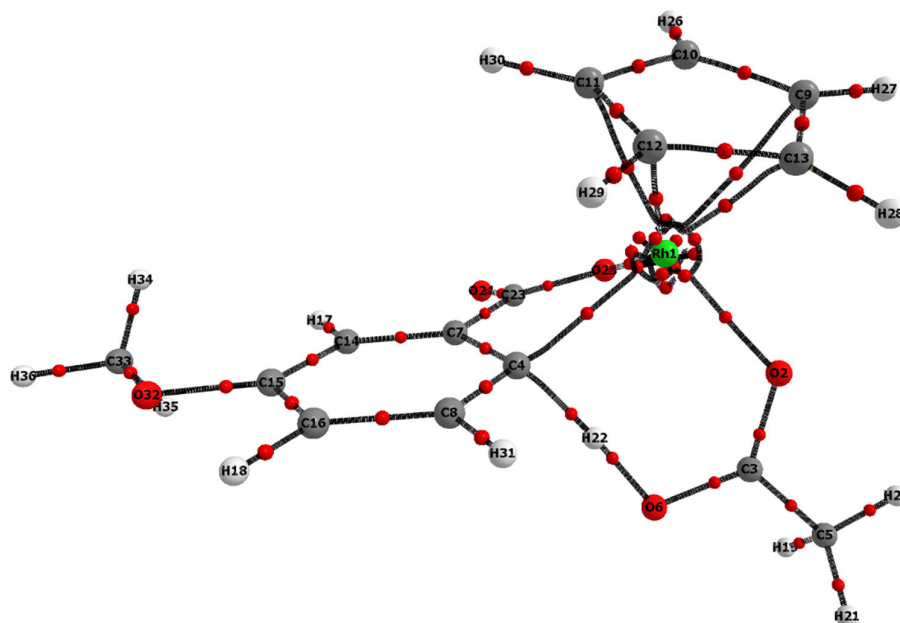
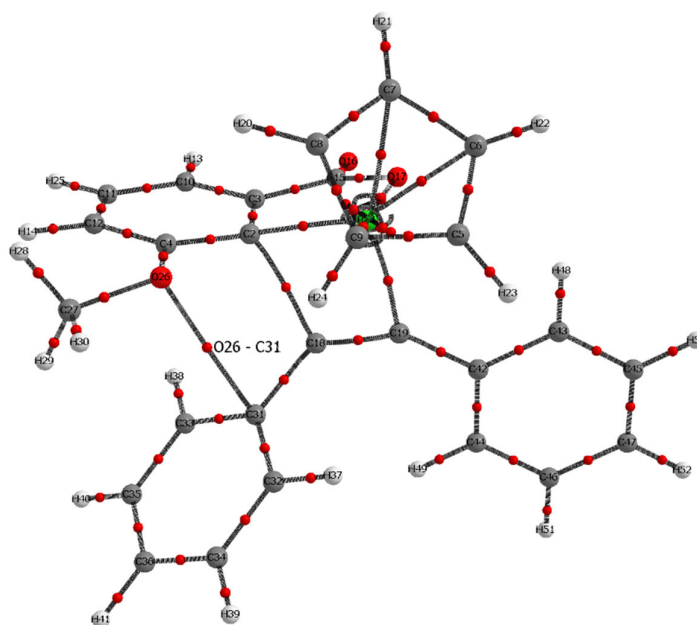


Figure S19. Theoretical molecular graph for TS'0_Cp. No bond critical points between the methoxy group and the Cp ligand were found.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_T_Cp	O26-C31	0.010373	0.041631	0.001703

Figure S20. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS1_T_Cp.

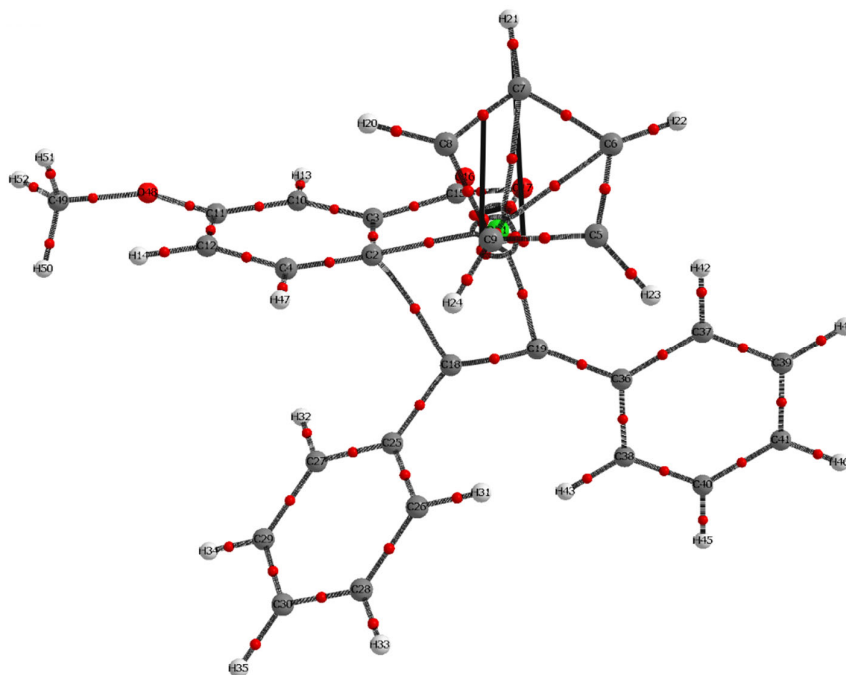
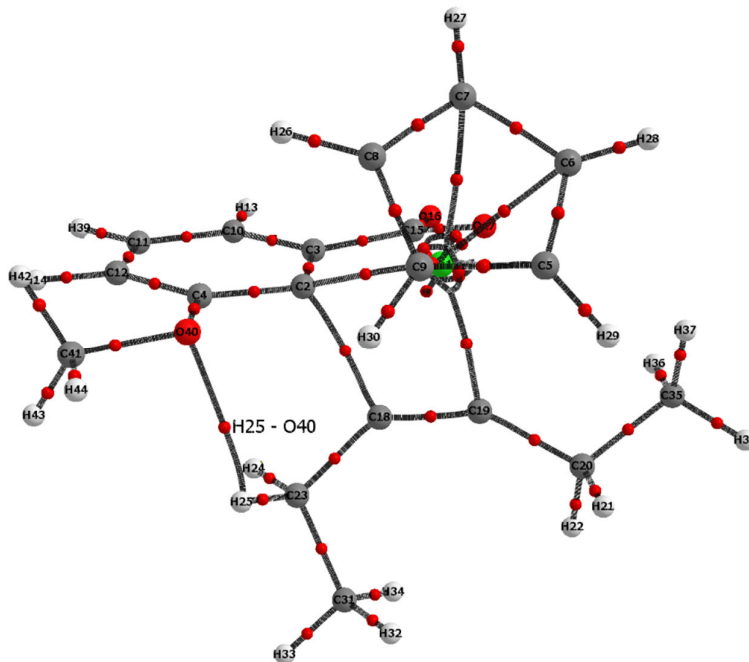


Figure S21. Theoretical molecular graph for **TS'1_T_Cp**. No bond critical points between the methoxy group or the alkyne moiety and the Cp ligand were found.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_H_Cp	H25-O40	0.010740	0.047124	0.002330

Figure S22. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for **TS1_H_Cp**.

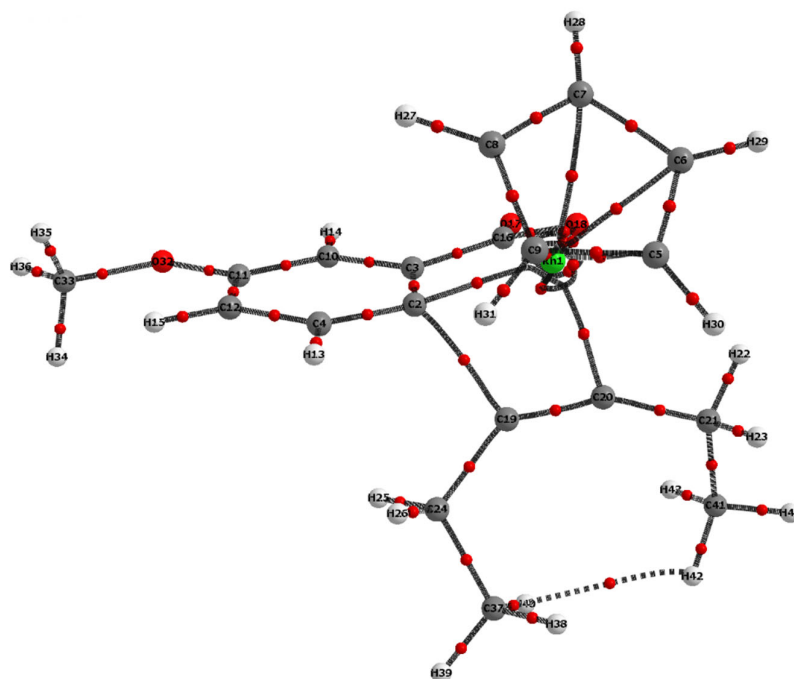
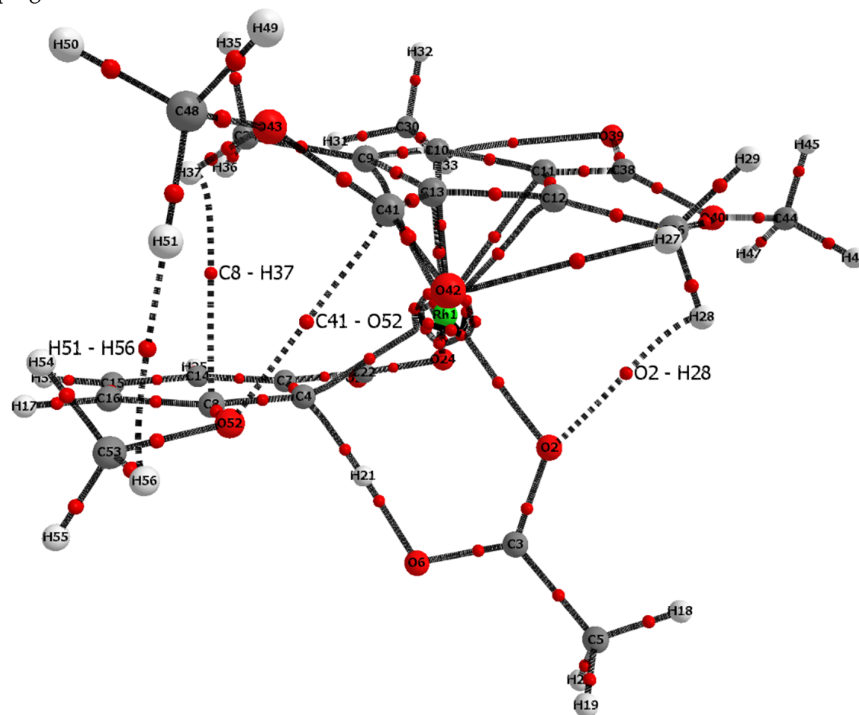
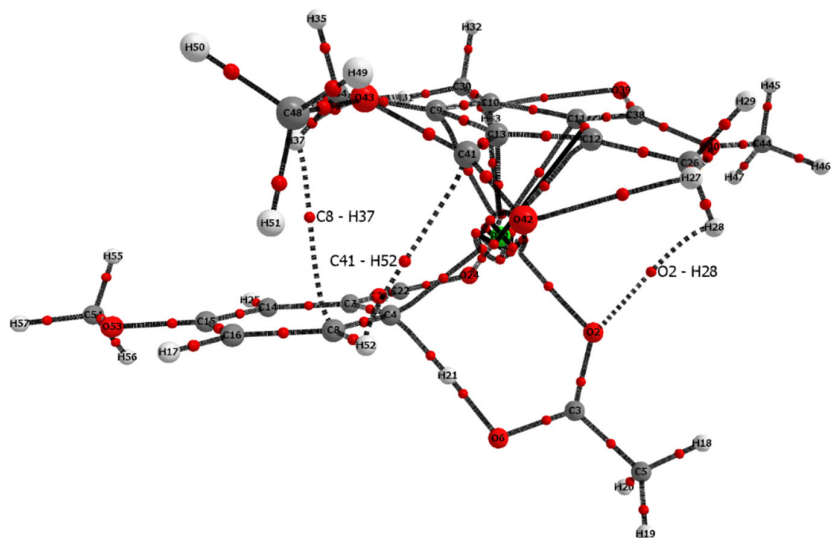


Figure S23. Theoretical molecular graph for TS'1_H_Cp. No bond critical points between the methoxy group or the alkyne moiety and the Cp ligand were found.



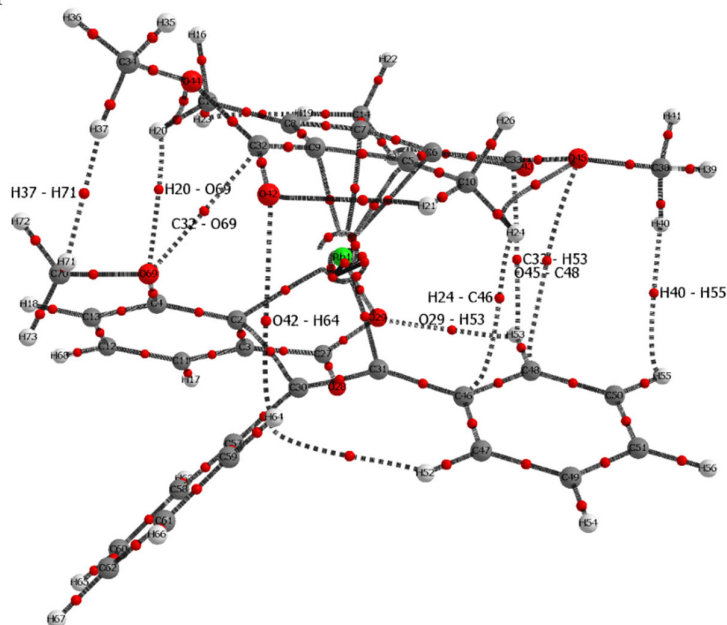
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS0_CpE	H51-H56	0.005136	0.024682	0.001842
	C8-H37	0.006510	0.026892	0.001652
	C41-O52	0.008280	0.033407	0.001423
	O2-H28	0.007081	0.033539	0.002057

Figure S24. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS0_CpE.



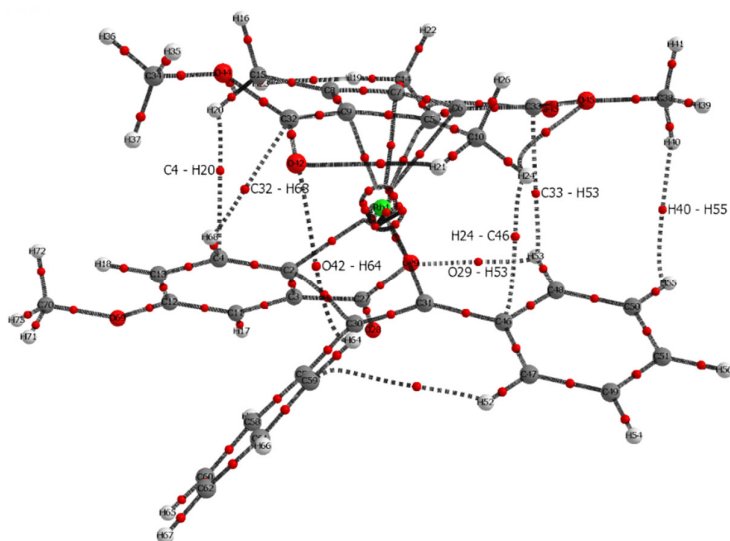
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'0_CpE	O2-H28	0.006141	0.028961	0.001778
	C8-H37	0.006773	0.026222	0.001674
	C41-H52	0.006378	0.027669	0.001683

Figure S25. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS'0_CpE.



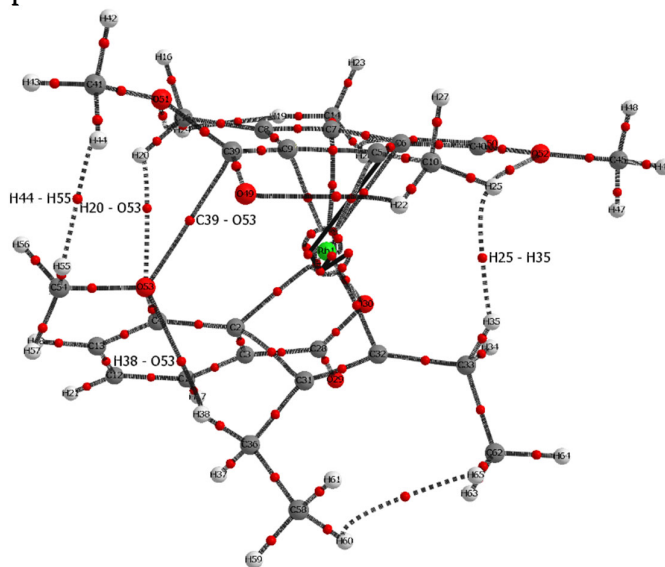
Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_T_CpE	H37-H71	0.005682	0.026869	0.001964
	H20-O69	0.008287	0.034508	0.001783
	C32-O69	0.009328	0.039216	0.001714
	O42-H64	0.001797	0.007456	0.000506
	O29-H53	0.006375	0.028574	0.001706
	H24-C46	0.006146	0.023750	0.001625
	O45-C48	0.004077	0.014532	0.000768
	C33-H53	0.004192	0.018712	0.001315
	H40-H55	0.002674	0.012316	0.000996

Figure S26. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS1_T_CpE.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS'1_T_CpE	C4-H20	0.006590	0.023777	0.001429
	C32-H68	0.005533	0.024324	0.001549
	O42-H64	0.003001	0.012862	0.000849
	O29-H53	0.006890	0.031318	0.001844
	H24-C46	0.004948	0.019235	0.001352
	C33-H53	0.005472	0.024011	0.001607
	H40-H55	0.002960	0.013248	0.001059
	H40-H55	0.002674	0.012316	0.000996

Figure S27. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS'1_T_CpE.



Transition state	BCP	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
TS1_H_CpE	H44-H55	0.005585	0.026770	0.001924
	H20-O53	0.007718	0.031778	0.001633
	C39-O53	0.010323	0.043411	0.001814
	H38-O53	0.013696	0.059812	0.002582
	H25-H35	0.006021	0.026651	0.001898

Figure S28. Theoretical molecular graph and calculated parameters of the electron density distribution at the selected bond critical points for TS1_H_CpE.