Supplementary Information for:

**Enantioselective Nazarov cyclization of indole enones cooperatively catalyzed by Lewis acids and chiral Brønsted acids**

Guo-Peng Wang,\textsuperscript{a} Meng-Qing Chen,\textsuperscript{a} Shou-Fei Zhu,\textsuperscript{*,a} and Qi-Lin Zhou\textsuperscript{*,a,b}

\textsuperscript{a} State Key Laboratory and Institute of Elemento-Organic Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China

\textsuperscript{b} Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300071, China

**Computational Methods**

**DFT Methods**

All DFT theoretical calculations have been carried out using the Gaussian 09 program package. The B3LYP\textsuperscript{1} method with DEF2SVP\textsuperscript{2} basis set has been selected for geometry optimizations and calculation of Gibbs energy corrections at 298 K temperature. Final energies were retrieved from single-point calculations at the B3LYP/DEF2TZVP\textsuperscript{2} level, including the D3BJ dispersion correction scheme developed by Grimme\textsuperscript{3}. All structures have been optimized considering solvent effects using the SMD\textsuperscript{4} model for 1,2-dichloroethane. Reaction paths were traced by the intrinsic reaction coordinate method for all transition states. All energetics reported throughout the text are in kcal/mol. Structures were generated using CYLview\textsuperscript{5}.

**Complete Citation for Gaussian 09**

Table S1. Sum of computed energies of stationary points (For Figure S1 and Figure S2)

<table>
<thead>
<tr>
<th>Structure</th>
<th>$\Delta G_{\text{sol}}$</th>
<th>$\Delta H_{\text{sol}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate</td>
<td>-633.29770445</td>
<td>-633.24290745</td>
</tr>
<tr>
<td>ZnCl$_2$</td>
<td>-2700.08507295</td>
<td>-2700.05343195</td>
</tr>
<tr>
<td>(R)-TRIP-SPA</td>
<td>-2469.22291068</td>
<td>-2469.08284268</td>
</tr>
<tr>
<td>INT I</td>
<td>-3333.37398600</td>
<td>-3333.30254300</td>
</tr>
<tr>
<td>TS I</td>
<td>-5802.56558656</td>
<td>-5802.37975856</td>
</tr>
<tr>
<td>INT II</td>
<td>-5802.60318700</td>
<td>-5802.41999600</td>
</tr>
<tr>
<td>CP II-Pre</td>
<td>-3102.52107157</td>
<td>-3102.35154957</td>
</tr>
<tr>
<td>TS II</td>
<td>-3102.49799870</td>
<td>-3102.33011570</td>
</tr>
<tr>
<td>CP II-Post</td>
<td>-3102.51322113</td>
<td>-3102.34268313</td>
</tr>
<tr>
<td>Enol</td>
<td>-633.29051703</td>
<td>-633.23724603</td>
</tr>
<tr>
<td>CP III-R-Pre</td>
<td>-3102.51322752</td>
<td>-3102.34109552</td>
</tr>
<tr>
<td>CP III-S-Pre</td>
<td>-3102.51387608</td>
<td>-3102.34194508</td>
</tr>
<tr>
<td>TS III-R</td>
<td>-3102.50432525</td>
<td>-3102.33562925</td>
</tr>
<tr>
<td>TS III-S</td>
<td>-3102.50742828</td>
<td>-3102.33908928</td>
</tr>
<tr>
<td>CP III-R-Post</td>
<td>-3102.54344755</td>
<td>-3102.37144155</td>
</tr>
<tr>
<td>CP III-S-Post</td>
<td>-3102.54550249</td>
<td>-3102.37255949</td>
</tr>
<tr>
<td>Product-R</td>
<td>-633.31653363</td>
<td>-633.26406363</td>
</tr>
<tr>
<td>Product-S</td>
<td>-633.31653194</td>
<td>-633.26406394</td>
</tr>
</tbody>
</table>

Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.
Figure S1. The computed energy surfaces for the co-catalyzed Nazarov cyclization (Ring-closing TS and [1,4]-proton transfer TS)
Figure S2. The computed energy surfaces for the co-catalyzed Nazarov cyclization ([1,3]-proton transfer TS)

Table S2. Comparision of energy barrier of the transition states with ZnCl$_2$ (SPA) and without ZnCl$_2$ (SPA)

<table>
<thead>
<tr>
<th>Structure</th>
<th>$\Delta G_{sol}$</th>
<th>$\Delta H_{sol}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS I’</td>
<td>-3333.33560805</td>
<td>-3333.26641105</td>
</tr>
<tr>
<td>INT II’</td>
<td>-3333.36808853</td>
<td>-3333.29857453</td>
</tr>
<tr>
<td>CP II-Pre’</td>
<td>-5802.60321019</td>
<td>-5802.41996619</td>
</tr>
<tr>
<td>TS II’</td>
<td>-5802.57222496</td>
<td>-5802.39167696</td>
</tr>
<tr>
<td>CP II-Post’</td>
<td>-5802.59336534</td>
<td>-5802.40666734</td>
</tr>
</tbody>
</table>

S4
Figure S3. The computed energy surfaces for the transition states with ZnCl₂ (SPA) and without ZnCl₂ (SPA)
Table S3. Comparison of energy barrier of the [1,3]-proton transfer transition state promoted by other species

<table>
<thead>
<tr>
<th>Structure</th>
<th>ΔG$_{sol}$</th>
<th>ΔH$_{sol}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS IV</td>
<td>-633.19775174</td>
<td>-633.14573474</td>
</tr>
<tr>
<td>CP V-Pre</td>
<td>-709.75277097</td>
<td>-709.69040197</td>
</tr>
<tr>
<td>TS V</td>
<td>-709.70654475</td>
<td>-709.65130975</td>
</tr>
<tr>
<td>CP V-Post</td>
<td>-709.77521984</td>
<td>-709.71542384</td>
</tr>
<tr>
<td>CP VI-Pre</td>
<td>-1266.57262375</td>
<td>-1266.48263675</td>
</tr>
<tr>
<td>TS VI</td>
<td>-1266.54231105</td>
<td>-1266.45709605</td>
</tr>
<tr>
<td>CP VI-Post</td>
<td>-1266.62191002</td>
<td>-1266.53092602</td>
</tr>
</tbody>
</table>

Figure S4. The computed energy surfaces for the [1,3]-proton transfer transition state promoted by other species
The Cartesian coordinates (Å) and energies at 298 K for the optimized structures.

Substrate

SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.48569745 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.18799300 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.29770445 a.u.

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.40754000</td>
<td>-0.93011300</td>
<td>0.16190300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.61509300</td>
<td>0.46635000</td>
<td>-0.02751800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.90332800</td>
<td>1.01358100</td>
<td>-0.13298300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.97913000</td>
<td>0.14372400</td>
<td>-0.02502100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.79318000</td>
<td>-1.24331100</td>
<td>0.17774500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.52198000</td>
<td>-1.78524300</td>
<td>0.27168800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.00077600</td>
<td>-1.12601100</td>
<td>0.19039200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.05825900</td>
<td>2.07646700</td>
<td>-0.29040600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.98927100</td>
<td>0.53779000</td>
<td>-0.09674300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.66339300</td>
<td>-1.88868600</td>
<td>0.25781100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.38180400</td>
<td>-2.85249000</td>
<td>0.42232800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.52434600</td>
<td>-2.05562900</td>
<td>0.35712800</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-0.38910800</td>
<td>1.08880300</td>
<td>-0.08096800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.22466200</td>
<td>2.50817100</td>
<td>-0.36762900</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.81330200</td>
<td>2.78243300</td>
<td>-0.19869100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.51155800</td>
<td>2.73085700</td>
<td>-1.40278200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.86058900</td>
<td>3.09112400</td>
<td>0.30660100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.60550700</td>
<td>0.11304800</td>
<td>0.03207200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.04368100</td>
<td>0.42612500</td>
<td>0.12555300</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>2.44989700</td>
<td>1.54301100</td>
<td>0.45449000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.04878000</td>
<td>-0.65438800</td>
<td>-0.16190300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.35543100</td>
<td>-0.52166300</td>
<td>0.57821200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.78982000</td>
<td>0.46755200</td>
<td>0.40266600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.20511700</td>
<td>-0.60856900</td>
<td>1.66152400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.06816400</td>
<td>-1.28890900</td>
<td>0.26276500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.83623600</td>
<td>-1.58080900</td>
<td>-1.10820400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.60484300</td>
<td>-2.30593600</td>
<td>-1.36541800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.91086800</td>
<td>-1.62847100</td>
<td>-1.67176700</td>
<td></td>
</tr>
</tbody>
</table>
ZnCl$_2$

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -2700.06118295 a.u.
Thermal correction to Gibbs free energy at 298 K: -0.02389000 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -2700.08507295 a.u.

\[
\begin{array}{ccc}
\text{Zn} & 1.55000000 & 0.31545741 & 0.00000000 \\
\text{Cl}  & -0.69000000 & 0.31545741 & 0.00000000 \\
\text{Cl}  & 3.79000000 & 0.31545741 & 0.00000000 \\
\end{array}
\]

\((R)-\text{TRIP-SPA}\)

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -2470.08964368 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.86673300 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -2469.22291068 a.u.

\[
\begin{array}{cccc}
P & -0.07818800 & 0.26266300 & -0.33847000 \\
O & 1.00768700 & -0.63435700 & 0.47017700 \\
O & -1.24855400 & -0.79229700 & -0.76055500 \\
O & -0.63987400 & 1.07508300 & 0.92715400 \\
O & 0.36095400 & 1.01193200 & -1.52883700 \\
C & 1.75791600 & -1.55268800 & -0.26931300 \\
C & 3.04546700 & -1.18706700 & -0.71471800 \\
C & 3.73207500 & -2.11205700 & -1.52056200 \\
C & 3.14883900 & -3.31496700 & -1.92802200 \\
C & 1.88078500 & -3.64911700 & -1.45865700 \\
C & 1.03381400 & -4.85847200 & -1.78833500 \\
C & -0.35026100 & -4.45969700 & -1.23787600 \\
\end{array}
\]
<table>
<thead>
<tr>
<th>X (A)</th>
<th>Y (A)</th>
<th>Z (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.03364500</td>
<td>-3.52393800</td>
<td>-0.02549900</td>
</tr>
<tr>
<td>1.20125100</td>
<td>-2.79970100</td>
<td>-0.56675600</td>
</tr>
<tr>
<td>0.33529400</td>
<td>-4.39514000</td>
<td>1.22439100</td>
</tr>
<tr>
<td>-1.02062600</td>
<td>-4.81258600</td>
<td>1.82472300</td>
</tr>
<tr>
<td>-1.90413000</td>
<td>-3.63594700</td>
<td>0.70084300</td>
</tr>
<tr>
<td>-3.14729500</td>
<td>-4.39451400</td>
<td>0.50479600</td>
</tr>
<tr>
<td>-3.75215300</td>
<td>-2.09671100</td>
<td>0.70084300</td>
</tr>
<tr>
<td>-3.12194400</td>
<td>-2.13429000</td>
<td>0.15490800</td>
</tr>
<tr>
<td>-1.88318600</td>
<td>-1.61833200</td>
<td>0.15490800</td>
</tr>
<tr>
<td>-1.28684800</td>
<td>-2.82972100</td>
<td>0.04796000</td>
</tr>
<tr>
<td>0.33529400</td>
<td>-4.39514000</td>
<td>1.22439100</td>
</tr>
<tr>
<td>1.20125100</td>
<td>-2.79970100</td>
<td>-0.56675600</td>
</tr>
<tr>
<td>3.68622000</td>
<td>-3.98221800</td>
<td>2.60720900</td>
</tr>
<tr>
<td>1.42054600</td>
<td>-5.76648500</td>
<td>1.29201000</td>
</tr>
<tr>
<td>0.97721100</td>
<td>-5.31883100</td>
<td>0.95803000</td>
</tr>
<tr>
<td>-0.90054200</td>
<td>-3.87795900</td>
<td>1.99462200</td>
</tr>
<tr>
<td>0.98684100</td>
<td>-5.24341300</td>
<td>0.97102200</td>
</tr>
<tr>
<td>0.87976500</td>
<td>-3.76073800</td>
<td>1.94264200</td>
</tr>
<tr>
<td>-1.39740300</td>
<td>-5.74343800</td>
<td>1.36401400</td>
</tr>
<tr>
<td>-0.97248500</td>
<td>-4.99667600</td>
<td>2.90977000</td>
</tr>
<tr>
<td>-3.64082900</td>
<td>-3.92900400</td>
<td>2.73823700</td>
</tr>
<tr>
<td>-4.72574300</td>
<td>-1.82047100</td>
<td>2.00217000</td>
</tr>
<tr>
<td>-3.71323100</td>
<td>0.13057000</td>
<td>0.38011400</td>
</tr>
<tr>
<td>-3.83877200</td>
<td>1.12035000</td>
<td>1.39789900</td>
</tr>
<tr>
<td>-4.13826500</td>
<td>0.43360700</td>
<td>-0.94208000</td>
</tr>
<tr>
<td>-4.35130600</td>
<td>2.38207600</td>
<td>1.05380300</td>
</tr>
<tr>
<td>-4.64757400</td>
<td>1.70844800</td>
<td>-1.22068500</td>
</tr>
<tr>
<td>-4.75755600</td>
<td>2.70456800</td>
<td>-0.24448100</td>
</tr>
<tr>
<td>-4.44662200</td>
<td>3.14363100</td>
<td>1.83207900</td>
</tr>
<tr>
<td>-4.97029600</td>
<td>1.92802200</td>
<td>-2.24125200</td>
</tr>
<tr>
<td>3.68706400</td>
<td>0.11919000</td>
<td>-0.34116700</td>
</tr>
<tr>
<td>4.08699200</td>
<td>0.35147800</td>
<td>1.00219400</td>
</tr>
<tr>
<td>3.94580400</td>
<td>1.10450100</td>
<td>-1.32965500</td>
</tr>
<tr>
<td>4.73330200</td>
<td>1.55170800</td>
<td>1.32293800</td>
</tr>
<tr>
<td>4.60285300</td>
<td>2.28401000</td>
<td>-0.94924000</td>
</tr>
<tr>
<td>5.00495000</td>
<td>2.53453800</td>
<td>0.36475700</td>
</tr>
<tr>
<td>5.04090400</td>
<td>1.71940500</td>
<td>2.35848900</td>
</tr>
<tr>
<td>4.80361900</td>
<td>3.04454800</td>
<td>-1.70852100</td>
</tr>
<tr>
<td>3.55206900</td>
<td>0.93645600</td>
<td>-2.79919600</td>
</tr>
<tr>
<td>2.87773300</td>
<td>0.07111100</td>
<td>-2.86626500</td>
</tr>
<tr>
<td>4.78310900</td>
<td>0.64958900</td>
<td>-3.68024200</td>
</tr>
<tr>
<td>5.33886500</td>
<td>-0.23880900</td>
<td>-3.34227300</td>
</tr>
<tr>
<td>4.48015700</td>
<td>0.48043100</td>
<td>-4.72692200</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>---</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>H</td>
<td>5.48565500</td>
<td>1.49953000</td>
</tr>
<tr>
<td>C</td>
<td>2.76815000</td>
<td>2.14227900</td>
</tr>
<tr>
<td>H</td>
<td>3.38308400</td>
<td>3.05677800</td>
</tr>
<tr>
<td>H</td>
<td>2.43921700</td>
<td>1.93686300</td>
</tr>
<tr>
<td>H</td>
<td>1.87429500</td>
<td>2.32927200</td>
</tr>
<tr>
<td>C</td>
<td>3.87335000</td>
<td>-0.67165700</td>
</tr>
<tr>
<td>H</td>
<td>3.36439500</td>
<td>-1.54411600</td>
</tr>
<tr>
<td>C</td>
<td>2.96439300</td>
<td>-0.12644000</td>
</tr>
<tr>
<td>H</td>
<td>1.99777500</td>
<td>0.20535000</td>
</tr>
<tr>
<td>H</td>
<td>2.76984700</td>
<td>-0.90583900</td>
</tr>
<tr>
<td>H</td>
<td>3.42812300</td>
<td>0.72753700</td>
</tr>
<tr>
<td>C</td>
<td>5.21137800</td>
<td>-1.18211400</td>
</tr>
<tr>
<td>H</td>
<td>5.84500900</td>
<td>-1.60964400</td>
</tr>
<tr>
<td>H</td>
<td>5.78428400</td>
<td>-0.37465600</td>
</tr>
<tr>
<td>H</td>
<td>5.03928300</td>
<td>-1.96579200</td>
</tr>
<tr>
<td>C</td>
<td>5.71057900</td>
<td>3.83427600</td>
</tr>
<tr>
<td>H</td>
<td>5.80189500</td>
<td>4.41887300</td>
</tr>
<tr>
<td>C</td>
<td>4.88737600</td>
<td>4.67774700</td>
</tr>
<tr>
<td>H</td>
<td>5.38252700</td>
<td>5.64283500</td>
</tr>
<tr>
<td>H</td>
<td>3.88001900</td>
<td>4.88496600</td>
</tr>
<tr>
<td>H</td>
<td>4.76792600</td>
<td>4.16103300</td>
</tr>
<tr>
<td>C</td>
<td>7.13515300</td>
<td>3.59015300</td>
</tr>
<tr>
<td>H</td>
<td>7.12316100</td>
<td>3.02496600</td>
</tr>
<tr>
<td>H</td>
<td>7.73625100</td>
<td>3.01681200</td>
</tr>
<tr>
<td>H</td>
<td>7.65107100</td>
<td>4.54562200</td>
</tr>
<tr>
<td>C</td>
<td>-3.48988500</td>
<td>0.86164500</td>
</tr>
<tr>
<td>H</td>
<td>-2.91310800</td>
<td>-0.07226100</td>
</tr>
<tr>
<td>C</td>
<td>-4.77124300</td>
<td>0.66404500</td>
</tr>
<tr>
<td>H</td>
<td>-4.52052900</td>
<td>0.39859700</td>
</tr>
<tr>
<td>H</td>
<td>-5.37364600</td>
<td>1.58713900</td>
</tr>
<tr>
<td>H</td>
<td>-5.41192600</td>
<td>-0.13227300</td>
</tr>
<tr>
<td>C</td>
<td>-2.61456800</td>
<td>1.95590800</td>
</tr>
<tr>
<td>H</td>
<td>-3.13004000</td>
<td>2.92860600</td>
</tr>
<tr>
<td>H</td>
<td>-2.36171200</td>
<td>1.67493100</td>
</tr>
<tr>
<td>H</td>
<td>-1.66757200</td>
<td>2.09198700</td>
</tr>
<tr>
<td>C</td>
<td>-4.11308800</td>
<td>-0.59604800</td>
</tr>
<tr>
<td>H</td>
<td>-3.61590700</td>
<td>-1.49953800</td>
</tr>
<tr>
<td>C</td>
<td>-5.54241700</td>
<td>-1.01159600</td>
</tr>
<tr>
<td>H</td>
<td>-6.10208000</td>
<td>-1.40369400</td>
</tr>
<tr>
<td>H</td>
<td>-6.11287300</td>
<td>-0.16178000</td>
</tr>
<tr>
<td>H</td>
<td>-5.51575900</td>
<td>-1.79756800</td>
</tr>
<tr>
<td>C</td>
<td>-3.31069600</td>
<td>-0.11406700</td>
</tr>
<tr>
<td>H</td>
<td>-3.79297100</td>
<td>0.74594300</td>
</tr>
<tr>
<td>H</td>
<td>-2.28975600</td>
<td>0.18069300</td>
</tr>
</tbody>
</table>
INT I

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3333.55485300 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.18086700 a.u.
Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-3333.37398600 a.u.
<table>
<thead>
<tr>
<th>Atoms</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.09702600</td>
<td>1.04971100</td>
<td>0.06947900</td>
</tr>
<tr>
<td>O</td>
<td>-0.96054000</td>
<td>0.15490500</td>
<td>0.18796100</td>
</tr>
<tr>
<td>C</td>
<td>-0.50030500</td>
<td>2.48692700</td>
<td>0.07252000</td>
</tr>
<tr>
<td>C</td>
<td>-1.64720100</td>
<td>2.85840700</td>
<td>0.97630300</td>
</tr>
<tr>
<td>H</td>
<td>-2.57735900</td>
<td>2.37050400</td>
<td>0.64167700</td>
</tr>
<tr>
<td>H</td>
<td>-1.45710500</td>
<td>2.53609400</td>
<td>2.01352700</td>
</tr>
<tr>
<td>H</td>
<td>-1.80748400</td>
<td>3.94564500</td>
<td>0.97239700</td>
</tr>
<tr>
<td>C</td>
<td>0.07737300</td>
<td>3.35069800</td>
<td>-0.78301000</td>
</tr>
<tr>
<td>H</td>
<td>-0.25914800</td>
<td>4.39022800</td>
<td>-0.83695600</td>
</tr>
<tr>
<td>H</td>
<td>0.86203300</td>
<td>3.04350500</td>
<td>-1.47698000</td>
</tr>
<tr>
<td>Zn</td>
<td>-2.83416700</td>
<td>-0.65955600</td>
<td>0.05056800</td>
</tr>
<tr>
<td>Cl</td>
<td>-2.52347200</td>
<td>-2.75470800</td>
<td>0.51081300</td>
</tr>
<tr>
<td>Cl</td>
<td>-4.33756300</td>
<td>0.77644000</td>
<td>-0.56287900</td>
</tr>
</tbody>
</table>

**TS I**

![Diagram of TS I](image)

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5803.63914156 a.u.

Thermal correction to Gibbs free energy at 298 K: 1.07355500 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5802.56558656 a.u.
<table>
<thead>
<tr>
<th>Atom</th>
<th>Cx</th>
<th>Cy</th>
<th>Cz</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-0.39481200</td>
<td>5.36472400</td>
<td>1.87752100</td>
</tr>
<tr>
<td>H</td>
<td>1.19352600</td>
<td>6.55590600</td>
<td>-1.33830500</td>
</tr>
<tr>
<td>H</td>
<td>0.90703500</td>
<td>5.04820800</td>
<td>-2.23288400</td>
</tr>
<tr>
<td>H</td>
<td>-1.19128200</td>
<td>7.15206100</td>
<td>-1.44770300</td>
</tr>
<tr>
<td>H</td>
<td>-1.01917800</td>
<td>6.31083400</td>
<td>-2.99314100</td>
</tr>
<tr>
<td>H</td>
<td>-3.70935300</td>
<td>5.46672600</td>
<td>-2.32443300</td>
</tr>
<tr>
<td>H</td>
<td>-4.80287500</td>
<td>3.48809400</td>
<td>-1.29007200</td>
</tr>
<tr>
<td>C</td>
<td>-3.70275900</td>
<td>1.53010700</td>
<td>0.20701300</td>
</tr>
<tr>
<td>C</td>
<td>-4.18981800</td>
<td>0.55259900</td>
<td>-0.70568000</td>
</tr>
<tr>
<td>C</td>
<td>-3.89623500</td>
<td>1.33768200</td>
<td>1.59842700</td>
</tr>
<tr>
<td>C</td>
<td>-4.81950800</td>
<td>-0.59077600</td>
<td>-0.20094200</td>
</tr>
<tr>
<td>C</td>
<td>-4.54437600</td>
<td>0.17504100</td>
<td>2.04635500</td>
</tr>
<tr>
<td>C</td>
<td>-5.01179000</td>
<td>-0.80735800</td>
<td>1.16944600</td>
</tr>
<tr>
<td>H</td>
<td>-5.16892600</td>
<td>-1.35649500</td>
<td>-0.89773900</td>
</tr>
<tr>
<td>H</td>
<td>-4.69236700</td>
<td>0.04680900</td>
<td>3.12017600</td>
</tr>
<tr>
<td>C</td>
<td>3.94281100</td>
<td>1.21633800</td>
<td>-0.00452800</td>
</tr>
<tr>
<td>C</td>
<td>4.21245700</td>
<td>0.85137600</td>
<td>-1.35022900</td>
</tr>
<tr>
<td>C</td>
<td>4.33965100</td>
<td>0.34962200</td>
<td>1.04806300</td>
</tr>
<tr>
<td>C</td>
<td>4.89091000</td>
<td>-0.34764200</td>
<td>1.60892500</td>
</tr>
<tr>
<td>C</td>
<td>5.01977300</td>
<td>-0.83513400</td>
<td>0.72894800</td>
</tr>
<tr>
<td>C</td>
<td>5.32030700</td>
<td>-1.20149400</td>
<td>-0.58650600</td>
</tr>
<tr>
<td>H</td>
<td>5.10960600</td>
<td>-0.60847100</td>
<td>-2.64752600</td>
</tr>
<tr>
<td>H</td>
<td>5.34116000</td>
<td>-1.49443000</td>
<td>1.54102600</td>
</tr>
<tr>
<td>C</td>
<td>4.06743500</td>
<td>0.65133300</td>
<td>2.52398700</td>
</tr>
<tr>
<td>H</td>
<td>3.45518100</td>
<td>1.56188200</td>
<td>2.57121200</td>
</tr>
<tr>
<td>C</td>
<td>5.36838400</td>
<td>0.92449800</td>
<td>3.30121800</td>
</tr>
<tr>
<td>H</td>
<td>5.95344900</td>
<td>1.74261900</td>
<td>2.85290300</td>
</tr>
<tr>
<td>H</td>
<td>5.14436200</td>
<td>1.20196300</td>
<td>4.34498000</td>
</tr>
<tr>
<td>H</td>
<td>6.01690000</td>
<td>0.03303600</td>
<td>3.32818200</td>
</tr>
<tr>
<td>C</td>
<td>3.24681100</td>
<td>-0.45797400</td>
<td>3.20264700</td>
</tr>
<tr>
<td>H</td>
<td>3.79388600</td>
<td>-1.41439400</td>
<td>3.23590200</td>
</tr>
<tr>
<td>H</td>
<td>3.02005300</td>
<td>-0.17720300</td>
<td>4.24470300</td>
</tr>
<tr>
<td>H</td>
<td>2.29570800</td>
<td>-0.60701200</td>
<td>2.67406700</td>
</tr>
<tr>
<td>C</td>
<td>3.83635400</td>
<td>1.73666300</td>
<td>-2.53898200</td>
</tr>
<tr>
<td>H</td>
<td>3.34050100</td>
<td>2.63498900</td>
<td>-2.14753700</td>
</tr>
<tr>
<td>C</td>
<td>2.83497800</td>
<td>1.04227600</td>
<td>-3.47925100</td>
</tr>
<tr>
<td>H</td>
<td>1.92236500</td>
<td>0.74890400</td>
<td>-2.94034800</td>
</tr>
<tr>
<td>H</td>
<td>2.54007200</td>
<td>1.71971700</td>
<td>-4.29762600</td>
</tr>
<tr>
<td>H</td>
<td>3.26920100</td>
<td>0.14013000</td>
<td>-3.94155700</td>
</tr>
<tr>
<td>C</td>
<td>5.08157500</td>
<td>2.22105700</td>
<td>-3.30445400</td>
</tr>
<tr>
<td>H</td>
<td>5.78429800</td>
<td>2.74493300</td>
<td>-2.63724000</td>
</tr>
<tr>
<td>H</td>
<td>5.62637900</td>
<td>1.38474900</td>
<td>-3.77250400</td>
</tr>
<tr>
<td>H</td>
<td>4.79368700</td>
<td>2.91797900</td>
<td>-4.10882300</td>
</tr>
<tr>
<td>C</td>
<td>6.14171200</td>
<td>-2.45343300</td>
<td>-0.87442000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>------------------</td>
<td>------------------</td>
<td>------------------</td>
</tr>
<tr>
<td>H</td>
<td>6.18689400</td>
<td>-3.02713100</td>
<td>0.06866700</td>
</tr>
<tr>
<td>C</td>
<td>5.50659400</td>
<td>-3.36523300</td>
<td>-1.93544500</td>
</tr>
<tr>
<td>H</td>
<td>6.08729700</td>
<td>-4.29529800</td>
<td>-2.04931900</td>
</tr>
<tr>
<td>H</td>
<td>4.47403800</td>
<td>-3.63728700</td>
<td>-1.66602800</td>
</tr>
<tr>
<td>H</td>
<td>5.47180100</td>
<td>-2.87889500</td>
<td>-2.92366600</td>
</tr>
<tr>
<td>C</td>
<td>7.58957800</td>
<td>-2.09214100</td>
<td>-1.25502500</td>
</tr>
<tr>
<td>H</td>
<td>7.61942500</td>
<td>-1.51501900</td>
<td>-2.19391800</td>
</tr>
<tr>
<td>H</td>
<td>8.06649600</td>
<td>-1.48087200</td>
<td>-0.47330400</td>
</tr>
<tr>
<td>C</td>
<td>8.19861500</td>
<td>-3.00021400</td>
<td>-1.39855400</td>
</tr>
<tr>
<td>H</td>
<td>-4.08782300</td>
<td>0.70395200</td>
<td>-2.22615900</td>
</tr>
<tr>
<td>H</td>
<td>-3.47389000</td>
<td>1.58803800</td>
<td>-2.44227900</td>
</tr>
<tr>
<td>C</td>
<td>-5.47442800</td>
<td>0.93326300</td>
<td>-2.85729400</td>
</tr>
<tr>
<td>H</td>
<td>-5.38491800</td>
<td>1.11033000</td>
<td>-3.94170000</td>
</tr>
<tr>
<td>H</td>
<td>-6.12711300</td>
<td>0.05664500</td>
<td>-2.71443700</td>
</tr>
<tr>
<td>H</td>
<td>-5.98700600</td>
<td>1.80025200</td>
<td>-2.41209100</td>
</tr>
<tr>
<td>C</td>
<td>-3.38735700</td>
<td>-0.48281800</td>
<td>-2.90624800</td>
</tr>
<tr>
<td>H</td>
<td>-3.93890400</td>
<td>-1.42448500</td>
<td>-2.74866400</td>
</tr>
<tr>
<td>H</td>
<td>-3.30715600</td>
<td>-0.33436700</td>
<td>-3.99369400</td>
</tr>
<tr>
<td>H</td>
<td>-2.35913500</td>
<td>-0.57394200</td>
<td>-2.52222900</td>
</tr>
<tr>
<td>C</td>
<td>-3.48579900</td>
<td>2.37850500</td>
<td>2.64212500</td>
</tr>
<tr>
<td>H</td>
<td>-2.96924800</td>
<td>3.19570700</td>
<td>2.12077800</td>
</tr>
<tr>
<td>C</td>
<td>-4.72032900</td>
<td>3.00156400</td>
<td>3.32058200</td>
</tr>
<tr>
<td>H</td>
<td>-5.40210800</td>
<td>3.44798700</td>
<td>2.57956500</td>
</tr>
<tr>
<td>H</td>
<td>-5.29293000</td>
<td>2.25182400</td>
<td>3.89082400</td>
</tr>
<tr>
<td>H</td>
<td>-4.41710300</td>
<td>3.79424200</td>
<td>4.02476700</td>
</tr>
<tr>
<td>C</td>
<td>-2.50171000</td>
<td>1.81621300</td>
<td>3.68289400</td>
</tr>
<tr>
<td>H</td>
<td>-2.96148400</td>
<td>1.01777800</td>
<td>4.28873100</td>
</tr>
<tr>
<td>H</td>
<td>-1.60115200</td>
<td>1.41104800</td>
<td>3.19883300</td>
</tr>
<tr>
<td>H</td>
<td>-2.18410900</td>
<td>2.61039000</td>
<td>4.37895700</td>
</tr>
<tr>
<td>C</td>
<td>-5.74636700</td>
<td>-2.06481700</td>
<td>1.62703000</td>
</tr>
<tr>
<td>H</td>
<td>-5.36672300</td>
<td>-2.88687900</td>
<td>0.99475800</td>
</tr>
<tr>
<td>C</td>
<td>-5.49229900</td>
<td>-2.45026000</td>
<td>3.08899200</td>
</tr>
<tr>
<td>H</td>
<td>-5.95334800</td>
<td>-3.42551200</td>
<td>3.31190700</td>
</tr>
<tr>
<td>H</td>
<td>-4.41656900</td>
<td>-2.52846200</td>
<td>3.31257500</td>
</tr>
<tr>
<td>H</td>
<td>-5.92744500</td>
<td>-1.71834400</td>
<td>3.78949300</td>
</tr>
<tr>
<td>C</td>
<td>-7.25948200</td>
<td>-1.94086000</td>
<td>1.36033600</td>
</tr>
<tr>
<td>H</td>
<td>-7.69731600</td>
<td>-1.12459900</td>
<td>1.95915900</td>
</tr>
<tr>
<td>H</td>
<td>-7.46585600</td>
<td>-1.72507900</td>
<td>0.30104400</td>
</tr>
<tr>
<td>H</td>
<td>-7.78256000</td>
<td>-2.87504200</td>
<td>1.62350700</td>
</tr>
</tbody>
</table>
INT II

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5803.68160200 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.07841500 a.u.
Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-5802.60318700 a.u.

Zn            -2.15212200  -2.95278000  -2.45166400
Cl            -3.44981300  -3.92592000  -0.95668700
Cl            -1.89585100  -3.12606800  -4.61729300
P             0.17935500   1.07522000   0.00073200
O             1.31760200   2.00579800  -0.71247700
O             -0.81813400  2.15506200   0.70573000
O             -0.56338900  0.51521200  -1.26797000
O             0.66638700   0.10301200  1.01294000
C             2.13995000   2.85064200   0.02086300
C             3.43457200   2.42130800   0.38751600
C             4.23184700   3.31642400   1.12406700
C             3.75242000   4.55439800   1.55476600
C             2.46732300   4.94392100   1.87559000
C             1.71550800   6.19697700   1.57354800
C             0.27199100   5.85555700   1.16045800
C             0.43030400   4.89740200  -0.06875200
C             1.67602600   4.12481900   0.36176100
C             0.69654200   5.74589300  -1.35628800
C            -0.69681200   6.25390400  -1.77642200
C            -1.61018600   5.15213400  -1.28735600
C            -2.95603200   4.94270900  -1.57555200
C            -3.59941300   3.82743400  -1.03387100
C            -2.91081000   2.86315200  -0.27676100
C            -1.54297800   3.10009200  -0.01265100
C            -0.91357300   4.27216900  -0.43905400
H            -0.57652500  -0.50842300  -1.34442800
H             5.24465900   3.00747100   1.39023200
H             4.37800500   5.20202700   2.17476200
H  2.09614700  7.07696200  1.02465900
H  1.81335400  6.42986000  2.64594100
H  -0.34316000  6.73854200  0.93405900
H  1.42674500  6.55155800 -1.19024900
H  1.10464600  5.08199600 -2.13519500
H  -0.22751800  5.30187000  1.97166200
H  1.81335400  6.42986000 -1.29582500
H  -0.34316000  6.73854200  0.93405900
H  1.42674500  6.55155800 -1.19024900
H  1.10464600  5.08199600 -2.13519500
H  -0.22751800  5.30187000  1.97166200
C  -3.62785500  1.64247700  0.22182500
C  -4.17747100  0.70438600 -0.69743200
C  -3.80711900  1.43488400  1.61338600
C  -4.85255600 -0.41600000 -0.19914400
C  -4.50592900  0.29920800  2.05405800
C  -5.03460400 -0.64530800  1.17052000
C  -5.24947900 -1.15265700 -0.90146800
C  -4.64407500  0.16175000  3.12806100
C  -3.99300600  1.07134600  0.04094900
C  -4.29676900  0.73661400 -1.30258200
C  -4.31045200  0.15237200  1.07916700
C  -4.92648300 -0.48781900 -1.57831900
C  -4.93654400 -1.05556400  0.74432700
C  -5.27279200 -1.39474700 -0.57314800
H  -5.17119600 -0.72117400 -2.61612900
H  -5.19673400 -1.75378900  1.54646900
C  -4.02105700  0.43204000  2.55702800
H  -4.34794310  1.38520400  2.61755900
C  -4.31970500  0.58805100  3.37009800
H  -4.97560400  1.36773800  2.95204700
H  -5.09209400  0.86161100  4.41360800
H  -5.89823300 -0.35049600  3.39305500
C  -3.10159900 -0.62662400  3.18828600
H  -3.56794200 -1.62603300  3.19914800
H  -2.88142900 -0.36260000  4.23604600
H  -2.14996400 -0.67563800  2.64141300
C  -4.01720600  1.68041700 -2.47265400
H  -3.54361600  2.58576400 -2.07007300
C  -3.03331900  1.07053300 -3.48670300
H  -2.08266300  0.80095600 -3.00454200
H  -2.81140800  1.79356100 -4.28883300
H  -3.44762600  0.16769100 -3.96540900
C  -5.31961800  2.13475400 -3.15748100
H  -6.00804600  2.60572100 -2.43794300
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>5.85255300</td>
<td>1.29162500</td>
<td>-3.62706500</td>
</tr>
<tr>
<td>H</td>
<td>5.10196900</td>
<td>2.86937500</td>
<td>-3.95022600</td>
</tr>
<tr>
<td>C</td>
<td>6.06104800</td>
<td>-2.67335400</td>
<td>-0.84490800</td>
</tr>
<tr>
<td>H</td>
<td>5.69990000</td>
<td>-3.42805100</td>
<td>-0.12148500</td>
</tr>
<tr>
<td>C</td>
<td>5.86703200</td>
<td>-3.25321700</td>
<td>-2.25173600</td>
</tr>
<tr>
<td>H</td>
<td>6.37121900</td>
<td>-4.22885100</td>
<td>-2.33778200</td>
</tr>
<tr>
<td>H</td>
<td>4.80285100</td>
<td>-3.39895400</td>
<td>-2.49529900</td>
</tr>
<tr>
<td>H</td>
<td>6.29809100</td>
<td>-2.59829900</td>
<td>-3.02595900</td>
</tr>
<tr>
<td>C</td>
<td>7.55964100</td>
<td>-2.45570300</td>
<td>-0.55477800</td>
</tr>
<tr>
<td>H</td>
<td>7.98300000</td>
<td>-1.70416000</td>
<td>-1.24136700</td>
</tr>
<tr>
<td>H</td>
<td>7.72284800</td>
<td>-2.09641000</td>
<td>0.47279300</td>
</tr>
<tr>
<td>H</td>
<td>8.12702900</td>
<td>-3.39237400</td>
<td>-0.68391800</td>
</tr>
<tr>
<td>C</td>
<td>-4.10362300</td>
<td>0.88013000</td>
<td>-2.21721700</td>
</tr>
<tr>
<td>H</td>
<td>-3.43412000</td>
<td>1.72384800</td>
<td>-2.43134700</td>
</tr>
<tr>
<td>C</td>
<td>-5.48854600</td>
<td>1.21874400</td>
<td>-2.80226400</td>
</tr>
<tr>
<td>H</td>
<td>-5.41534200</td>
<td>1.42097900</td>
<td>-3.88347100</td>
</tr>
<tr>
<td>H</td>
<td>-6.19296100</td>
<td>0.38188800</td>
<td>-2.66598600</td>
</tr>
<tr>
<td>H</td>
<td>-5.93342400</td>
<td>2.10310900</td>
<td>-2.32001400</td>
</tr>
<tr>
<td>C</td>
<td>-3.50903900</td>
<td>-0.33726100</td>
<td>-2.94147100</td>
</tr>
<tr>
<td>H</td>
<td>-4.10095800</td>
<td>-1.25068200</td>
<td>-2.76407000</td>
</tr>
<tr>
<td>H</td>
<td>-3.48197400</td>
<td>-0.18416800</td>
<td>-4.03100600</td>
</tr>
<tr>
<td>H</td>
<td>-2.46843300</td>
<td>-0.49440900</td>
<td>-2.62283600</td>
</tr>
<tr>
<td>C</td>
<td>-3.32307000</td>
<td>2.43046800</td>
<td>2.66924000</td>
</tr>
<tr>
<td>H</td>
<td>-2.78530200</td>
<td>3.23750700</td>
<td>2.15394400</td>
</tr>
<tr>
<td>C</td>
<td>-4.50810200</td>
<td>3.09002400</td>
<td>3.39941000</td>
</tr>
<tr>
<td>H</td>
<td>-5.19160200</td>
<td>3.58178900</td>
<td>2.68929900</td>
</tr>
<tr>
<td>H</td>
<td>-5.09602600</td>
<td>2.35350900</td>
<td>3.97131500</td>
</tr>
<tr>
<td>H</td>
<td>-4.15048700</td>
<td>3.85352600</td>
<td>4.11035600</td>
</tr>
<tr>
<td>C</td>
<td>-2.33521500</td>
<td>1.79713700</td>
<td>3.66511000</td>
</tr>
<tr>
<td>H</td>
<td>-2.81469400</td>
<td>1.00824300</td>
<td>4.26840600</td>
</tr>
<tr>
<td>H</td>
<td>-1.47270000</td>
<td>1.36069400</td>
<td>3.14027600</td>
</tr>
<tr>
<td>H</td>
<td>-1.95508100</td>
<td>2.55745900</td>
<td>4.36763100</td>
</tr>
<tr>
<td>C</td>
<td>-5.81932000</td>
<td>-1.87446700</td>
<td>1.62102800</td>
</tr>
<tr>
<td>H</td>
<td>-5.48435000</td>
<td>-2.70310200</td>
<td>0.97247800</td>
</tr>
<tr>
<td>C</td>
<td>-5.56201200</td>
<td>-2.29165200</td>
<td>3.07374200</td>
</tr>
<tr>
<td>H</td>
<td>-6.06461500</td>
<td>-3.24752600</td>
<td>3.29076200</td>
</tr>
<tr>
<td>H</td>
<td>-4.48779000</td>
<td>-2.42372700</td>
<td>3.27928900</td>
</tr>
<tr>
<td>H</td>
<td>-5.95141700</td>
<td>-1.55031700</td>
<td>3.79119400</td>
</tr>
<tr>
<td>C</td>
<td>-7.32882000</td>
<td>-1.67923000</td>
<td>1.37817100</td>
</tr>
<tr>
<td>H</td>
<td>-7.72273400</td>
<td>-0.85524600</td>
<td>1.99669900</td>
</tr>
<tr>
<td>H</td>
<td>-7.53978200</td>
<td>-1.43639900</td>
<td>0.32564600</td>
</tr>
<tr>
<td>H</td>
<td>-7.88900600</td>
<td>-2.59416100</td>
<td>1.63244400</td>
</tr>
<tr>
<td>C</td>
<td>1.72768000</td>
<td>-5.02929200</td>
<td>4.43225000</td>
</tr>
<tr>
<td>C</td>
<td>0.50448600</td>
<td>-4.47479500</td>
<td>4.82446700</td>
</tr>
</tbody>
</table>
TS I'

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3333.51682905 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.18122100 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3333.33560805 a.u.
INT II'

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3333.55119753 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.18310900 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3333.36808853 a.u.
SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.60340257 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.08233100 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3102.52107157 a.u.
<table>
<thead>
<tr>
<th>At.</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.88576500</td>
<td>-4.28156300</td>
<td>-0.85761700</td>
</tr>
<tr>
<td>C</td>
<td>-0.50029100</td>
<td>-4.07313500</td>
<td>-1.00747500</td>
</tr>
<tr>
<td>C</td>
<td>0.24658200</td>
<td>-4.68401600</td>
<td>-2.00885400</td>
</tr>
<tr>
<td>C</td>
<td>-0.43625700</td>
<td>-5.54619500</td>
<td>-2.87871500</td>
</tr>
<tr>
<td>C</td>
<td>-1.81089600</td>
<td>-5.77033400</td>
<td>-2.74375500</td>
</tr>
<tr>
<td>C</td>
<td>-2.54983000</td>
<td>-5.12861800</td>
<td>-1.73666000</td>
</tr>
<tr>
<td>C</td>
<td>-2.34395800</td>
<td>-3.37241400</td>
<td>0.25200000</td>
</tr>
<tr>
<td>H</td>
<td>1.31722500</td>
<td>-4.50588300</td>
<td>-2.11795900</td>
</tr>
<tr>
<td>H</td>
<td>0.11772400</td>
<td>-6.04845400</td>
<td>-3.67512700</td>
</tr>
<tr>
<td>H</td>
<td>-2.31661900</td>
<td>-6.44926600</td>
<td>-3.43411100</td>
</tr>
<tr>
<td>H</td>
<td>-3.62568300</td>
<td>-5.29746700</td>
<td>-1.64778500</td>
</tr>
<tr>
<td>H</td>
<td>-2.86025100</td>
<td>-2.50331200</td>
<td>-0.20604600</td>
</tr>
<tr>
<td>N</td>
<td>-0.03535100</td>
<td>-3.20560500</td>
<td>0.02493700</td>
</tr>
<tr>
<td>C</td>
<td>1.36793000</td>
<td>-2.85741200</td>
<td>0.19579200</td>
</tr>
<tr>
<td>H</td>
<td>1.74193400</td>
<td>-2.40949200</td>
<td>-0.73423100</td>
</tr>
<tr>
<td>H</td>
<td>1.46796700</td>
<td>-2.11677900</td>
<td>0.99288100</td>
</tr>
<tr>
<td>H</td>
<td>1.94933000</td>
<td>-3.76049600</td>
<td>0.43335300</td>
</tr>
<tr>
<td>C</td>
<td>-1.05324200</td>
<td>-2.85707000</td>
<td>0.78819900</td>
</tr>
<tr>
<td>C</td>
<td>-1.21177200</td>
<td>-2.37682800</td>
<td>2.14482100</td>
</tr>
<tr>
<td>O</td>
<td>-0.35606600</td>
<td>-1.68224300</td>
<td>2.86713700</td>
</tr>
<tr>
<td>C</td>
<td>-2.39343500</td>
<td>-2.92952600</td>
<td>2.59951000</td>
</tr>
<tr>
<td>C</td>
<td>-2.89186800</td>
<td>-2.78610200</td>
<td>3.99441200</td>
</tr>
<tr>
<td>H</td>
<td>-2.22592300</td>
<td>-2.13733300</td>
<td>4.57898700</td>
</tr>
<tr>
<td>H</td>
<td>-3.90681500</td>
<td>-2.35041100</td>
<td>3.99897600</td>
</tr>
<tr>
<td>H</td>
<td>-2.96835500</td>
<td>-3.76172000</td>
<td>4.49835400</td>
</tr>
<tr>
<td>C</td>
<td>-3.10288700</td>
<td>-3.75260600</td>
<td>1.54728900</td>
</tr>
<tr>
<td>H</td>
<td>-4.18271700</td>
<td>-3.53737100</td>
<td>1.50859400</td>
</tr>
<tr>
<td>H</td>
<td>-2.99439600</td>
<td>-4.83280400</td>
<td>1.74892900</td>
</tr>
<tr>
<td>P</td>
<td>0.25865800</td>
<td>0.58748400</td>
<td>0.17382600</td>
</tr>
<tr>
<td>O</td>
<td>-0.68116500</td>
<td>1.91327600</td>
<td>0.51480400</td>
</tr>
<tr>
<td>O</td>
<td>1.55324400</td>
<td>1.27197200</td>
<td>-0.60612000</td>
</tr>
<tr>
<td>O</td>
<td>0.71941200</td>
<td>0.10746800</td>
<td>1.54438900</td>
</tr>
<tr>
<td>O</td>
<td>-0.39529700</td>
<td>-0.34447100</td>
<td>-0.79603800</td>
</tr>
<tr>
<td>C</td>
<td>-1.17197800</td>
<td>2.72711000</td>
<td>-0.48069200</td>
</tr>
<tr>
<td>C</td>
<td>-2.48077700</td>
<td>2.53298800</td>
<td>-0.97958500</td>
</tr>
<tr>
<td>C</td>
<td>-2.93388600</td>
<td>3.40084500</td>
<td>-1.99016600</td>
</tr>
<tr>
<td>C</td>
<td>-2.11379600</td>
<td>4.83291100</td>
<td>-2.54785400</td>
</tr>
<tr>
<td>C</td>
<td>-0.82630000</td>
<td>4.54897700</td>
<td>-2.04368200</td>
</tr>
<tr>
<td>C</td>
<td>0.25331500</td>
<td>5.50118600</td>
<td>-2.50564800</td>
</tr>
<tr>
<td>C</td>
<td>1.50680000</td>
<td>4.94203600</td>
<td>-1.80786000</td>
</tr>
<tr>
<td>C</td>
<td>0.97174400</td>
<td>4.30665900</td>
<td>-0.47962200</td>
</tr>
<tr>
<td>C</td>
<td>-0.37026300</td>
<td>3.76580300</td>
<td>-0.96918900</td>
</tr>
<tr>
<td>C</td>
<td>0.78435800</td>
<td>5.42791000</td>
<td>0.59489400</td>
</tr>
<tr>
<td>C</td>
<td>2.20196500</td>
<td>5.67207300</td>
<td>1.14978500</td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td>H</td>
<td>-1.80656600</td>
<td>-1.23866100</td>
<td>-2.33229600</td>
</tr>
<tr>
<td>C</td>
<td>-3.54876000</td>
<td>2.59226600</td>
<td>1.83435700</td>
</tr>
<tr>
<td>H</td>
<td>-2.80377500</td>
<td>3.24199700</td>
<td>1.35722600</td>
</tr>
<tr>
<td>C</td>
<td>-2.88494000</td>
<td>1.99119600</td>
<td>3.08590600</td>
</tr>
<tr>
<td>H</td>
<td>-1.99690600</td>
<td>1.40086700</td>
<td>2.81818400</td>
</tr>
<tr>
<td>H</td>
<td>-2.56339300</td>
<td>2.79236600</td>
<td>3.77211200</td>
</tr>
<tr>
<td>H</td>
<td>-3.58083900</td>
<td>1.34136100</td>
<td>3.64314300</td>
</tr>
<tr>
<td>C</td>
<td>-4.74337100</td>
<td>3.48907100</td>
<td>2.20852200</td>
</tr>
<tr>
<td>H</td>
<td>-5.19609700</td>
<td>3.94824200</td>
<td>1.31534100</td>
</tr>
<tr>
<td>H</td>
<td>-5.53328100</td>
<td>2.92410000</td>
<td>2.73062600</td>
</tr>
<tr>
<td>H</td>
<td>-4.42025400</td>
<td>4.30135400</td>
<td>2.88047200</td>
</tr>
<tr>
<td>C</td>
<td>-6.52479000</td>
<td>-1.36509800</td>
<td>0.70089500</td>
</tr>
<tr>
<td>H</td>
<td>-6.27959000</td>
<td>-2.34631900</td>
<td>0.25231100</td>
</tr>
<tr>
<td>C</td>
<td>-6.72914300</td>
<td>-1.58327900</td>
<td>2.20490000</td>
</tr>
<tr>
<td>H</td>
<td>-7.49397800</td>
<td>-2.35632300</td>
<td>2.38175600</td>
</tr>
<tr>
<td>H</td>
<td>-7.80146800</td>
<td>-1.90306700</td>
<td>2.70466800</td>
</tr>
<tr>
<td>H</td>
<td>-7.07573100</td>
<td>-0.66501000</td>
<td>2.70583600</td>
</tr>
<tr>
<td>C</td>
<td>-7.83787100</td>
<td>-0.88916500</td>
<td>0.44745700</td>
</tr>
<tr>
<td>H</td>
<td>-8.13436100</td>
<td>0.09451100</td>
<td>0.44742400</td>
</tr>
<tr>
<td>H</td>
<td>-7.73067100</td>
<td>-0.78521800</td>
<td>-1.04295800</td>
</tr>
<tr>
<td>H</td>
<td>-8.65861500</td>
<td>-1.59896000</td>
<td>0.24474900</td>
</tr>
<tr>
<td>C</td>
<td>4.01065500</td>
<td>-0.20182500</td>
<td>2.94258200</td>
</tr>
<tr>
<td>H</td>
<td>3.43721600</td>
<td>0.73405500</td>
<td>2.90038100</td>
</tr>
<tr>
<td>C</td>
<td>5.31626000</td>
<td>0.06688000</td>
<td>3.71698100</td>
</tr>
<tr>
<td>H</td>
<td>5.09562400</td>
<td>0.44362000</td>
<td>4.72950600</td>
</tr>
<tr>
<td>H</td>
<td>5.90973400</td>
<td>-0.85621100</td>
<td>3.82753000</td>
</tr>
<tr>
<td>H</td>
<td>5.95518200</td>
<td>0.80806400</td>
<td>3.21420100</td>
</tr>
<tr>
<td>C</td>
<td>3.14847600</td>
<td>-1.21199200</td>
<td>3.71885000</td>
</tr>
<tr>
<td>H</td>
<td>3.66344700</td>
<td>-2.17707100</td>
<td>3.85858100</td>
</tr>
<tr>
<td>H</td>
<td>2.92546400</td>
<td>-0.81831000</td>
<td>4.72406400</td>
</tr>
<tr>
<td>H</td>
<td>2.18803400</td>
<td>-1.39874900</td>
<td>3.22224300</td>
</tr>
<tr>
<td>C</td>
<td>4.22480300</td>
<td>0.58999700</td>
<td>-2.18243400</td>
</tr>
<tr>
<td>H</td>
<td>3.83186700</td>
<td>1.56913300</td>
<td>-1.88049200</td>
</tr>
<tr>
<td>C</td>
<td>5.58301900</td>
<td>0.85141600</td>
<td>-2.85946300</td>
</tr>
<tr>
<td>H</td>
<td>6.29486000</td>
<td>1.32034500</td>
<td>-2.16167000</td>
</tr>
<tr>
<td>H</td>
<td>6.04317900</td>
<td>-0.07929000</td>
<td>-3.23053900</td>
</tr>
<tr>
<td>H</td>
<td>5.46021800</td>
<td>1.52601200</td>
<td>-3.72304500</td>
</tr>
<tr>
<td>C</td>
<td>3.21107300</td>
<td>-0.01514800</td>
<td>-3.16968700</td>
</tr>
<tr>
<td>H</td>
<td>3.55175800</td>
<td>-0.99078200</td>
<td>-3.55635900</td>
</tr>
<tr>
<td>H</td>
<td>2.22959300</td>
<td>-0.14860600</td>
<td>-2.69201600</td>
</tr>
<tr>
<td>H</td>
<td>3.07635400</td>
<td>0.65091800</td>
<td>-4.03827600</td>
</tr>
<tr>
<td>C</td>
<td>5.74939900</td>
<td>-3.78858700</td>
<td>-0.15827200</td>
</tr>
<tr>
<td>H</td>
<td>5.71485300</td>
<td>-4.27896000</td>
<td>0.83047800</td>
</tr>
<tr>
<td>C</td>
<td>4.97302700</td>
<td>-4.68270200</td>
<td>-1.13899900</td>
</tr>
</tbody>
</table>
TS II

SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.57777370 a.u.

Thermal correction to Gibbs free energy at 298 K: 1.07977500 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3102.49799870 a.u.
H  3.35931900 -1.89902500 -2.63232000
H  3.23215300 -3.56195600 -3.23218600
C  1.90755300 -3.42851800 -0.57401500
H  2.74704500 -2.86325700 -0.13837600
H  2.20320000 -4.49328800 -0.57681000
P  0.09747900  0.42980700 -0.29258000
O  1.34766100  1.49040000 -0.47876600
O  -1.02999600  1.29358100  0.54962900
O  -0.38531400  0.07826600 -1.66829700
O  0.52448500 -0.65791100  0.70772500
C  1.98803300  2.13480000  0.56448600
C  3.25223900  1.68709600  1.01452400
C  3.85879900  2.39031300  2.07293400
C  3.22929400  3.45190300  2.72109800
C  1.99187800  3.88063700  2.25104500
C  1.11925100  4.99233300  2.78606500
C  -0.20625600  4.75978600  2.04048800
C  0.21633300  4.12147900  0.67362000
C  1.39878200  3.27241300  1.13040800
C  0.67943700  5.24994900 -0.30623700
C  -0.63209700  5.85481600 -0.84259200
C  -1.58465700  4.68189900 -0.78297900
C  -2.86917000  4.57636900 -1.30777400
C  -3.57157800  3.38627000 -1.12098800
C  -2.99475900  2.25336500 -0.51386300
C  -1.67571200  2.37944800 -0.01903000
C  -1.01717600  3.61401700 -0.06656300
H  -0.45431600 -1.17121100 -2.89082400
H  4.84761100  2.06807300  2.40485000
H  3.70694400  3.94067700  3.57443700
H  1.54782700  5.98349700  2.55225700
H  1.01103600  4.94900300  3.88187400
H  -0.80915400  5.67067900  1.91342800
H  -0.82111200  4.02874700  2.58958500
H  1.33971400  5.98571700  0.17603000
H  1.24421500  4.78575400 -1.13054500
H  -0.98428300  6.68888600 -0.20942800
H  -0.53268600  6.25864900 -1.86316200
H  -3.33092900  5.41230500 -1.83999400
H  -4.60043700  3.31059100 -1.47605900
C  -3.85082100  1.02412400 -0.39780300
C  -4.39666100  0.43287200 -1.56909300
C  -4.26204800  0.54641500  0.87702400
C  -5.37456900 -0.56734200 -1.43435300
<table>
<thead>
<tr>
<th>Atoms</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-5.22406600</td>
<td>-0.47165200</td>
<td>0.94824100</td>
</tr>
<tr>
<td>C</td>
<td>-5.81863600</td>
<td>-1.02633500</td>
<td>-0.19074600</td>
</tr>
<tr>
<td>H</td>
<td>-5.81591600</td>
<td>-1.00064300</td>
<td>-2.33679300</td>
</tr>
<tr>
<td>H</td>
<td>-5.54483300</td>
<td>-0.81402100</td>
<td>1.93561300</td>
</tr>
<tr>
<td>C</td>
<td>4.01175400</td>
<td>0.53429200</td>
<td>0.42542500</td>
</tr>
<tr>
<td>C</td>
<td>4.53269700</td>
<td>0.61094200</td>
<td>-0.89253300</td>
</tr>
<tr>
<td>C</td>
<td>4.34415300</td>
<td>-0.58254700</td>
<td>1.24115300</td>
</tr>
<tr>
<td>C</td>
<td>5.37806400</td>
<td>-0.40990400</td>
<td>-1.35606200</td>
</tr>
<tr>
<td>C</td>
<td>5.18602200</td>
<td>-1.57543000</td>
<td>0.72137800</td>
</tr>
<tr>
<td>C</td>
<td>5.73319500</td>
<td>-1.50739500</td>
<td>-0.56501000</td>
</tr>
<tr>
<td>H</td>
<td>5.79230700</td>
<td>-0.32316500</td>
<td>-2.36291100</td>
</tr>
<tr>
<td>H</td>
<td>5.44817700</td>
<td>-2.42907100</td>
<td>1.35409300</td>
</tr>
<tr>
<td>C</td>
<td>3.84931000</td>
<td>-0.74260600</td>
<td>2.68241100</td>
</tr>
<tr>
<td>H</td>
<td>3.19952400</td>
<td>0.11148700</td>
<td>2.91228700</td>
</tr>
<tr>
<td>C</td>
<td>5.01321200</td>
<td>-0.72120300</td>
<td>3.69071000</td>
</tr>
<tr>
<td>H</td>
<td>5.62607300</td>
<td>0.18829400</td>
<td>3.59080700</td>
</tr>
<tr>
<td>H</td>
<td>4.62977400</td>
<td>-0.75825100</td>
<td>4.72372300</td>
</tr>
<tr>
<td>H</td>
<td>5.68363000</td>
<td>-1.58597000</td>
<td>3.55575000</td>
</tr>
<tr>
<td>C</td>
<td>2.98688400</td>
<td>-2.00079600</td>
<td>2.87232100</td>
</tr>
<tr>
<td>H</td>
<td>3.54354000</td>
<td>-2.92370700</td>
<td>2.63717700</td>
</tr>
<tr>
<td>H</td>
<td>2.64804900</td>
<td>-2.07682200</td>
<td>3.91877700</td>
</tr>
<tr>
<td>H</td>
<td>2.09452000</td>
<td>-1.95255300</td>
<td>2.23535600</td>
</tr>
<tr>
<td>C</td>
<td>4.27090300</td>
<td>1.80243300</td>
<td>-1.81556500</td>
</tr>
<tr>
<td>H</td>
<td>3.63713300</td>
<td>2.51539200</td>
<td>-1.27251800</td>
</tr>
<tr>
<td>C</td>
<td>3.50192300</td>
<td>1.39626000</td>
<td>-3.08496600</td>
</tr>
<tr>
<td>H</td>
<td>2.53919000</td>
<td>0.92931000</td>
<td>-2.83182600</td>
</tr>
<tr>
<td>H</td>
<td>3.29254400</td>
<td>2.28236100</td>
<td>-3.70688500</td>
</tr>
<tr>
<td>H</td>
<td>4.08098800</td>
<td>0.69067200</td>
<td>-3.70404100</td>
</tr>
<tr>
<td>C</td>
<td>5.57307200</td>
<td>2.54794700</td>
<td>-2.16148500</td>
</tr>
<tr>
<td>H</td>
<td>6.10636100</td>
<td>2.86662600</td>
<td>-1.25178300</td>
</tr>
<tr>
<td>H</td>
<td>6.26250300</td>
<td>1.92102800</td>
<td>-2.75046700</td>
</tr>
<tr>
<td>H</td>
<td>5.35441000</td>
<td>3.44810700</td>
<td>-2.75957400</td>
</tr>
<tr>
<td>C</td>
<td>6.74555700</td>
<td>-2.55692300</td>
<td>-1.01467300</td>
</tr>
<tr>
<td>H</td>
<td>6.51315100</td>
<td>-3.48013500</td>
<td>-0.45384000</td>
</tr>
<tr>
<td>C</td>
<td>6.68070500</td>
<td>-2.90051400</td>
<td>-2.50881300</td>
</tr>
<tr>
<td>H</td>
<td>7.36792600</td>
<td>-3.72972700</td>
<td>-2.74160500</td>
</tr>
<tr>
<td>H</td>
<td>5.66783000</td>
<td>-3.20389900</td>
<td>-2.81348400</td>
</tr>
<tr>
<td>H</td>
<td>6.98009100</td>
<td>-2.04752900</td>
<td>-3.13948100</td>
</tr>
<tr>
<td>C</td>
<td>8.17275100</td>
<td>-2.13157700</td>
<td>-0.61619900</td>
</tr>
<tr>
<td>H</td>
<td>8.46535000</td>
<td>-1.20725700</td>
<td>-1.14136000</td>
</tr>
<tr>
<td>H</td>
<td>8.24642400</td>
<td>-1.93719200</td>
<td>0.46493900</td>
</tr>
<tr>
<td>H</td>
<td>8.90475400</td>
<td>-2.91496400</td>
<td>-0.87431400</td>
</tr>
<tr>
<td>C</td>
<td>-3.97966400</td>
<td>0.83767400</td>
<td>-2.98534500</td>
</tr>
<tr>
<td>H</td>
<td>-3.16896200</td>
<td>1.57288300</td>
<td>-2.89544900</td>
</tr>
</tbody>
</table>

S27
CP II-Post

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.59500213 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.08178100 a.u.
Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3102.51322113 a.u.

C    -5.12931100  1.49325300  -3.77237200
H    -4.77680100  1.82937500  -4.76138400
H    -5.95753900  0.78521800  -3.94072600
H    -5.54571900  2.36737600  -3.24890100
C    -3.40238700  -0.34859800  -3.77522100
H    -4.15650300  -1.13268900  -3.95729300
H    -3.03774100  -0.01196200  -4.75946200
H    -2.55641400  -0.80070300  -3.24339900
C    -3.75471600  1.13932900  2.19299200
H    -3.06904700  1.96133500  1.95222900
C    -4.89943700  1.75403400  3.01986100
H    -5.45650200  2.50576100  2.43829000
H    -5.62034600  0.99179800  3.35767700
H    -4.49977400  2.24971700  3.91998500
C    -2.95429500  0.11332600  3.01445300
H    -5.57474200  -0.75219400  3.30138900
H    -2.08583400  -0.25400400  2.44930700
H    -2.58053200  0.57383300  3.94174400
C    -6.94476000  -2.05349900  -0.09331600
H    -7.18957300  -2.35176400  -1.12698900
C    -6.53864600  -3.32272000  0.66830200
H    -7.36952000  -4.04673400  0.69073600
H    -5.67753400  -3.81677100  0.19155000
H    -6.26467500  -3.10078300  1.71264100
C    -8.21654300  -1.42878200  0.51223700
H    -8.05004700  -1.11489400  1.55581600
H    -8.53501300  -0.54084200  -0.05581000
H    -9.04782500  -2.15321500  0.50919500

C    1.45612300  -4.50031900  1.17408900
C    0.28124600  -3.75305000  1.49654700

S28
<p>| C  | -4.24607100 | 2.73886200 | -1.40733000 |
| C  | -3.50444300 | 1.78701400 | -0.68410100 |
| C  | -2.27556500 | 2.21373500 | -0.13654000 |
| C  | -1.84536100 | 3.53697700 | -0.24737000 |
| C  | 0.23772100  | 6.47210900 | 2.23837700  |
| C  | 2.67493200  | 4.85775100 | 3.42749100  |
| C  | -0.15303900 | 5.45092600 | 3.62761900  |
| H  | 0.04734800  | 6.29897500 | 2.39237700  |
| C  | 0.02088600  | 5.01454500 | 1.38201000  |
| H  | 0.237831100 | 6.53757600 | -0.61096000 |
| C  | -2.35831100 | -1.06199600 | 0.17635000  |
| C  | -1.78351600 | 6.10039000 | -2.22435400 |
| C  | -4.34836400 | 4.72410100 | -2.60041000 |
| C  | 0.51241100  | 2.43973900 | -1.81529100 |
| C  | -0.50763900 | 0.40412900 | -0.48720100 |
| C  | -4.26963500 | -0.45597200 | -1.59874800 |
| C  | -4.45470200 | -0.02094000 | 0.80994800  |
| C  | -4.87711500 | -1.70212700 | -1.38269400 |
| C  | 0.50439400  | 1.27872800 | 0.96312600  |
| C  | -5.28516300 | -2.13629200 | -0.11827600 |
| H  | 0.50533700  | -2.36176000 | -2.53800700 |
| C  | -5.36980100 | -1.58793000 | 1.96302400  |
| C  | 3.58265300  | 1.37617400 | 0.44732000  |
| C  | 4.07492000  | 1.49001900 | -0.88109000 |
| C  | 4.05470000  | 0.32655400 | 1.27978600  |
| C  | 5.03311400  | 0.57327300 | -1.33255300 |
| C  | 5.01584500  | -0.55955000 | 0.77202100  |
| C  | 4.35295350  | -0.45387100 | -0.52282000 |
| C  | 5.41581800  | 0.67873700 | -2.53085400 |
| H  | 5.38460600  | -1.36429800 | 1.41409700  |
| C  | 3.57142500  | 0.11806700 | 2.71746100  |
| H  | 2.72257300  | 0.79536200 | 2.88754000  |
| C  | 4.66531300  | 0.47052500 | 3.74390500  |
| H  | 5.02411900  | 1.50496000 | 3.63067600  |
| H  | 4.28400100  | 0.35618500 | 4.77215600  |
| H  | 5.35882900  | -0.19357100 | 3.63718400  |
| C  | 3.05785900  | -1.31047800 | 2.96432000  |
| H  | 3.86486400  | -2.05785900 | 2.90216000  |
| H  | 2.61766800  | -1.39031600 | 3.97141100  |
| H  | 2.28516600  | -1.59188900 | 2.23728400  |
| C  | 3.64685200  | 2.60519200 | -1.83704400 |</p>
<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.9006</td>
<td>3.2266</td>
<td>-1.3246</td>
</tr>
<tr>
<td>C</td>
<td>2.9763</td>
<td>2.0508</td>
<td>-3.1066</td>
</tr>
<tr>
<td>H</td>
<td>2.1099</td>
<td>1.4213</td>
<td>-2.8570</td>
</tr>
<tr>
<td>H</td>
<td>2.6241</td>
<td>2.8761</td>
<td>-3.7480</td>
</tr>
<tr>
<td>H</td>
<td>3.6766</td>
<td>1.4457</td>
<td>-3.7055</td>
</tr>
<tr>
<td>C</td>
<td>4.8241</td>
<td>3.5349</td>
<td>-2.1857</td>
</tr>
<tr>
<td>H</td>
<td>5.2808</td>
<td>3.9620</td>
<td>-1.2788</td>
</tr>
<tr>
<td>H</td>
<td>5.6153</td>
<td>3.0021</td>
<td>-2.7381</td>
</tr>
<tr>
<td>H</td>
<td>4.4830</td>
<td>4.3699</td>
<td>-2.8199</td>
</tr>
<tr>
<td>C</td>
<td>6.6179</td>
<td>-1.4029</td>
<td>-3.1562</td>
</tr>
<tr>
<td>H</td>
<td>6.7341</td>
<td>-2.1776</td>
<td>-0.2310</td>
</tr>
<tr>
<td>C</td>
<td>6.2440</td>
<td>-2.1198</td>
<td>-2.3164</td>
</tr>
<tr>
<td>H</td>
<td>7.0172</td>
<td>-2.8559</td>
<td>-2.5913</td>
</tr>
<tr>
<td>H</td>
<td>5.2839</td>
<td>-2.6497</td>
<td>-2.2218</td>
</tr>
<tr>
<td>H</td>
<td>6.1524</td>
<td>-1.4119</td>
<td>-3.1562</td>
</tr>
<tr>
<td>C</td>
<td>7.9720</td>
<td>-0.6819</td>
<td>-1.1407</td>
</tr>
<tr>
<td>H</td>
<td>7.9297</td>
<td>0.1063</td>
<td>-1.9104</td>
</tr>
<tr>
<td>H</td>
<td>8.2655</td>
<td>-0.2059</td>
<td>-0.1920</td>
</tr>
<tr>
<td>H</td>
<td>8.7676</td>
<td>-1.3891</td>
<td>-1.4290</td>
</tr>
<tr>
<td>C</td>
<td>-3.8921</td>
<td>-0.0758</td>
<td>-3.0335</td>
</tr>
<tr>
<td>H</td>
<td>-3.2454</td>
<td>0.8116</td>
<td>-2.9828</td>
</tr>
<tr>
<td>C</td>
<td>-5.1411</td>
<td>0.2860</td>
<td>-3.8622</td>
</tr>
<tr>
<td>H</td>
<td>-4.8531</td>
<td>0.6107</td>
<td>-4.8756</td>
</tr>
<tr>
<td>H</td>
<td>-5.8072</td>
<td>-0.5862</td>
<td>-3.9679</td>
</tr>
<tr>
<td>H</td>
<td>-5.7305</td>
<td>1.0941</td>
<td>-3.4039</td>
</tr>
<tr>
<td>C</td>
<td>-3.0916</td>
<td>-1.1691</td>
<td>-3.7623</td>
</tr>
<tr>
<td>H</td>
<td>-3.6988</td>
<td>-2.0704</td>
<td>-3.9477</td>
</tr>
<tr>
<td>H</td>
<td>-2.7618</td>
<td>-0.7974</td>
<td>-4.7460</td>
</tr>
<tr>
<td>H</td>
<td>-2.1940</td>
<td>-1.4722</td>
<td>-3.2091</td>
</tr>
<tr>
<td>C</td>
<td>-4.3111</td>
<td>0.8579</td>
<td>2.0549</td>
</tr>
<tr>
<td>H</td>
<td>-3.8375</td>
<td>1.8018</td>
<td>1.7539</td>
</tr>
<tr>
<td>C</td>
<td>-5.6842</td>
<td>1.2277</td>
<td>2.6461</td>
</tr>
<tr>
<td>H</td>
<td>-6.3224</td>
<td>1.7223</td>
<td>1.8969</td>
</tr>
<tr>
<td>H</td>
<td>-6.2254</td>
<td>0.3394</td>
<td>3.0106</td>
</tr>
<tr>
<td>H</td>
<td>-5.5655</td>
<td>1.9163</td>
<td>3.4990</td>
</tr>
<tr>
<td>C</td>
<td>-3.3989</td>
<td>0.2172</td>
<td>3.1159</td>
</tr>
<tr>
<td>H</td>
<td>-3.8194</td>
<td>-0.7278</td>
<td>3.4983</td>
</tr>
<tr>
<td>H</td>
<td>-2.3998</td>
<td>0.0109</td>
<td>2.7046</td>
</tr>
<tr>
<td>H</td>
<td>-3.2753</td>
<td>0.8931</td>
<td>3.9783</td>
</tr>
<tr>
<td>C</td>
<td>-5.9979</td>
<td>-3.4729</td>
<td>0.0528</td>
</tr>
<tr>
<td>H</td>
<td>-5.9150</td>
<td>-4.0014</td>
<td>-0.9128</td>
</tr>
<tr>
<td>C</td>
<td>-5.3514</td>
<td>-4.3683</td>
<td>1.1218</td>
</tr>
<tr>
<td>H</td>
<td>-5.8537</td>
<td>-5.3484</td>
<td>1.1632</td>
</tr>
<tr>
<td>H</td>
<td>-4.2850</td>
<td>-4.5442</td>
<td>0.9109</td>
</tr>
</tbody>
</table>
CP II-Pre'

![Chemical Structure](image)

SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5803.68160419 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.07839400 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-5802.60321019 a.u.

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-5.42480500</td>
<td>-3.92057900</td>
<td>2.12647200</td>
</tr>
<tr>
<td>C</td>
<td>-7.49823800</td>
<td>-3.26990800</td>
<td>0.33486600</td>
</tr>
<tr>
<td>H</td>
<td>-7.65549200</td>
<td>-2.74809200</td>
<td>1.29343600</td>
</tr>
<tr>
<td>H</td>
<td>-7.97503700</td>
<td>-2.66759900</td>
<td>-0.45408400</td>
</tr>
<tr>
<td>H</td>
<td>-8.02271800</td>
<td>-4.23821500</td>
<td>0.38981000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.49911200</td>
<td>-4.03556900</td>
<td>2.25509500</td>
</tr>
<tr>
<td>C</td>
<td>0.26450500</td>
<td>-3.49063800</td>
<td>2.66762600</td>
</tr>
<tr>
<td>C</td>
<td>-0.25245500</td>
<td>-3.68718200</td>
<td>3.94322100</td>
</tr>
<tr>
<td>C</td>
<td>0.50246100</td>
<td>-4.47430800</td>
<td>4.82481000</td>
</tr>
<tr>
<td>C</td>
<td>1.72573300</td>
<td>-5.02886100</td>
<td>4.43292200</td>
</tr>
<tr>
<td>C</td>
<td>2.24021900</td>
<td>-4.80257100</td>
<td>3.14573100</td>
</tr>
<tr>
<td>C</td>
<td>1.76490600</td>
<td>-3.49812400</td>
<td>0.87209000</td>
</tr>
<tr>
<td>H</td>
<td>-1.20694700</td>
<td>-3.25644700</td>
<td>4.24870200</td>
</tr>
<tr>
<td>H</td>
<td>0.12427000</td>
<td>-4.65787800</td>
<td>5.83312200</td>
</tr>
<tr>
<td>H</td>
<td>2.28929000</td>
<td>-5.64355600</td>
<td>5.13847500</td>
</tr>
<tr>
<td>H</td>
<td>3.20264900</td>
<td>-5.22881500</td>
<td>2.85256800</td>
</tr>
<tr>
<td>H</td>
<td>2.48775500</td>
<td>-2.66287400</td>
<td>0.97639200</td>
</tr>
<tr>
<td>N</td>
<td>-0.33128600</td>
<td>-2.78510200</td>
<td>1.57929300</td>
</tr>
<tr>
<td>C</td>
<td>-1.64607600</td>
<td>-2.15958500</td>
<td>1.63427700</td>
</tr>
<tr>
<td>H</td>
<td>-1.61430200</td>
<td>-1.30812900</td>
<td>2.32821800</td>
</tr>
<tr>
<td>H</td>
<td>-1.91526000</td>
<td>-1.81276000</td>
<td>0.63382800</td>
</tr>
<tr>
<td>H</td>
<td>-2.39131800</td>
<td>-2.89763100</td>
<td>1.95972800</td>
</tr>
<tr>
<td>C</td>
<td>0.46372800</td>
<td>-2.86583400</td>
<td>0.53088500</td>
</tr>
<tr>
<td>C</td>
<td>0.30072900</td>
<td>-2.72462800</td>
<td>-0.89553300</td>
</tr>
<tr>
<td>O</td>
<td>-0.64942800</td>
<td>-2.02426600</td>
<td>-1.49050500</td>
</tr>
<tr>
<td>C</td>
<td>1.26731700</td>
<td>-3.53492800</td>
<td>-1.46749800</td>
</tr>
<tr>
<td>C</td>
<td>1.45385500</td>
<td>-3.74291200</td>
<td>-2.92908600</td>
</tr>
<tr>
<td>H</td>
<td>0.64884500</td>
<td>-3.28153700</td>
<td>-3.51804600</td>
</tr>
<tr>
<td>H</td>
<td>2.41659700</td>
<td>-3.30170000</td>
<td>-3.24830900</td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>H</td>
<td>1.50241200</td>
<td>-4.81654800</td>
<td>-3.17934500</td>
</tr>
<tr>
<td>C</td>
<td>2.11426900</td>
<td>-4.24928600</td>
<td>-0.43387700</td>
</tr>
<tr>
<td>H</td>
<td>3.18661600</td>
<td>-4.22773500</td>
<td>-0.68493300</td>
</tr>
<tr>
<td>H</td>
<td>1.81811500</td>
<td>-5.31033700</td>
<td>-0.36197600</td>
</tr>
<tr>
<td>Zn</td>
<td>-2.15226900</td>
<td>-2.95221600</td>
<td>-2.45204600</td>
</tr>
<tr>
<td>Cl</td>
<td>-3.44952000</td>
<td>-3.92548000</td>
<td>-0.95669600</td>
</tr>
<tr>
<td>Cl</td>
<td>-1.89596000</td>
<td>-3.12562300</td>
<td>-4.61764100</td>
</tr>
<tr>
<td>P</td>
<td>0.17973700</td>
<td>1.07497600</td>
<td>0.00043900</td>
</tr>
<tr>
<td>O</td>
<td>1.31801600</td>
<td>2.00564400</td>
<td>-0.71264500</td>
</tr>
<tr>
<td>O</td>
<td>-0.81774300</td>
<td>2.15481000</td>
<td>0.70562500</td>
</tr>
<tr>
<td>O</td>
<td>-0.56294900</td>
<td>0.51510200</td>
<td>-1.26825000</td>
</tr>
<tr>
<td>O</td>
<td>0.66675000</td>
<td>0.10274100</td>
<td>1.01264100</td>
</tr>
<tr>
<td>C</td>
<td>2.14047900</td>
<td>2.85021100</td>
<td>0.02083100</td>
</tr>
<tr>
<td>C</td>
<td>3.43505000</td>
<td>2.42067100</td>
<td>0.38748700</td>
</tr>
<tr>
<td>C</td>
<td>4.23242800</td>
<td>3.31562400</td>
<td>1.12411500</td>
</tr>
<tr>
<td>C</td>
<td>3.75316400</td>
<td>4.55361500</td>
<td>1.55495700</td>
</tr>
<tr>
<td>C</td>
<td>2.46809600</td>
<td>4.94330600</td>
<td>1.18784100</td>
</tr>
<tr>
<td>C</td>
<td>1.71640800</td>
<td>6.19638800</td>
<td>1.57399200</td>
</tr>
<tr>
<td>C</td>
<td>0.27286000</td>
<td>5.85517100</td>
<td>1.16084400</td>
</tr>
<tr>
<td>C</td>
<td>0.43108300</td>
<td>4.89715300</td>
<td>-0.06847900</td>
</tr>
<tr>
<td>C</td>
<td>1.67672300</td>
<td>4.12439000</td>
<td>0.36193700</td>
</tr>
<tr>
<td>C</td>
<td>0.69742900</td>
<td>5.74576600</td>
<td>-1.35591400</td>
</tr>
<tr>
<td>C</td>
<td>-0.69585300</td>
<td>6.25402200</td>
<td>-1.77595600</td>
</tr>
<tr>
<td>C</td>
<td>-1.60936700</td>
<td>5.15229900</td>
<td>-1.28704100</td>
</tr>
<tr>
<td>C</td>
<td>-2.95525600</td>
<td>4.94314000</td>
<td>-1.57521400</td>
</tr>
<tr>
<td>C</td>
<td>-3.59880300</td>
<td>3.82791500</td>
<td>-1.03364700</td>
</tr>
<tr>
<td>C</td>
<td>-2.91032700</td>
<td>2.86341300</td>
<td>-0.27669900</td>
</tr>
<tr>
<td>C</td>
<td>-1.54243400</td>
<td>3.10006900</td>
<td>-0.01259200</td>
</tr>
<tr>
<td>C</td>
<td>-0.91286500</td>
<td>4.27212100</td>
<td>-0.43886300</td>
</tr>
<tr>
<td>H</td>
<td>-0.57651600</td>
<td>-0.50874800</td>
<td>-1.34473300</td>
</tr>
<tr>
<td>H</td>
<td>5.24521200</td>
<td>3.00653100</td>
<td>1.39023400</td>
</tr>
<tr>
<td>H</td>
<td>4.37884800</td>
<td>5.20110300</td>
<td>2.17500000</td>
</tr>
<tr>
<td>H</td>
<td>2.09715100</td>
<td>7.07641000</td>
<td>1.02523400</td>
</tr>
<tr>
<td>H</td>
<td>1.81426000</td>
<td>6.42911300</td>
<td>2.64641900</td>
</tr>
<tr>
<td>H</td>
<td>-0.34220900</td>
<td>6.73824100</td>
<td>0.93456100</td>
</tr>
<tr>
<td>H</td>
<td>-0.22670500</td>
<td>5.30143800</td>
<td>1.97197600</td>
</tr>
<tr>
<td>H</td>
<td>1.42776800</td>
<td>6.55128800</td>
<td>-1.18979000</td>
</tr>
<tr>
<td>H</td>
<td>1.10540800</td>
<td>5.08187600</td>
<td>-2.13489500</td>
</tr>
<tr>
<td>H</td>
<td>-0.93756200</td>
<td>7.21879900</td>
<td>-1.29517400</td>
</tr>
<tr>
<td>H</td>
<td>-0.78323900</td>
<td>6.41578900</td>
<td>-2.86229300</td>
</tr>
<tr>
<td>H</td>
<td>-3.50601300</td>
<td>5.63989800</td>
<td>-2.21267600</td>
</tr>
<tr>
<td>H</td>
<td>-4.66211100</td>
<td>3.67366600</td>
<td>-1.22554600</td>
</tr>
<tr>
<td>C</td>
<td>-3.62763900</td>
<td>1.64280500</td>
<td>0.22168000</td>
</tr>
<tr>
<td>C</td>
<td>-4.17727100</td>
<td>0.70487900</td>
<td>-0.69774100</td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>C</td>
<td>-3.80720500</td>
<td>1.43513500</td>
<td>1.61319200</td>
</tr>
<tr>
<td>C</td>
<td>-4.85266100</td>
<td>-0.41542000</td>
<td>-0.19967600</td>
</tr>
<tr>
<td>C</td>
<td>-4.50637900</td>
<td>0.29958900</td>
<td>2.05363200</td>
</tr>
<tr>
<td>C</td>
<td>-5.03505400</td>
<td>-0.64477300</td>
<td>1.16992900</td>
</tr>
<tr>
<td>H</td>
<td>-5.24955100</td>
<td>-1.15196800</td>
<td>-0.90213300</td>
</tr>
<tr>
<td>H</td>
<td>-4.64476500</td>
<td>0.16207700</td>
<td>3.12759800</td>
</tr>
<tr>
<td>C</td>
<td>3.99326500</td>
<td>1.07062800</td>
<td>0.04091300</td>
</tr>
<tr>
<td>C</td>
<td>4.29690300</td>
<td>0.73578700</td>
<td>-1.30260200</td>
</tr>
<tr>
<td>C</td>
<td>4.31064600</td>
<td>0.15163300</td>
<td>1.07915500</td>
</tr>
<tr>
<td>C</td>
<td>4.92640400</td>
<td>-0.48877300</td>
<td>-1.57834100</td>
</tr>
<tr>
<td>C</td>
<td>4.93652400</td>
<td>-1.05639900</td>
<td>0.74432200</td>
</tr>
<tr>
<td>C</td>
<td>5.27264600</td>
<td>-1.39570300</td>
<td>-0.57317200</td>
</tr>
<tr>
<td>H</td>
<td>5.17104200</td>
<td>-0.72215900</td>
<td>-2.61616100</td>
</tr>
<tr>
<td>H</td>
<td>5.19664300</td>
<td>-1.75461800</td>
<td>1.54649000</td>
</tr>
<tr>
<td>C</td>
<td>4.02136100</td>
<td>0.43138600</td>
<td>2.55702800</td>
</tr>
<tr>
<td>H</td>
<td>3.47991500</td>
<td>1.38464700</td>
<td>2.61757100</td>
</tr>
<tr>
<td>C</td>
<td>5.32006700</td>
<td>0.58718600</td>
<td>3.37003600</td>
</tr>
<tr>
<td>H</td>
<td>5.97611100</td>
<td>1.36670800</td>
<td>2.95189300</td>
</tr>
<tr>
<td>H</td>
<td>5.09256100</td>
<td>0.86086900</td>
<td>4.41353500</td>
</tr>
<tr>
<td>H</td>
<td>5.89840400</td>
<td>-0.35147500</td>
<td>3.39303400</td>
</tr>
<tr>
<td>C</td>
<td>3.10170400</td>
<td>-0.62708200</td>
<td>3.18835000</td>
</tr>
<tr>
<td>H</td>
<td>3.56790600</td>
<td>-1.62655600</td>
<td>3.19930700</td>
</tr>
<tr>
<td>H</td>
<td>2.88157200</td>
<td>-0.36295700</td>
<td>4.23609400</td>
</tr>
<tr>
<td>H</td>
<td>2.15007300</td>
<td>-0.67600300</td>
<td>2.64145700</td>
</tr>
<tr>
<td>C</td>
<td>4.01752500</td>
<td>1.67962700</td>
<td>-2.47269200</td>
</tr>
<tr>
<td>H</td>
<td>3.54377100</td>
<td>2.58491200</td>
<td>-2.07016000</td>
</tr>
<tr>
<td>C</td>
<td>3.03393700</td>
<td>1.06974800</td>
<td>-3.48703100</td>
</tr>
<tr>
<td>H</td>
<td>2.08324200</td>
<td>0.79991300</td>
<td>-3.00509300</td>
</tr>
<tr>
<td>H</td>
<td>2.81204300</td>
<td>1.79287500</td>
<td>-4.28907400</td>
</tr>
<tr>
<td>H</td>
<td>3.44850500</td>
<td>0.16707300</td>
<td>-3.96582700</td>
</tr>
<tr>
<td>C</td>
<td>5.32007800</td>
<td>2.13411000</td>
<td>-3.15716200</td>
</tr>
<tr>
<td>H</td>
<td>6.00829900</td>
<td>2.60506400</td>
<td>-2.43741800</td>
</tr>
<tr>
<td>H</td>
<td>5.85318400</td>
<td>1.29105100</td>
<td>-3.62667900</td>
</tr>
<tr>
<td>H</td>
<td>5.10257900</td>
<td>2.86878300</td>
<td>-3.94900000</td>
</tr>
<tr>
<td>C</td>
<td>6.06066900</td>
<td>-2.67448700</td>
<td>-0.84484800</td>
</tr>
<tr>
<td>H</td>
<td>5.69906600</td>
<td>-3.42917800</td>
<td>-0.12164100</td>
</tr>
<tr>
<td>C</td>
<td>5.86697300</td>
<td>-3.25411900</td>
<td>-2.25180500</td>
</tr>
<tr>
<td>H</td>
<td>6.37108300</td>
<td>-4.22979300</td>
<td>-2.33785400</td>
</tr>
<tr>
<td>H</td>
<td>4.80284500</td>
<td>-3.39974100</td>
<td>-2.49567600</td>
</tr>
<tr>
<td>H</td>
<td>6.29830000</td>
<td>-2.59113300</td>
<td>-3.02581900</td>
</tr>
<tr>
<td>C</td>
<td>7.55922100</td>
<td>-2.45726000</td>
<td>-0.55421900</td>
</tr>
<tr>
<td>H</td>
<td>7.98296900</td>
<td>-1.70576700</td>
<td>-1.24062300</td>
</tr>
<tr>
<td>H</td>
<td>7.72223700</td>
<td>-2.09808300</td>
<td>0.47342100</td>
</tr>
<tr>
<td>H</td>
<td>8.12640600</td>
<td>-3.39406600</td>
<td>-0.68326200</td>
</tr>
</tbody>
</table>
TS II'

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5803.64774096 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.07551600 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5802.57222496 a.u.

S35
<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.17110800</td>
<td>-2.67593200</td>
<td>3.41284700</td>
</tr>
<tr>
<td>C</td>
<td>-1.23993200</td>
<td>-2.51804600</td>
<td>3.50514400</td>
</tr>
<tr>
<td>C</td>
<td>-1.91497800</td>
<td>-2.49194800</td>
<td>4.72647400</td>
</tr>
<tr>
<td>C</td>
<td>-1.15457500</td>
<td>-2.66852400</td>
<td>5.88527500</td>
</tr>
<tr>
<td>C</td>
<td>0.23573900</td>
<td>-2.85703600</td>
<td>5.81604800</td>
</tr>
<tr>
<td>C</td>
<td>0.90688700</td>
<td>-2.85319200</td>
<td>4.59006700</td>
</tr>
<tr>
<td>C</td>
<td>0.49830600</td>
<td>-2.53565300</td>
<td>1.98685600</td>
</tr>
<tr>
<td>H</td>
<td>-2.99554500</td>
<td>-2.34906600</td>
<td>4.78047900</td>
</tr>
<tr>
<td>H</td>
<td>-1.65163000</td>
<td>-2.66380200</td>
<td>6.85815600</td>
</tr>
<tr>
<td>H</td>
<td>0.80273000</td>
<td>-3.00432000</td>
<td>6.73838900</td>
</tr>
<tr>
<td>H</td>
<td>1.98852900</td>
<td>-2.99023500</td>
<td>4.55287700</td>
</tr>
<tr>
<td>H</td>
<td>0.69080200</td>
<td>-1.18655700</td>
<td>1.71225200</td>
</tr>
<tr>
<td>N</td>
<td>-1.78107500</td>
<td>-2.42516100</td>
<td>2.20312900</td>
</tr>
<tr>
<td>C</td>
<td>-3.19924500</td>
<td>-2.30963000</td>
<td>1.89842100</td>
</tr>
<tr>
<td>H</td>
<td>-3.55246900</td>
<td>-1.28543100</td>
<td>2.08798900</td>
</tr>
<tr>
<td>H</td>
<td>-3.37859800</td>
<td>-2.55778400</td>
<td>0.84568100</td>
</tr>
<tr>
<td>H</td>
<td>-3.76332000</td>
<td>-3.01504300</td>
<td>2.52466600</td>
</tr>
<tr>
<td>C</td>
<td>-0.76667800</td>
<td>-2.50531100</td>
<td>1.33510200</td>
</tr>
<tr>
<td>C</td>
<td>-0.58186100</td>
<td>-2.63697800</td>
<td>-0.09228800</td>
</tr>
<tr>
<td>O</td>
<td>-1.45411300</td>
<td>-2.12482600</td>
<td>-1.01681400</td>
</tr>
<tr>
<td>C</td>
<td>0.69438200</td>
<td>-3.05894400</td>
<td>-0.32711500</td>
</tr>
<tr>
<td>C</td>
<td>1.31863600</td>
<td>-3.24055400</td>
<td>-1.66583600</td>
</tr>
<tr>
<td>H</td>
<td>0.58529600</td>
<td>-3.12756800</td>
<td>-2.47625500</td>
</tr>
<tr>
<td>H</td>
<td>2.13098400</td>
<td>-2.50794400</td>
<td>-1.81168400</td>
</tr>
<tr>
<td>H</td>
<td>1.77866200</td>
<td>-4.23994100</td>
<td>-1.74605900</td>
</tr>
<tr>
<td>C</td>
<td>1.45210600</td>
<td>-3.19270500</td>
<td>0.98154400</td>
</tr>
<tr>
<td>H</td>
<td>2.44499900</td>
<td>-2.72232600</td>
<td>0.90011600</td>
</tr>
<tr>
<td>H</td>
<td>1.61977300</td>
<td>-4.25451000</td>
<td>1.23679900</td>
</tr>
<tr>
<td>Zn</td>
<td>-2.69781200</td>
<td>-3.02788200</td>
<td>-2.40504100</td>
</tr>
<tr>
<td>Cl</td>
<td>-4.58979400</td>
<td>-3.51766300</td>
<td>-1.42205500</td>
</tr>
<tr>
<td>Cl</td>
<td>-1.62401600</td>
<td>-3.41939200</td>
<td>-4.25272500</td>
</tr>
<tr>
<td>P</td>
<td>0.46865300</td>
<td>0.77344700</td>
<td>0.08171500</td>
</tr>
<tr>
<td>O</td>
<td>1.79526500</td>
<td>1.39646800</td>
<td>-0.64875600</td>
</tr>
<tr>
<td>O</td>
<td>-0.34226300</td>
<td>2.08031600</td>
<td>0.64583000</td>
</tr>
<tr>
<td>O</td>
<td>-0.31020900</td>
<td>0.08044100</td>
<td>-1.01070300</td>
</tr>
<tr>
<td>O</td>
<td>0.88521800</td>
<td>0.01432500</td>
<td>1.35227400</td>
</tr>
<tr>
<td>C</td>
<td>2.76386400</td>
<td>2.15489200</td>
<td>-0.00284000</td>
</tr>
<tr>
<td>C</td>
<td>4.02191400</td>
<td>1.58128300</td>
<td>0.29636300</td>
</tr>
<tr>
<td>C</td>
<td>4.96503700</td>
<td>2.39111100</td>
<td>0.95796900</td>
</tr>
<tr>
<td>C</td>
<td>4.66448800</td>
<td>3.68125300</td>
<td>1.39457700</td>
</tr>
<tr>
<td>C</td>
<td>3.42376700</td>
<td>4.22347500</td>
<td>1.07462800</td>
</tr>
<tr>
<td>C</td>
<td>2.86715000</td>
<td>5.58195000</td>
<td>1.43716000</td>
</tr>
<tr>
<td>C</td>
<td>1.39562100</td>
<td>5.47073200</td>
<td>0.99461300</td>
</tr>
</tbody>
</table>
C   1.42618200  4.45980500  -0.19772600
C   2.50390000  3.49736200   0.29613200
C   1.92484700  5.19586000  -1.48829000
C   0.68207000  5.93075900  -2.01859500
C  -0.44185900  5.02454600  -1.57332500
C  -1.77416700  5.04017500  -1.97207100
C  -2.63769200  4.07328900  -1.45945500
C  -2.19654200  3.04066000  -0.61032600
C  -0.84044200  3.05902600  -0.21017200
C   0.01689300  4.07807100  -0.63902200
H  -1.10708100 -1.14299700  -1.11759900
H   5.95303600  1.97349200   1.15942200
H   5.39893100  4.25583600   1.96522900
H   3.39485300  6.38898000   0.89841700
H   2.97688600  5.80077600   2.51161000
H   0.94256400  6.43476700   0.72102200
H   0.78941100  5.03593300   1.80540200
H   2.78209700  5.85631600  -1.29399400
H   2.24951100  4.43671500  -2.21795800
H   0.58472100  6.93744700  -1.57387300
H   0.69776800  6.07130200  -3.11123300
H  -2.14197600  5.79302700  -2.67419400
H  -3.69108080  4.08902800  -1.74425400
C  -3.20708900  2.01198100  -0.19241400
C  -3.83091600  1.19288300  -1.17767400
C  -3.65773900  1.94675100   1.14959700
C  -4.87597900  0.34691100  -0.79012000
C  -4.73106500  1.09869700   1.47344100
C  -5.36599400  0.29659700   0.52146300
H  -5.34450400 -0.29578400  -1.53995700
H  -5.08598400  1.08627400   2.50564100
C   4.41427700  0.17729600  -0.05995400
C   4.50067000 -0.23026800  -1.41920800
C   4.81551800 -0.72652600   0.96266100
C   4.97253300 -1.51648000  -1.71922700
C   5.27637100 -2.00124200   0.60070300
C   5.37532200 -2.42039500  -0.72958800
H   5.05395000 -1.80762900  -2.76928500
H   5.59253400 -2.69206100   1.38821400
C   4.80092800  0.37176500   2.45337100
H   4.40705200  0.64677800   2.55635600
C   6.21828200 -0.37919300   3.05522800
H   6.90279300  0.28035100   2.49893500
H   6.19514900 -0.03679400   4.10292200
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-1.92551800</td>
<td>2.60425400</td>
<td>4.11705600</td>
</tr>
<tr>
<td>C</td>
<td>-6.57688300</td>
<td>-0.58259700</td>
<td>0.82737600</td>
</tr>
<tr>
<td>H</td>
<td>-6.38710200</td>
<td>-1.55126700</td>
<td>0.33102200</td>
</tr>
<tr>
<td>C</td>
<td>-6.80783100</td>
<td>-0.85777500</td>
<td>2.31774000</td>
</tr>
<tr>
<td>H</td>
<td>-7.63629400</td>
<td>-1.57168300</td>
<td>2.44822500</td>
</tr>
<tr>
<td>H</td>
<td>-5.91919600</td>
<td>-1.28703100</td>
<td>2.80590800</td>
</tr>
<tr>
<td>H</td>
<td>-7.08068000</td>
<td>0.05977400</td>
<td>2.86507200</td>
</tr>
<tr>
<td>C</td>
<td>-7.85278300</td>
<td>0.01099400</td>
<td>0.19694200</td>
</tr>
<tr>
<td>H</td>
<td>-8.09390000</td>
<td>0.98770100</td>
<td>0.64889200</td>
</tr>
<tr>
<td>H</td>
<td>-7.73755200</td>
<td>0.16352400</td>
<td>-0.88664100</td>
</tr>
<tr>
<td>H</td>
<td>-8.71429100</td>
<td>-0.65881200</td>
<td>0.35336800</td>
</tr>
</tbody>
</table>

**CP II-Post'**

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5803.66830134 a.u.

Thermal correction to Gibbs free energy at 298 K: 1.07493600 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -5802.59336534 a.u.
O   -1.42613200  -1.74896700  -1.10893000
C    0.75552900  -2.88372700  -1.13824600
C    1.34752300  -2.31891700  -2.38854900
H    0.64562200  -1.65402400  -2.90703800
H    2.27977500  -1.76529700  -2.18478900
H    1.60448100  -3.12858100  -3.09326900
C    1.44109200  -3.94517100  -0.28441400
H    2.41255200  -3.58343000  0.09758200
H    1.66745000  -4.83161300  -0.90560000
Zn  -2.73488500  -2.33718900  -2.64062500
Cl  -4.64902600  -2.92310600  -1.77890500
Cl  -1.66971700  -2.37058300  -4.53100100
P    0.45190300  1.11307200  -0.01774400
O    1.82677800  1.81297500  -0.49420900
O  -0.33499900  2.20651700  0.86386300
O  -0.25390900  0.55170400  -1.20765000
O    0.80034200  0.06214300  1.13401500
C    2.73706300  2.37716500  0.41011500
C    3.89862800  1.65382800  0.75547000
C    4.77656900  2.25309000  1.67682700
C    4.49394700  3.47592600  2.28672400
C    3.34121000  4.16340600  1.91897100
C    2.81536300  5.47573900  2.45255900
C    1.37808500  5.50903000  1.90263800
C    1.45465000  4.71330600  0.55370700
C    2.48374900  3.64909300  0.92862300
C    1.99016900  5.65344100  -0.57659100
C    0.76124800  6.48006700  -1.00474800
C  -0.38475500  5.53109000  -0.73523200
C  -1.71663600  5.63070400  -1.12854300
C  -2.60509900  4.61077500  -0.78214400
C  -2.18584900  3.44050800  -0.12125000
C  -0.82647300  3.37085100  0.24723000
C    0.05370200  4.42960600  0.02087900
H  -1.02474500  -0.82619500  -1.19828900
H    5.69685700  1.72486500  1.93013200
H    5.17401600  3.88602200  3.03784900
H    3.41225100  6.32542200  2.07573500
H    2.85664000  5.52688600  3.55216500
H    0.97592100  6.52103700  1.77324900
H    0.70433300  4.96703100  2.58799700
H    2.84132300  6.26741200  -0.24793000
H    2.33470800  5.03059300  -1.41764600
H    0.66500700  7.40352800  -0.40648700
<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>5.33615000</td>
<td>-3.24975500</td>
<td>-3.53025100</td>
</tr>
<tr>
<td>C</td>
<td>7.35913900</td>
<td>-3.32294300</td>
<td>-1.58129500</td>
</tr>
<tr>
<td>H</td>
<td>7.60843200</td>
<td>-2.57549400</td>
<td>-2.35258700</td>
</tr>
<tr>
<td>H</td>
<td>7.85250600</td>
<td>-3.01480000</td>
<td>-0.64629600</td>
</tr>
<tr>
<td>H</td>
<td>7.79315700</td>
<td>-4.28651900</td>
<td>-1.89515600</td>
</tr>
<tr>
<td>C</td>
<td>-3.56086800</td>
<td>1.97266600</td>
<td>-2.37403900</td>
</tr>
<tr>
<td>H</td>
<td>-2.71178200</td>
<td>2.66731600</td>
<td>-2.43215600</td>
</tr>
<tr>
<td>C</td>
<td>-4.76602100</td>
<td>2.65403100</td>
<td>-3.05020200</td>
</tr>
<tr>
<td>H</td>
<td>-4.52625600</td>
<td>2.92383100</td>
<td>-4.09175700</td>
</tr>
<tr>
<td>H</td>
<td>-5.64188000</td>
<td>1.98554400</td>
<td>-3.07191600</td>
</tr>
<tr>
<td>H</td>
<td>-5.06773300</td>
<td>3.57213700</td>
<td>-2.52222400</td>
</tr>
<tr>
<td>C</td>
<td>-3.14590100</td>
<td>0.71913200</td>
<td>-3.16128400</td>
</tr>
<tr>
<td>H</td>
<td>-3.93029500</td>
<td>-0.05678000</td>
<td>-3.13447700</td>
</tr>
<tr>
<td>H</td>
<td>-2.97243500</td>
<td>0.95487400</td>
<td>-4.22290200</td>
</tr>
<tr>
<td>H</td>
<td>-2.20070000</td>
<td>0.31464600</td>
<td>-2.77461300</td>
</tr>
<tr>
<td>C</td>
<td>-2.92621200</td>
<td>2.77314700</td>
<td>2.71602500</td>
</tr>
<tr>
<td>H</td>
<td>-2.15835500</td>
<td>3.46707000</td>
<td>2.34767400</td>
</tr>
<tr>
<td>C</td>
<td>-3.97240400</td>
<td>3.63103300</td>
<td>3.45186000</td>
</tr>
<tr>
<td>H</td>
<td>-4.44584000</td>
<td>4.35631900</td>
<td>2.77146200</td>
</tr>
<tr>
<td>H</td>
<td>-4.77316900</td>
<td>3.01188600</td>
<td>3.88775900</td>
</tr>
<tr>
<td>H</td>
<td>-3.50266400</td>
<td>4.19379800</td>
<td>4.27566200</td>
</tr>
<tr>
<td>C</td>
<td>-2.22506300</td>
<td>1.79881400</td>
<td>3.67909300</td>
</tr>
<tr>
<td>H</td>
<td>-2.93756000</td>
<td>1.09158200</td>
<td>4.13468300</td>
</tr>
<tr>
<td>H</td>
<td>-1.45006500</td>
<td>1.21583000</td>
<td>3.15995600</td>
</tr>
<tr>
<td>H</td>
<td>-1.74116000</td>
<td>2.35082100</td>
<td>4.50194100</td>
</tr>
<tr>
<td>C</td>
<td>-6.34526600</td>
<td>-0.55132400</td>
<td>0.96328700</td>
</tr>
<tr>
<td>H</td>
<td>-6.19759900</td>
<td>-1.37012700</td>
<td>0.23816400</td>
</tr>
<tr>
<td>C</td>
<td>-6.36411900</td>
<td>-1.17114400</td>
<td>2.36539400</td>
</tr>
<tr>
<td>H</td>
<td>-7.13334000</td>
<td>-1.95746700</td>
<td>2.42237900</td>
</tr>
<tr>
<td>H</td>
<td>-5.39709400</td>
<td>-1.62818400</td>
<td>2.62632500</td>
</tr>
<tr>
<td>H</td>
<td>-6.60532000</td>
<td>-0.42681500</td>
<td>3.14253400</td>
</tr>
<tr>
<td>C</td>
<td>-7.70517600</td>
<td>0.10309900</td>
<td>0.64784100</td>
</tr>
<tr>
<td>H</td>
<td>-7.90727600</td>
<td>0.94021400</td>
<td>1.33706300</td>
</tr>
<tr>
<td>H</td>
<td>-7.73505000</td>
<td>0.50060600</td>
<td>-0.37813400</td>
</tr>
<tr>
<td>H</td>
<td>-8.52407500</td>
<td>-0.62779500</td>
<td>0.75076100</td>
</tr>
</tbody>
</table>

**Enol**

![Enol structure]

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.480678032 a.u.

Thermal correction to Gibbs free energy at 298 K: 0.19016100 a.u.

S42
Gibbs free energy at 298 K \([\text{B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)}]\):
\(-633.29051703\) a.u.

\begin{align*}
\text{C} & : 3.52787200 \quad -1.38395200 \quad 0.00016200 \\
\text{C} & : 3.85386000 \quad -0.01142800 \quad 0.00026700 \\
\text{C} & : 2.85818300 \quad 0.96571800 \quad 0.00018400 \\
\text{C} & : 1.52334400 \quad 0.54309300 \quad 0.00009600 \\
\text{C} & : 1.16881500 \quad -0.85206400 \quad -0.00014700 \\
\text{C} & : 2.02242000 \quad -1.80982900 \quad -0.00007300 \\
\text{N} & : 0.36157700 \quad 1.30672800 \quad 0.00005200 \\
\text{C} & : -0.69336000 \quad 0.42337300 \quad -0.00043600 \\
\text{C} & : -0.26096200 \quad -0.88463900 \quad -0.00058500 \\
\text{C} & : 0.29647100 \quad 2.75218900 \quad 0.00025500 \\
\text{C} & : -2.14874000 \quad 0.47208400 \quad 0.00012000 \\
\text{C} & : -2.63153100 \quad -0.80476200 \quad 0.00013800 \\
\text{C} & : -1.46410900 \quad -1.78746700 \quad -0.00014300 \\
\text{C} & : -4.06537300 \quad -1.23151000 \quad 0.00023600 \\
\text{H} & : 4.33246900 \quad -2.12389400 \quad 0.00021800 \\
\text{H} & : 4.90369900 \quad 0.29258700 \quad 0.00037900 \\
\text{H} & : 3.11698900 \quad 2.02710600 \quad 0.00016800 \\
\text{H} & : 1.96452000 \quad -2.87679900 \quad -0.00023100 \\
\text{H} & : -0.75625600 \quad 3.06002000 \quad 0.00283500 \\
\text{H} & : 0.79103800 \quad 3.17259700 \quad 0.89187200 \\
\text{H} & : 0.78566500 \quad 3.17236400 \quad -0.89553000 \\
\text{H} & : -1.50247000 \quad -2.45137500 \quad -0.88429100 \\
\text{H} & : -1.50180100 \quad -2.45095500 \quad 0.88436900 \\
\text{H} & : -4.75883100 \quad -0.37254300 \quad -0.00045100 \\
\text{H} & : -4.31687000 \quad -1.84312500 \quad -0.88545300 \\
\text{H} & : -4.31721300 \quad -1.84197800 \quad 0.88663200 \\
\text{O} & : -2.81329700 \quad 1.65672200 \quad 0.00022600 \\
\text{H} & : -3.76586700 \quad 1.49029000 \quad 0.00054200 \\
\end{align*}

**CP III-R-Pre**

![Diagram](image)

SCF energy[\text{B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)}]: -3103.59363952 a.u.

Thermal correction to Gibbs free energy at 298 K: 1.08041200 a.u.

Gibbs free energy at 298 K [\text{B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)}]:
-3102.51322752 a.u.

\[
\begin{array}{cccc}
C & -0.54211300 & 7.74096900 & 2.03132100 \\
C & 0.84345900 & 7.66619700 & 2.28795200 \\
C & 1.62329100 & 6.64378000 & 1.74690100 \\
C & 0.98899200 & 5.69047800 & 0.94060000 \\
C & -0.42274700 & 5.74976300 & 0.66498200 \\
C & -1.17750200 & 6.79746600 & 1.22876500 \\
N & 1.53172800 & 4.58653000 & 0.29582200 \\
C & 0.49963300 & 3.97038600 & -0.37351000 \\
C & -0.69344100 & 4.63318100 & -0.18659700 \\
C & 2.91724100 & 2.78573200 & 2.28795200 \\
C & 0.98899200 & 5.69047800 & 0.94060000 \\
C & -0.42274700 & 5.74976300 & 0.66498200 \\
C & -1.17750200 & 6.79746600 & 1.22876500 \\
N & 1.53172800 & 4.58653000 & 0.29582200 \\
C & 0.49963300 & 3.97038600 & -0.37351000 \\
C & -0.69344100 & 4.63318100 & -0.18659700 \\
C & 2.91724100 & 2.78573200 & 2.28795200 \\
C & 0.98899200 & 5.69047800 & 0.94060000 \\
C & -0.42274700 & 5.74976300 & 0.66498200 \\
C & -1.17750200 & 6.79746600 & 1.22876500 \\
H & -1.12349100 & 8.55558900 & 2.47100100 \\
H & 1.31456200 & 8.42192600 & 2.92169200 \\
H & 2.69546900 & 6.59239100 & 1.94962600 \\
H & -2.25127300 & 6.86822000 & 1.03634600 \\
H & 3.03111500 & 3.24576000 & -0.23630300 \\
H & 3.57892700 & 4.94366900 & -0.08612300 \\
H & 3.23485800 & 3.98042100 & 1.38033700 \\
H & -2.59954500 & 3.56412900 & -0.25558200 \\
H & -2.24158600 & 4.48841500 & -1.71795000 \\
H & -2.06113200 & 2.37485200 & -3.38501700 \\
H & -0.97396500 & 1.04274900 & -2.92369800 \\
H & -2.53902300 & 1.24363800 & -2.11170900 \\
O & 1.34096800 & 2.00132000 & -1.55342600 \\
H & 1.04262200 & 1.09225700 & -1.79235400 \\
P & -0.05437300 & -0.91319500 & -0.31254500 \\
O & 1.03019800 & -1.60838400 & 0.67078900 \\
O & -1.28649000 & -1.96315400 & -0.40804800 \\
O & -0.53106600 & 0.29780700 & 0.60429500 \\
O & 0.42105800 & -0.56455400 & -1.68026200 \\
C & 1.69670700 & -2.75111100 & 0.20729400 \\
C & 2.98253200 & -2.62922300 & -0.36107100 \\
C & 3.57482400 & -3.80580100 & -0.85550100 \\
C & 2.90678100 & -5.03216600 & -0.86308300 \\
C & 1.64350700 & -5.11672900 & -0.28491200 \\
C & 0.71817300 & -6.30918800 & -0.18998700 \\
C & -0.60834900 & -5.66876400 & 0.26407200 \\
C & -0.17448500 & -4.42172700 & 1.10360900 \\
C & 1.05972600 & -3.98856800 & 0.31800000
\end{array}
\]
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.22130300</td>
<td>-4.87544200</td>
<td>2.54925700</td>
</tr>
<tr>
<td>C</td>
<td>-1.11872600</td>
<td>-5.00617500</td>
<td>3.29635800</td>
</tr>
<tr>
<td>C</td>
<td>-1.97782500</td>
<td>-3.96930200</td>
<td>2.60965100</td>
</tr>
<tr>
<td>C</td>
<td>-3.20894700</td>
<td>-3.45675500</td>
<td>3.00841400</td>
</tr>
<tr>
<td>C</td>
<td>-3.81634000</td>
<td>-2.47210800</td>
<td>2.22780200</td>
</tr>
<tr>
<td>C</td>
<td>-3.19430900</td>
<td>-1.92635300</td>
<td>1.08932000</td>
</tr>
<tr>
<td>C</td>
<td>-1.94614600</td>
<td>-2.46932100</td>
<td>0.71430200</td>
</tr>
<tr>
<td>C</td>
<td>-1.36729100</td>
<td>-3.52491200</td>
<td>1.42305400</td>
</tr>
<tr>
<td>H</td>
<td>-0.71247500</td>
<td>1.11568100</td>
<td>0.07617500</td>
</tr>
<tr>
<td>H</td>
<td>4.58408700</td>
<td>-3.74093800</td>
<td>-1.26412600</td>
</tr>
<tr>
<td>H</td>
<td>3.37754400</td>
<td>-5.91114900</td>
<td>-1.31112400</td>
</tr>
<tr>
<td>H</td>
<td>1.08758300</td>
<td>-7.04370300</td>
<td>-0.54773300</td>
</tr>
<tr>
<td>H</td>
<td>0.62902300</td>
<td>-6.84585600</td>
<td>-1.14797700</td>
</tr>
<tr>
<td>H</td>
<td>-1.25857100</td>
<td>-6.35247300</td>
<td>-0.82917700</td>
</tr>
<tr>
<td>H</td>
<td>-1.17507300</td>
<td>-5.31899900</td>
<td>-0.61367000</td>
</tr>
<tr>
<td>H</td>
<td>0.82134100</td>
<td>-5.79697900</td>
<td>2.55244100</td>
</tr>
<tr>
<td>H</td>
<td>0.82982700</td>
<td>-4.08140200</td>
<td>3.01089800</td>
</tr>
<tr>
<td>H</td>
<td>-1.54948800</td>
<td>-6.01735600</td>
<td>3.18440400</td>
</tr>
<tr>
<td>H</td>
<td>-1.02682700</td>
<td>-4.82339000</td>
<td>4.37887300</td>
</tr>
<tr>
<td>H</td>
<td>-3.69849400</td>
<td>-3.81839700</td>
<td>3.91645200</td>
</tr>
<tr>
<td>H</td>
<td>-4.79604500</td>
<td>-2.08652200</td>
<td>2.51411500</td>
</tr>
<tr>
<td>C</td>
<td>-3.89142100</td>
<td>-0.83101800</td>
<td>0.33474100</td>
</tr>
<tr>
<td>C</td>
<td>-4.13825200</td>
<td>0.42211400</td>
<td>0.95926500</td>
</tr>
<tr>
<td>C</td>
<td>-4.40261100</td>
<td>-1.07510300</td>
<td>-0.96845400</td>
</tr>
<tr>
<td>C</td>
<td>-4.88823400</td>
<td>1.38574100</td>
<td>0.26802200</td>
</tr>
<tr>
<td>C</td>
<td>-5.14390500</td>
<td>-0.07303200</td>
<td>-1.60875500</td>
</tr>
<tr>
<td>C</td>
<td>-5.40827900</td>
<td>1.16408300</td>
<td>-1.01040800</td>
</tr>
<tr>
<td>H</td>
<td>-5.08802400</td>
<td>2.34620400</td>
<td>0.75114900</td>
</tr>
<tr>
<td>H</td>
<td>-5.54310900</td>
<td>-0.27700500</td>
<td>-2.60556800</td>
</tr>
<tr>
<td>C</td>
<td>3.76043500</td>
<td>-1.34403200</td>
<td>-0.41439800</td>
</tr>
<tr>
<td>C</td>
<td>4.27601500</td>
<td>-0.78351300</td>
<td>0.78071900</td>
</tr>
<tr>
<td>C</td>
<td>4.07928500</td>
<td>-0.74233600</td>
<td>-1.66464100</td>
</tr>
<tr>
<td>C</td>
<td>5.11729100</td>
<td>0.33822500</td>
<td>0.70498700</td>
</tr>
<tr>
<td>C</td>
<td>4.92092300</td>
<td>0.37554900</td>
<td>-1.67642000</td>
</tr>
<tr>
<td>C</td>
<td>5.46964000</td>
<td>0.92680200</td>
<td>-0.51130700</td>
</tr>
<tr>
<td>H</td>
<td>5.51435700</td>
<td>0.74932500</td>
<td>1.63462500</td>
</tr>
<tr>
<td>H</td>
<td>5.16523700</td>
<td>0.83970200</td>
<td>-2.63567900</td>
</tr>
<tr>
<td>C</td>
<td>3.55666500</td>
<td>-1.27680700</td>
<td>-3.00209700</td>
</tr>
<tr>
<td>H</td>
<td>2.71961400</td>
<td>-1.95512000</td>
<td>-2.78209300</td>
</tr>
<tr>
<td>C</td>
<td>4.63813800</td>
<td>-2.07299500</td>
<td>-3.75940900</td>
</tr>
<tr>
<td>H</td>
<td>5.02368200</td>
<td>-2.92085400</td>
<td>-3.17544200</td>
</tr>
<tr>
<td>H</td>
<td>4.23411500</td>
<td>-2.47260500</td>
<td>-4.70435400</td>
</tr>
<tr>
<td>H</td>
<td>5.49639100</td>
<td>-1.42733000</td>
<td>-4.00938500</td>
</tr>
<tr>
<td>C</td>
<td>3.00612900</td>
<td>-0.17249100</td>
<td>-3.92256900</td>
</tr>
</tbody>
</table>
H  -6.23461900   3.11923500   -1.05798300
C  -5.71569800   2.62499500   -3.07786500
H  -6.31882900   3.43904400   -3.51200400
H  -4.67330100   2.97205100   -3.01026000
H  -5.74114900   1.78218400   -3.78806000
C  -7.73442400   1.77625200   -1.79582900
H  -7.83952300   0.88145500   -2.43144400
H  -8.14453200   1.53055800   -0.80378400
H  -8.35693200   2.57314700   -2.23518300

CP III-S-Pre

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.59416008 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.08028400 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-3102.51387608 a.u.
<table>
<thead>
<tr>
<th>Atoms</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.07758000</td>
<td>4.70737100</td>
<td>-1.79558800</td>
</tr>
<tr>
<td>H</td>
<td>1.48585000</td>
<td>3.13938100</td>
<td>-2.49822100</td>
</tr>
<tr>
<td>H</td>
<td>-1.45159300</td>
<td>2.55895200</td>
<td>0.18586900</td>
</tr>
<tr>
<td>H</td>
<td>-1.29230900</td>
<td>4.13866300</td>
<td>-0.59715600</td>
</tr>
<tr>
<td>H</td>
<td>-1.30099900</td>
<td>2.66905400</td>
<td>-1.57965000</td>
</tr>
<tr>
<td>O</td>
<td>0.93092600</td>
<td>2.25362100</td>
<td>1.81543100</td>
</tr>
<tr>
<td>H</td>
<td>0.18599800</td>
<td>1.60701000</td>
<td>1.72296700</td>
</tr>
<tr>
<td>P</td>
<td>-0.71181500</td>
<td>-0.53016900</td>
<td>0.14394400</td>
</tr>
<tr>
<td>O</td>
<td>-2.11851200</td>
<td>-0.80018400</td>
<td>-0.62144600</td>
</tr>
<tr>
<td>O</td>
<td>-0.11370000</td>
<td>-1.99538200</td>
<td>0.47633400</td>
</tr>
<tr>
<td>O</td>
<td>0.16580400</td>
<td>0.06904600</td>
<td>-1.03589700</td>
</tr>
<tr>
<td>O</td>
<td>-0.80678100</td>
<td>0.27688200</td>
<td>1.39223100</td>
</tr>
<tr>
<td>C</td>
<td>-3.16668800</td>
<td>-1.40619700</td>
<td>0.07908000</td>
</tr>
<tr>
<td>C</td>
<td>-4.18240800</td>
<td>-0.60925600</td>
<td>0.64801900</td>
</tr>
<tr>
<td>C</td>
<td>-5.17880300</td>
<td>-1.27439000</td>
<td>1.38545700</td>
</tr>
<tr>
<td>C</td>
<td>-5.14769400</td>
<td>-2.65345200</td>
<td>1.60519400</td>
</tr>
<tr>
<td>C</td>
<td>-4.14241000</td>
<td>-3.41056200</td>
<td>1.00974400</td>
</tr>
<tr>
<td>C</td>
<td>-3.88697100</td>
<td>-4.89752900</td>
<td>1.10834800</td>
</tr>
<tr>
<td>C</td>
<td>-2.47183000</td>
<td>-5.03415500</td>
<td>0.51360300</td>
</tr>
<tr>
<td>C</td>
<td>-2.36637600</td>
<td>-3.87099600</td>
<td>-0.52968700</td>
</tr>
<tr>
<td>C</td>
<td>-3.17987000</td>
<td>-2.79783600</td>
<td>0.18847700</td>
</tr>
<tr>
<td>C</td>
<td>-3.05599600</td>
<td>-4.30028300</td>
<td>-1.86766500</td>
</tr>
<tr>
<td>C</td>
<td>-2.00042300</td>
<td>-5.15832500</td>
<td>-2.59181100</td>
</tr>
<tr>
<td>C</td>
<td>-0.69917900</td>
<td>-4.56455100</td>
<td>-2.10088300</td>
</tr>
<tr>
<td>C</td>
<td>0.59238700</td>
<td>-4.77525900</td>
<td>-2.57648100</td>
</tr>
<tr>
<td>C</td>
<td>1.65741400</td>
<td>-4.11051600</td>
<td>-1.96461100</td>
</tr>
<tr>
<td>C</td>
<td>1.46292900</td>
<td>-3.16812900</td>
<td>-0.93835900</td>
</tr>
<tr>
<td>C</td>
<td>0.13674900</td>
<td>-2.95565300</td>
<td>-0.50606000</td>
</tr>
<tr>
<td>C</td>
<td>-0.92845800</td>
<td>-3.70167100</td>
<td>-1.01445700</td>
</tr>
<tr>
<td>H</td>
<td>0.46584800</td>
<td>1.00371800</td>
<td>-0.86233400</td>
</tr>
<tr>
<td>H</td>
<td>-5.98927000</td>
<td>-0.67988800</td>
<td>1.81016800</td>
</tr>
<tr>
<td>H</td>
<td>-5.90992900</td>
<td>-3.12717100</td>
<td>2.22945400</td>
</tr>
<tr>
<td>H</td>
<td>-4.62988300</td>
<td>-5.46862700</td>
<td>0.52325500</td>
</tr>
<tr>
<td>H</td>
<td>-3.95388000</td>
<td>-5.26620600</td>
<td>2.14433700</td>
</tr>
<tr>
<td>H</td>
<td>-2.27282200</td>
<td>-6.02008800</td>
<td>0.06868000</td>
</tr>
<tr>
<td>H</td>
<td>-1.71912300</td>
<td>-4.86676600</td>
<td>1.30067200</td>
</tr>
<tr>
<td>H</td>
<td>-4.01018500</td>
<td>-4.82163500</td>
<td>-1.70216400</td>
</tr>
<tr>
<td>H</td>
<td>-3.26962300</td>
<td>-3.39401500</td>
<td>-2.45678100</td>
</tr>
<tr>
<td>H</td>
<td>-2.08228700</td>
<td>-6.22378000</td>
<td>-2.31178800</td>
</tr>
<tr>
<td>H</td>
<td>-2.09252100</td>
<td>-5.11540400</td>
<td>-3.68887200</td>
</tr>
<tr>
<td>H</td>
<td>0.77769900</td>
<td>-5.46026100</td>
<td>-3.40808500</td>
</tr>
<tr>
<td>H</td>
<td>2.67803700</td>
<td>-4.30734700</td>
<td>-2.29677900</td>
</tr>
<tr>
<td>C</td>
<td>2.65497600</td>
<td>-2.49125500</td>
<td>-0.32355900</td>
</tr>
<tr>
<td>C</td>
<td>3.46883600</td>
<td>-1.61898500</td>
<td>-1.09758300</td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>C</td>
<td>3.03545000</td>
<td>-2.79996700</td>
<td>1.00771900</td>
</tr>
<tr>
<td>C</td>
<td>4.64013200</td>
<td>-1.10456600</td>
<td>-0.52837700</td>
</tr>
<tr>
<td>C</td>
<td>4.22100800</td>
<td>-2.25458300</td>
<td>1.52406200</td>
</tr>
<tr>
<td>C</td>
<td>5.04825900</td>
<td>-1.41520100</td>
<td>0.77423000</td>
</tr>
<tr>
<td>H</td>
<td>5.26490900</td>
<td>-0.43177400</td>
<td>-1.12234900</td>
</tr>
<tr>
<td>H</td>
<td>4.50551400</td>
<td>-2.51063900</td>
<td>2.54616000</td>
</tr>
<tr>
<td>C</td>
<td>-4.28364300</td>
<td>0.87769000</td>
<td>0.45197000</td>
</tr>
<tr>
<td>C</td>
<td>-4.65267000</td>
<td>1.39346600</td>
<td>-0.81860900</td>
</tr>
<tr>
<td>C</td>
<td>-4.11627600</td>
<td>1.76645700</td>
<td>1.54713800</td>
</tr>
<tr>
<td>C</td>
<td>-4.85951500</td>
<td>2.77233100</td>
<td>-0.96077000</td>
</tr>
<tr>
<td>C</td>
<td>-4.34231900</td>
<td>3.13582100</td>
<td>1.34484900</td>
</tr>
<tr>
<td>C</td>
<td>-4.72133200</td>
<td>3.66466700</td>
<td>0.10754100</td>
</tr>
<tr>
<td>H</td>
<td>-5.15361600</td>
<td>3.15716400</td>
<td>-1.94036600</td>
</tr>
<tr>
<td>H</td>
<td>-4.21956700</td>
<td>3.82144700</td>
<td>2.18729900</td>
</tr>
<tr>
<td>C</td>
<td>-3.71676100</td>
<td>1.29236500</td>
<td>2.94666300</td>
</tr>
<tr>
<td>H</td>
<td>-3.34267000</td>
<td>0.26283000</td>
<td>2.85245100</td>
</tr>
<tr>
<td>C</td>
<td>-4.92340200</td>
<td>1.27915900</td>
<td>3.90576400</td>
</tr>
<tr>
<td>H</td>
<td>-5.74543800</td>
<td>0.64970900</td>
<td>3.53459300</td>
</tr>
<tr>
<td>H</td>
<td>-4.62725500</td>
<td>0.89584000</td>
<td>4.89626700</td>
</tr>
<tr>
<td>H</td>
<td>-5.32495000</td>
<td>2.29636200</td>
<td>4.04766200</td>
</tr>
<tr>
<td>C</td>
<td>-2.57760700</td>
<td>2.12363400</td>
<td>3.56319800</td>
</tr>
<tr>
<td>H</td>
<td>-2.90033400</td>
<td>3.14876900</td>
<td>3.80812500</td>
</tr>
<tr>
<td>H</td>
<td>-2.24162200</td>
<td>1.65831100</td>
<td>4.50401800</td>
</tr>
<tr>
<td>H</td>
<td>-1.70955300</td>
<td>2.18868000</td>
<td>2.89513900</td>
</tr>
<tr>
<td>C</td>
<td>-4.87374000</td>
<td>0.50239800</td>
<td>-2.04286800</td>
</tr>
<tr>
<td>H</td>
<td>-4.71350100</td>
<td>-0.54066000</td>
<td>-1.73701000</td>
</tr>
<tr>
<td>C</td>
<td>-3.86003100</td>
<td>0.80268300</td>
<td>-3.16155800</td>
</tr>
<tr>
<td>H</td>
<td>-2.82803700</td>
<td>0.68268600</td>
<td>-2.80013700</td>
</tr>
<tr>
<td>H</td>
<td>-4.00496500</td>
<td>0.11413700</td>
<td>-4.01076200</td>
</tr>
<tr>
<td>H</td>
<td>-3.97208300</td>
<td>1.82953700</td>
<td>-3.54721700</td>
</tr>
<tr>
<td>C</td>
<td>-6.32144300</td>
<td>0.58834900</td>
<td>-2.55952200</td>
</tr>
<tr>
<td>H</td>
<td>-7.04496200</td>
<td>0.33993300</td>
<td>-1.76702600</td>
</tr>
<tr>
<td>H</td>
<td>-6.56596000</td>
<td>1.59726300</td>
<td>-2.92983800</td>
</tr>
<tr>
<td>H</td>
<td>-6.47667700</td>
<td>-0.11564900</td>
<td>-3.39379700</td>
</tr>
<tr>
<td>C</td>
<td>-5.01206800</td>
<td>5.15329600</td>
<td>-0.04462500</td>
</tr>
<tr>
<td>H</td>
<td>-4.65628800</td>
<td>5.64106800</td>
<td>0.87975300</td>
</tr>
<tr>
<td>C</td>
<td>-4.26114300</td>
<td>5.79866100</td>
<td>-1.22002000</td>
</tr>
<tr>
<td>H</td>
<td>-4.43756700</td>
<td>6.88645100</td>
<td>-1.24228900</td>
</tr>
<tr>
<td>H</td>
<td>-3.17541200</td>
<td>5.63205200</td>
<td>-1.14391000</td>
</tr>
<tr>
<td>H</td>
<td>-4.59512000</td>
<td>5.39361100</td>
<td>-2.18941000</td>
</tr>
<tr>
<td>C</td>
<td>-6.52632300</td>
<td>5.41536100</td>
<td>-0.14522500</td>
</tr>
<tr>
<td>H</td>
<td>-6.94954400</td>
<td>4.95120700</td>
<td>-1.05145200</td>
</tr>
<tr>
<td>H</td>
<td>-7.06259500</td>
<td>5.00049700</td>
<td>0.72251700</td>
</tr>
<tr>
<td>H</td>
<td>-6.73633400</td>
<td>6.49682500</td>
<td>-0.19208700</td>
</tr>
<tr>
<td>C</td>
<td>3.12440400</td>
<td>-1.21835200</td>
<td>-2.53437000</td>
</tr>
<tr>
<td>H</td>
<td>2.09606300</td>
<td>-1.55071900</td>
<td>-2.73569600</td>
</tr>
<tr>
<td>C</td>
<td>4.05104700</td>
<td>-1.90258200</td>
<td>-3.55793000</td>
</tr>
<tr>
<td>H</td>
<td>3.76296100</td>
<td>-1.62875700</td>
<td>-4.58633700</td>
</tr>
<tr>
<td>H</td>
<td>5.09894900</td>
<td>-1.59279500</td>
<td>-3.41157100</td>
</tr>
<tr>
<td>H</td>
<td>4.01838400</td>
<td>-2.99979000</td>
<td>-3.48027700</td>
</tr>
<tr>
<td>C</td>
<td>3.15145500</td>
<td>0.30584300</td>
<td>-2.74267400</td>
</tr>
<tr>
<td>H</td>
<td>4.17212600</td>
<td>0.71534000</td>
<td>-2.68437000</td>
</tr>
<tr>
<td>H</td>
<td>2.75449000</td>
<td>0.56047200</td>
<td>-3.73907400</td>
</tr>
<tr>
<td>H</td>
<td>2.54495300</td>
<td>0.82567000</td>
<td>-1.98903500</td>
</tr>
<tr>
<td>C</td>
<td>2.23510000</td>
<td>-3.74445400</td>
<td>1.90641900</td>
</tr>
<tr>
<td>H</td>
<td>1.35837500</td>
<td>-4.09033700</td>
<td>1.34265100</td>
</tr>
<tr>
<td>C</td>
<td>3.04372600</td>
<td>-5.00352500</td>
<td>2.27005300</td>
</tr>
<tr>
<td>H</td>
<td>3.39100100</td>
<td>-5.53124300</td>
<td>1.36762700</td>
</tr>
<tr>
<td>H</td>
<td>3.93168200</td>
<td>-4.75919600</td>
<td>2.87588900</td>
</tr>
<tr>
<td>H</td>
<td>2.42645700</td>
<td>-5.70399500</td>
<td>2.85672400</td>
</tr>
<tr>
<td>C</td>
<td>1.70873600</td>
<td>-3.03309800</td>
<td>3.16591200</td>
</tr>
<tr>
<td>H</td>
<td>2.53284300</td>
<td>-2.69316600</td>
<td>3.81473000</td>
</tr>
<tr>
<td>H</td>
<td>1.09813800</td>
<td>-2.15732800</td>
<td>2.90181800</td>
</tr>
<tr>
<td>H</td>
<td>1.08268900</td>
<td>-3.71783800</td>
<td>3.76215600</td>
</tr>
<tr>
<td>C</td>
<td>6.37834200</td>
<td>-0.87837200</td>
<td>1.29482800</td>
</tr>
<tr>
<td>H</td>
<td>6.49081400</td>
<td>0.13846800</td>
<td>0.87699100</td>
</tr>
<tr>
<td>C</td>
<td>6.45693700</td>
<td>-0.76123100</td>
<td>2.82212600</td>
</tr>
<tr>
<td>H</td>
<td>7.38589600</td>
<td>-0.24927600</td>
<td>3.12002200</td>
</tr>
<tr>
<td>H</td>
<td>5.60781100</td>
<td>-0.19388100</td>
<td>3.23445100</td>
</tr>
<tr>
<td>H</td>
<td>6.46410000</td>
<td>-1.75027300</td>
<td>3.30880800</td>
</tr>
<tr>
<td>C</td>
<td>7.55144400</td>
<td>-1.72072500</td>
<td>0.75576300</td>
</tr>
<tr>
<td>H</td>
<td>7.49316700</td>
<td>-2.75593600</td>
<td>1.13134400</td>
</tr>
<tr>
<td>H</td>
<td>7.54318100</td>
<td>-1.76465100</td>
<td>-0.34411600</td>
</tr>
<tr>
<td>H</td>
<td>8.51917300</td>
<td>-1.29749500</td>
<td>1.07241000</td>
</tr>
</tbody>
</table>

**TS III-R**

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.58294325 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.07861800 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3102.50432525 a.u.
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.94692000</td>
<td>-1.35056600</td>
<td>-4.72533800</td>
</tr>
<tr>
<td>H</td>
<td>2.65363000</td>
<td>-0.32211000</td>
<td>-3.30374500</td>
</tr>
<tr>
<td>C</td>
<td>2.66828300</td>
<td>-2.64410200</td>
<td>2.31189000</td>
</tr>
<tr>
<td>H</td>
<td>1.78927100</td>
<td>-3.22691000</td>
<td>2.00153900</td>
</tr>
<tr>
<td>C</td>
<td>2.15731000</td>
<td>-1.47672900</td>
<td>3.17396900</td>
</tr>
<tr>
<td>H</td>
<td>1.49162100</td>
<td>-0.82078700</td>
<td>2.59444400</td>
</tr>
<tr>
<td>H</td>
<td>1.58997800</td>
<td>-1.85982300</td>
<td>4.03863600</td>
</tr>
<tr>
<td>H</td>
<td>2.98822900</td>
<td>-0.86962100</td>
<td>3.57076700</td>
</tr>
<tr>
<td>C</td>
<td>3.55578900</td>
<td>-3.60156200</td>
<td>3.12898200</td>
</tr>
<tr>
<td>H</td>
<td>3.88684400</td>
<td>-4.45953100</td>
<td>2.52234500</td>
</tr>
<tr>
<td>H</td>
<td>4.45758800</td>
<td>-3.09730900</td>
<td>3.51341100</td>
</tr>
<tr>
<td>H</td>
<td>3.00117300</td>
<td>-3.99383800</td>
<td>3.99757900</td>
</tr>
<tr>
<td>C</td>
<td>6.63527900</td>
<td>-0.19646200</td>
<td>0.35193900</td>
</tr>
<tr>
<td>H</td>
<td>6.83668000</td>
<td>0.34179900</td>
<td>-0.59226700</td>
</tr>
<tr>
<td>C</td>
<td>6.58172200</td>
<td>0.84813300</td>
<td>1.47676600</td>
</tr>
<tr>
<td>H</td>
<td>7.50788300</td>
<td>1.44573400</td>
<td>1.49550400</td>
</tr>
<tr>
<td>H</td>
<td>5.73021600</td>
<td>1.53643800</td>
<td>1.35612500</td>
</tr>
<tr>
<td>H</td>
<td>6.48416200</td>
<td>0.37620200</td>
<td>2.46763900</td>
</tr>
<tr>
<td>C</td>
<td>7.80408600</td>
<td>-1.17635400</td>
<td>0.56956100</td>
</tr>
<tr>
<td>H</td>
<td>7.65962200</td>
<td>-1.75678700</td>
<td>1.49568500</td>
</tr>
<tr>
<td>H</td>
<td>7.88386100</td>
<td>-1.89282600</td>
<td>-0.26251600</td>
</tr>
<tr>
<td>H</td>
<td>8.76335700</td>
<td>-0.63832600</td>
<td>0.65249700</td>
</tr>
<tr>
<td>C</td>
<td>-3.48664000</td>
<td>1.65637800</td>
<td>2.65833100</td>
</tr>
<tr>
<td>H</td>
<td>-3.18475500</td>
<td>0.61678200</td>
<td>2.84277600</td>
</tr>
<tr>
<td>C</td>
<td>-4.58716000</td>
<td>2.00963600</td>
<td>3.67689200</td>
</tr>
<tr>
<td>H</td>
<td>-4.22029200</td>
<td>1.87162600</td>
<td>4.70754200</td>
</tr>
<tr>
<td>H</td>
<td>-4.90739000</td>
<td>3.06002300</td>
<td>3.57637800</td>
</tr>
<tr>
<td>H</td>
<td>-5.48173700</td>
<td>1.38033700</td>
<td>3.55036300</td>
</tr>
<tr>
<td>C</td>
<td>-2.23355500</td>
<td>2.51611100</td>
<td>2.89433700</td>
</tr>
<tr>
<td>H</td>
<td>-2.43213700</td>
<td>3.58951100</td>
<td>2.73558100</td>
</tr>
<tr>
<td>H</td>
<td>-1.88355300</td>
<td>2.39841200</td>
<td>3.93332600</td>
</tr>
<tr>
<td>H</td>
<td>-1.42342100</td>
<td>2.19365000</td>
<td>2.22541100</td>
</tr>
<tr>
<td>C</td>
<td>-4.94614100</td>
<td>-0.41633900</td>
<td>-1.86033600</td>
</tr>
<tr>
<td>H</td>
<td>-4.65031800</td>
<td>-1.33314100</td>
<td>-1.3318800</td>
</tr>
<tr>
<td>C</td>
<td>-6.44484000</td>
<td>-0.56039800</td>
<td>-2.18463900</td>
</tr>
<tr>
<td>H</td>
<td>-7.04729100</td>
<td>-0.64782000</td>
<td>-1.26654400</td>
</tr>
<tr>
<td>H</td>
<td>-6.82696200</td>
<td>0.30294000</td>
<td>-2.75402600</td>
</tr>
<tr>
<td>H</td>
<td>-6.62252400</td>
<td>-1.46188700</td>
<td>-2.79429700</td>
</tr>
<tr>
<td>C</td>
<td>-4.09995600</td>
<td>-0.34368300</td>
<td>-3.14339300</td>
</tr>
<tr>
<td>H</td>
<td>-4.34307100</td>
<td>0.54959200</td>
<td>-3.74291900</td>
</tr>
<tr>
<td>H</td>
<td>-3.02643900</td>
<td>-0.32331000</td>
<td>-2.90628200</td>
</tr>
<tr>
<td>H</td>
<td>-4.28852000</td>
<td>-1.22614800</td>
<td>-3.77728800</td>
</tr>
<tr>
<td>C</td>
<td>-5.30475000</td>
<td>4.56977000</td>
<td>-1.04552000</td>
</tr>
<tr>
<td>H</td>
<td>-4.95348600</td>
<td>5.28941600</td>
<td>-0.28501300</td>
</tr>
</tbody>
</table>

S53
TS III-S

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.58656328 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.07913500 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-3102.50742828 a.u.
C  -3.02344400  -2.64275100  -0.96894200
C  -4.48294300  -1.20027900  0.92623900
C  -4.22720600  -2.00475900  1.66468500
C  -4.98137600  -1.28419400  -0.37996700
H  -5.05172600  -0.62769500  1.04151900
H  -4.58335700  -2.09079000  -2.33680300
C  4.23982800  1.03500300  -0.34712400
C  4.52532800  1.45128400  0.98099400
C  4.10018400  2.01195100  -1.36935000
C  4.67906300  2.81792500  1.24994000
C  4.27613300  3.36454500  -1.04151900
C  4.57224200  3.79511800  0.25451900
H  4.90808300  3.12506300  2.27366200
H  4.17859000  4.11619900  -1.82952900
C  3.77661300  1.65484400  -2.82292500
H  3.46047700  0.60245700  -2.84270600
C  5.01004600  1.80567700  -3.73432200
H  5.85815000  1.93788000  -3.39331500
H  4.76934200  1.50180100  -4.76657200
H  5.35210900  2.85357000  -3.76594700
C  2.60772900  2.47649600  -3.39441000
H  2.86683400  3.54192600  -3.50798200
H  2.33768000  2.10555500  -4.39474800
H  1.71531200  2.40650900  -2.75992200
C  4.71239900  0.46672500  2.13718900
H  4.59998600  -0.55028000  1.73790200
C  3.63549800  0.64629200  3.22216900
H  2.62742200  0.53158500  2.79791300
H  3.75762800  -0.10835200  4.01712400
H  3.70093000  1.63902800  3.69775400
C  6.12954000  0.54815400  2.73361500
H  6.89917300  0.38746100  1.96209700
H  6.32357700  1.52831100  3.19920800
H  6.26528800  -0.21952000  3.51345400
C  4.79595700  5.27282000  0.55430700
H  4.57645000  5.82170800  -0.37821000
C  3.84304600  5.80884200  1.63547800
H  3.98703900  6.89220600  1.78035300
H  2.79013200  5.63882100  1.36164500
H  4.01828500  5.32009200  2.60800600
C  6.26414900  5.55826300  0.91799300
H  6.55137400  5.04385600  1.84992500
H  6.94622300  5.21493500  0.12452900
H  6.42960200  6.63814700  1.06769000
CP III-R-Post

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.62470155 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.08125400 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3102.54344755 a.u.

S57
<table>
<thead>
<tr>
<th>Atoms</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.83302000</td>
<td>-1.84946300</td>
<td>-4.52822400</td>
</tr>
<tr>
<td>H</td>
<td>1.87692100</td>
<td>-0.98681700</td>
<td>-2.97006200</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>-0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
<tr>
<td>C</td>
<td>0.89841700</td>
<td>-2.85696300</td>
<td>3.32080300</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>H</td>
<td>1.88161300</td>
<td>-0.06016400</td>
<td>4.11470400</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.55257700</td>
<td>-1.90732200</td>
<td>2.88785700</td>
</tr>
<tr>
<td>H</td>
<td>0.19830100</td>
<td>-3.13996600</td>
<td>4.12446700</td>
</tr>
<tr>
<td>C</td>
<td>0.96264700</td>
<td>-3.96391000</td>
<td>2.25358700</td>
</tr>
<tr>
<td>H</td>
<td>0.06016400</td>
<td>-4.11470400</td>
<td>1.88501100</td>
</tr>
</tbody>
</table>
CP III-S-Post

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -3103.62568349 a.u.
Thermal correction to Gibbs free energy at 298 K: 1.08018100 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-3102.54550249 a.u.

<table>
<thead>
<tr>
<th></th>
<th>x1</th>
<th>y1</th>
<th>z1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.57095600</td>
<td>6.32428900</td>
<td>-2.06594800</td>
</tr>
<tr>
<td>H</td>
<td>-1.29442500</td>
<td>7.36716800</td>
<td>-2.29322900</td>
</tr>
<tr>
<td>H</td>
<td>-0.65650300</td>
<td>5.78376400</td>
<td>-1.77664800</td>
</tr>
<tr>
<td>H</td>
<td>-1.94429400</td>
<td>5.87201300</td>
<td>-2.99929600</td>
</tr>
<tr>
<td>C</td>
<td>-3.88743500</td>
<td>7.06641000</td>
<td>-1.34300500</td>
</tr>
<tr>
<td>H</td>
<td>-4.37146600</td>
<td>6.63206300</td>
<td>-2.23328000</td>
</tr>
<tr>
<td>H</td>
<td>-4.62854900</td>
<td>7.06809300</td>
<td>-0.52852200</td>
</tr>
<tr>
<td>H</td>
<td>-3.63474600</td>
<td>8.11379600</td>
<td>-1.57790700</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>x2</th>
<th>y2</th>
<th>z2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>8.03723200</td>
<td>3.69866900</td>
<td>-0.60048200</td>
</tr>
<tr>
<td>C</td>
<td>8.20809700</td>
<td>3.48876500</td>
<td>0.78892900</td>
</tr>
<tr>
<td>C</td>
<td>7.16593000</td>
<td>3.04459900</td>
<td>1.59505700</td>
</tr>
<tr>
<td>C</td>
<td>5.92332400</td>
<td>2.80694800</td>
<td>0.98338100</td>
</tr>
<tr>
<td>C</td>
<td>5.73034900</td>
<td>3.01607600</td>
<td>-0.42722900</td>
</tr>
<tr>
<td>C</td>
<td>6.81302600</td>
<td>3.46698600</td>
<td>-1.21167400</td>
</tr>
<tr>
<td>N</td>
<td>4.74238200</td>
<td>2.36862300</td>
<td>1.54709900</td>
</tr>
<tr>
<td>C</td>
<td>3.81572500</td>
<td>2.30215000</td>
<td>0.52678600</td>
</tr>
<tr>
<td>C</td>
<td>4.36615600</td>
<td>2.68314300</td>
<td>-0.68320900</td>
</tr>
<tr>
<td>C</td>
<td>4.51538100</td>
<td>2.03959800</td>
<td>2.94136900</td>
</tr>
<tr>
<td>C</td>
<td>2.43108400</td>
<td>1.92180600</td>
<td>0.39024000</td>
</tr>
<tr>
<td>C</td>
<td>2.06243600</td>
<td>2.11386200</td>
<td>-1.08751000</td>
</tr>
<tr>
<td>C</td>
<td>3.36311600</td>
<td>2.60715800</td>
<td>-1.79631900</td>
</tr>
<tr>
<td>C</td>
<td>0.85913600</td>
<td>3.05048700</td>
<td>-1.25562600</td>
</tr>
<tr>
<td>H</td>
<td>8.88450500</td>
<td>4.04844800</td>
<td>-1.19487100</td>
</tr>
<tr>
<td>H</td>
<td>9.18527500</td>
<td>3.68098200</td>
<td>1.23939100</td>
</tr>
<tr>
<td>H</td>
<td>7.31191600</td>
<td>2.88637100</td>
<td>2.66538300</td>
</tr>
<tr>
<td>H</td>
<td>6.68540900</td>
<td>3.63091100</td>
<td>-2.28448900</td>
</tr>
<tr>
<td>H</td>
<td>3.47265300</td>
<td>1.71839600</td>
<td>3.05550700</td>
</tr>
<tr>
<td>H</td>
<td>5.17834100</td>
<td>1.22065500</td>
<td>3.26477700</td>
</tr>
<tr>
<td>H</td>
<td>4.69436200</td>
<td>2.91466400</td>
<td>3.58767900</td>
</tr>
<tr>
<td>Atom</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>H</td>
<td>3.21014800</td>
<td>3.58728100</td>
<td>-2.27986800</td>
</tr>
<tr>
<td>H</td>
<td>3.67975000</td>
<td>1.91310100</td>
<td>-2.59299300</td>
</tr>
<tr>
<td>H</td>
<td>-0.00871500</td>
<td>2.68380700</td>
<td>-0.69063000</td>
</tr>
<tr>
<td>H</td>
<td>1.09508600</td>
<td>4.06902000</td>
<td>-0.90469300</td>
</tr>
<tr>
<td>H</td>
<td>0.56469600</td>
<td>3.10839700</td>
<td>-2.31420400</td>
</tr>
<tr>
<td>O</td>
<td>1.67655700</td>
<td>1.51580900</td>
<td>1.28186200</td>
</tr>
<tr>
<td>H</td>
<td>0.24255100</td>
<td>0.89621400</td>
<td>1.09901800</td>
</tr>
<tr>
<td>P</td>
<td>-0.93909800</td>
<td>-0.48545600</td>
<td>-0.15685800</td>
</tr>
<tr>
<td>O</td>
<td>-2.52630200</td>
<td>-0.35500300</td>
<td>-0.49340200</td>
</tr>
<tr>
<td>O</td>
<td>-0.81698600</td>
<td>-1.93584500</td>
<td>0.59405200</td>
</tr>
<tr>
<td>O</td>
<td>-0.13655900</td>
<td>-0.32880600</td>
<td>-1.39153300</td>
</tr>
<tr>
<td>O</td>
<td>-0.68836200</td>
<td>0.49584900</td>
<td>1.05230200</td>
</tr>
<tr>
<td>C</td>
<td>-3.51308700</td>
<td>-0.39940500</td>
<td>0.48158200</td>
</tr>
<tr>
<td>C</td>
<td>-4.08049000</td>
<td>0.81024500</td>
<td>0.94084500</td>
</tr>
<tr>
<td>C</td>
<td>-5.05936900</td>
<td>0.72167800</td>
<td>1.94613800</td>
</tr>
<tr>
<td>C</td>
<td>-5.41826500</td>
<td>-0.49719500</td>
<td>2.52706300</td>
</tr>
<tr>
<td>C</td>
<td>-4.84773100</td>
<td>-1.67140900</td>
<td>2.04303300</td>
</tr>
<tr>
<td>C</td>
<td>-5.04985200</td>
<td>-3.09114400</td>
<td>2.52327100</td>
</tr>
<tr>
<td>C</td>
<td>-3.90864900</td>
<td>-3.84837100</td>
<td>1.81674500</td>
</tr>
<tr>
<td>C</td>
<td>-3.68056600</td>
<td>-3.06311200</td>
<td>0.48206700</td>
</tr>
<tr>
<td>C</td>
<td>-3.94132600</td>
<td>-1.63737400</td>
<td>0.96790700</td>
</tr>
<tr>
<td>C</td>
<td>-4.74932100</td>
<td>-3.50543200</td>
<td>-0.57300000</td>
</tr>
<tr>
<td>C</td>
<td>-4.20185700</td>
<td>-4.82579600</td>
<td>-1.15066600</td>
</tr>
<tr>
<td>C</td>
<td>-2.70546300</td>
<td>-4.63593800</td>
<td>-1.03974500</td>
</tr>
<tr>
<td>C</td>
<td>-1.68211400</td>
<td>-5.37518900</td>
<td>-1.62820800</td>
</tr>
<tr>
<td>C</td>
<td>-0.35623600</td>
<td>-4.98841800</td>
<td>-1.41633200</td>
</tr>
<tr>
<td>C</td>
<td>-0.02269800</td>
<td>-3.83219200</td>
<td>-0.68794400</td>
</tr>
<tr>
<td>C</td>
<td>-1.08437800</td>
<td>-3.10261700</td>
<td>-0.11007000</td>
</tr>
<tr>
<td>C</td>
<td>-2.40881900</td>
<td>-3.53191000</td>
<td>-0.22174900</td>
</tr>
<tr>
<td>H</td>
<td>1.75922200</td>
<td>1.11950500</td>
<td>-1.45791000</td>
</tr>
<tr>
<td>H</td>
<td>-5.53058100</td>
<td>1.64259800</td>
<td>2.29333600</td>
</tr>
<tr>
<td>H</td>
<td>-6.14085600</td>
<td>-0.52311100</td>
<td>3.34715200</td>
</tr>
<tr>
<td>H</td>
<td>-6.03999200</td>
<td>-3.47798200</td>
<td>2.22204300</td>
</tr>
<tr>
<td>H</td>
<td>-5.00339700</td>
<td>-3.17219400</td>
<td>3.62115800</td>
</tr>
<tr>
<td>H</td>
<td>-4.12389200</td>
<td>-4.91381600</td>
<td>1.64858500</td>
</tr>
<tr>
<td>H</td>
<td>-2.98879800</td>
<td>-3.78565000</td>
<td>2.41998000</td>
</tr>
<tr>
<td>H</td>
<td>-5.75721100</td>
<td>-3.59645200</td>
<td>-0.14192500</td>
</tr>
<tr>
<td>H</td>
<td>-4.79377300</td>
<td>-2.74160400</td>
<td>-1.36582400</td>
</tr>
<tr>
<td>H</td>
<td>-4.53930300</td>
<td>-5.69660300</td>
<td>-0.56009700</td>
</tr>
<tr>
<td>H</td>
<td>-4.52565500</td>
<td>-5.00684700</td>
<td>-2.18812800</td>
</tr>
<tr>
<td>H</td>
<td>-1.90700900</td>
<td>-6.24698700</td>
<td>-2.24850100</td>
</tr>
<tr>
<td>H</td>
<td>0.45299100</td>
<td>-5.57845400</td>
<td>-1.85111500</td>
</tr>
<tr>
<td>C</td>
<td>1.41459900</td>
<td>-3.42383600</td>
<td>-0.54127100</td>
</tr>
<tr>
<td>C</td>
<td>2.17173300</td>
<td>-3.04341500</td>
<td>-1.68071600</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>C</td>
<td>1.58427500</td>
<td>-2.97426600</td>
<td>-3.09279300</td>
</tr>
<tr>
<td>H</td>
<td>0.49975200</td>
<td>-3.12883800</td>
<td>-3.01290000</td>
</tr>
<tr>
<td>C</td>
<td>2.14989600</td>
<td>-4.09186900</td>
<td>-3.98969300</td>
</tr>
<tr>
<td>H</td>
<td>1.67245000</td>
<td>-4.07145700</td>
<td>-4.98344700</td>
</tr>
<tr>
<td>H</td>
<td>3.23595200</td>
<td>-3.97419500</td>
<td>-4.14023100</td>
</tr>
<tr>
<td>H</td>
<td>1.98571700</td>
<td>-5.09112200</td>
<td>-3.55649400</td>
</tr>
<tr>
<td>C</td>
<td>1.77801200</td>
<td>-1.59630200</td>
<td>-3.74967500</td>
</tr>
<tr>
<td>H</td>
<td>2.84405300</td>
<td>-1.35250900</td>
<td>-3.89300100</td>
</tr>
<tr>
<td>H</td>
<td>1.30484200</td>
<td>-1.58428400</td>
<td>-4.74579300</td>
</tr>
<tr>
<td>H</td>
<td>1.30636200</td>
<td>-0.81566300</td>
<td>-3.13805500</td>
</tr>
<tr>
<td>C</td>
<td>1.31421500</td>
<td>-3.91469300</td>
<td>2.00118500</td>
</tr>
<tr>
<td>H</td>
<td>0.26800000</td>
<td>-4.12002400</td>
<td>1.73779300</td>
</tr>
<tr>
<td>C</td>
<td>1.89425300</td>
<td>-5.23118800</td>
<td>2.55075200</td>
</tr>
<tr>
<td>H</td>
<td>1.86503100</td>
<td>-6.02911500</td>
<td>1.79192900</td>
</tr>
<tr>
<td>H</td>
<td>2.94288600</td>
<td>-5.11346300</td>
<td>2.86985000</td>
</tr>
<tr>
<td>H</td>
<td>1.31753500</td>
<td>-5.57334000</td>
<td>3.42621000</td>
</tr>
<tr>
<td>C</td>
<td>1.29873600</td>
<td>-2.81597000</td>
<td>3.07850800</td>
</tr>
<tr>
<td>H</td>
<td>2.31487900</td>
<td>-2.58329800</td>
<td>3.43814200</td>
</tr>
<tr>
<td>H</td>
<td>0.85100400</td>
<td>-1.88970100</td>
<td>2.69063500</td>
</tr>
<tr>
<td>H</td>
<td>0.70834000</td>
<td>-3.14082800</td>
<td>3.95154700</td>
</tr>
<tr>
<td>C</td>
<td>5.65401010</td>
<td>-2.45716900</td>
<td>-0.15008000</td>
</tr>
<tr>
<td>H</td>
<td>5.99283300</td>
<td>-2.12012400</td>
<td>-1.14564200</td>
</tr>
<tr>
<td>C</td>
<td>5.93466400</td>
<td>-1.31244900</td>
<td>0.83767900</td>
</tr>
<tr>
<td>H</td>
<td>7.00778400</td>
<td>-1.06020100</td>
<td>0.85005900</td>
</tr>
<tr>
<td>H</td>
<td>5.37585700</td>
<td>-0.40357100</td>
<td>0.56652300</td>
</tr>
<tr>
<td>H</td>
<td>5.64805000</td>
<td>-1.58969400</td>
<td>1.86586700</td>
</tr>
<tr>
<td>C</td>
<td>6.47109300</td>
<td>-3.71156400</td>
<td>0.20991500</td>
</tr>
<tr>
<td>H</td>
<td>6.18563000</td>
<td>-4.10171500</td>
<td>1.20092400</td>
</tr>
<tr>
<td>H</td>
<td>6.30970000</td>
<td>-4.51698500</td>
<td>-0.52349600</td>
</tr>
<tr>
<td>H</td>
<td>7.54998900</td>
<td>-3.48501500</td>
<td>0.23747900</td>
</tr>
</tbody>
</table>

**Product-R**

![Chemical Structure](image)

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.508416633 a.u.

Thermal correction to Gibbs free energy at 298 K: 0.1918830 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.31653363 a.u.

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-3.46354700</td>
<td>-1.41656000</td>
<td>-0.05091000</td>
</tr>
</tbody>
</table>
### Product-S

![Product-S Image]

SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.508415944 a.u.

Thermal correction to Gibbs free energy at 298 K: 0.19188400 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.31653194 a.u.

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-3.81262900</td>
<td>-0.04791700</td>
<td>-0.12264900</td>
</tr>
<tr>
<td>C</td>
<td>-2.84586200</td>
<td>0.95258900</td>
<td>-0.11058400</td>
</tr>
<tr>
<td>C</td>
<td>-1.50006400</td>
<td>0.56043600</td>
<td>-0.02384000</td>
</tr>
<tr>
<td>C</td>
<td>-1.12556800</td>
<td>-0.82669700</td>
<td>0.05238900</td>
</tr>
<tr>
<td>C</td>
<td>-2.13453300</td>
<td>-1.81150800</td>
<td>0.03559400</td>
</tr>
<tr>
<td>N</td>
<td>-0.36028300</td>
<td>1.34021500</td>
<td>0.00595600</td>
</tr>
<tr>
<td>C</td>
<td>0.71149000</td>
<td>0.47940100</td>
<td>0.10384100</td>
</tr>
<tr>
<td>C</td>
<td>0.30239900</td>
<td>-0.83664300</td>
<td>0.13200900</td>
</tr>
<tr>
<td>C</td>
<td>-0.29090300</td>
<td>2.78729400</td>
<td>-0.04727800</td>
</tr>
<tr>
<td>C</td>
<td>2.16187100</td>
<td>0.61290900</td>
<td>0.16962500</td>
</tr>
<tr>
<td>C</td>
<td>2.70030500</td>
<td>-0.83237100</td>
<td>0.33801500</td>
</tr>
<tr>
<td>C</td>
<td>1.46798200</td>
<td>-1.78260600</td>
<td>0.20840300</td>
</tr>
<tr>
<td>O</td>
<td>2.84338000</td>
<td>1.62045000</td>
<td>0.11124100</td>
</tr>
<tr>
<td>C</td>
<td>3.86130900</td>
<td>-1.12143100</td>
<td>-0.61359300</td>
</tr>
<tr>
<td>H</td>
<td>-4.25457300</td>
<td>-2.17019500</td>
<td>-0.06376200</td>
</tr>
<tr>
<td>H</td>
<td>-4.86757200</td>
<td>0.23033000</td>
<td>-0.18947700</td>
</tr>
<tr>
<td>H</td>
<td>-3.12777900</td>
<td>2.00607100</td>
<td>-0.16682400</td>
</tr>
<tr>
<td>H</td>
<td>-1.87183800</td>
<td>-2.87095300</td>
<td>0.09110400</td>
</tr>
<tr>
<td>H</td>
<td>0.76664800</td>
<td>3.08020100</td>
<td>-0.02687700</td>
</tr>
<tr>
<td>H</td>
<td>-0.75120700</td>
<td>3.17058300</td>
<td>-0.97295500</td>
</tr>
<tr>
<td>H</td>
<td>-0.80752200</td>
<td>3.24231900</td>
<td>0.81428800</td>
</tr>
<tr>
<td>H</td>
<td>3.08261800</td>
<td>-0.87709600</td>
<td>1.37442600</td>
</tr>
<tr>
<td>H</td>
<td>1.39317500</td>
<td>-2.48180000</td>
<td>1.05840500</td>
</tr>
<tr>
<td>H</td>
<td>1.54404200</td>
<td>-2.40644000</td>
<td>-0.69985800</td>
</tr>
<tr>
<td>H</td>
<td>4.63769000</td>
<td>-0.34886300</td>
<td>-0.50664500</td>
</tr>
<tr>
<td>H</td>
<td>4.31472600</td>
<td>-2.10360400</td>
<td>-0.40634800</td>
</tr>
<tr>
<td>H</td>
<td>3.52303400</td>
<td>-1.11702500</td>
<td>-1.66322200</td>
</tr>
</tbody>
</table>

S65
TS IV

SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -633.38331274 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.18556100 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-633.19775174 a.u.
SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -76.47109086 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.00357200 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-76.46751886 a.u.

O                  0.00000000    0.00000000    0.12020700
H                  0.00000000    0.75703900    -0.48082800
H                  0.00000000   -0.75703900    -0.48082800
CPV-Pre

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -709.96157397 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.20880300 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -709.75277097 a.u.

C  -4.19763600 -0.94487200  0.00040300
  -4.31666400  0.46040800  0.00048800
  -3.18576000  1.27832700  0.00035000
  -1.92884800  0.66233000  0.00016100
  -1.78448100 -0.77063200 -0.00002700
  -2.94942500 -1.56316100  0.00015400
  -0.66619600  1.24387700  0.00010700
  0.24748900  0.21364700 -0.00039300
  -0.37541100 -1.01416000 -0.00043700
  -0.38626900  2.66264800 -0.00097100
  1.69869700  0.05735500 -0.00016200
  1.98454300 -1.28046600 -0.00007700
  0.68395900 -2.08085100 -0.00018800
  3.32999000 -1.93662700 -0.00042700
  -5.10313500 -1.55752000  0.00053400
  -5.30968000  0.91720800  0.00065000
  -3.28372100  2.36656800  0.00039200
  -2.87319000 -2.65372100  0.00006500
  0.70102400  2.80597600 -0.00038300
  -0.80952800  3.15209700 -0.89507800
  -0.81066200  3.15355300  0.89177800
  0.62521700 -2.74381400  0.88390400
  0.62557300 -2.74391900 -0.88423200
  3.46794300 -2.58588100 -0.88533900
  4.15102500 -1.20471100  0.00017300
  3.46776500 -2.58729200  0.88345100
  2.50427400  1.14259500 -0.00011500
  3.45436500  0.90543300  0.00049000
  5.27548100  0.94776300  0.00086800
  5.60079100  1.43963400  0.76842200
H 5.60043600  1.44271000  -0.76485800

TS V

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:  -709.91535875 a.u.
Thermal correction to Gibbs free energy at 298 K:  0.20881400 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-709.70654475 a.u.

C   -3.88035300  -1.30984600  0.28243800
C   -4.18207000   0.06729900  0.18177300
C   -3.18129300  1.02021300  0.01154900
C   -1.85341300  0.57084700 -0.05253300
C   -1.52640400 -0.82808100  0.03897700
C   -2.56813400 -1.76229400  0.21182200
N   -0.68811100  1.30222200 -0.20244000
C    0.34926800  0.39503100 -0.23315700
C   -0.10492500 -0.90318500 -0.09801100
C   -0.57855600  2.74072300 -0.33201800
C    1.79504600  0.42856200 -0.25364800
C    2.28264200 -0.91991800 -0.12962600
C    1.05928900 -1.85221400 -0.03841100
C    3.47511200 -1.38815000 -0.95931200
H   -4.69484000 -2.02613500  0.41527200
H   -5.22429700  0.39169400  0.23897700
H   -3.42561300  2.08186100 -0.06509000
H   -2.34372600 -2.82936600  0.28589200
H    0.48607000  3.00692100 -0.34822200
H   -1.05224000  3.09828300 -1.26216700
H   -1.05944900  3.24865700  0.52021800
H    1.05212100 -2.45126600  0.89099200
H    1.04911300 -2.58059400 -0.86947800
H    3.16506700 -1.67179000 -1.98246600
H    4.23824300 -0.60141500 -1.04869900
H    3.96439100 -2.26694400 -0.50795600
O    2.53289000  1.48323400 -0.17736000
H    3.41846900  1.09191600  0.56745500
O    3.95607800  0.34699200  1.37238100

S69
SCF energy [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -709.98779584 a.u.

Thermal correction to Gibbs free energy at 298 K: 0.21257600 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -709.77521984 a.u.

C  -4.10754800 -1.05333400 -0.03423800
C  -4.28184200  0.34830300 -0.11692100
C  -3.19828000  1.22026500 -0.11326000
C  -1.91173600  0.66303700 -0.02440600
C  -1.71482500 -0.75972700  0.06129300
C  -2.83919800 -1.61127300  0.05398900
N  -0.68421900  1.29495000 -0.00229800
C   0.27179900  0.30644900  0.09714600
C  -0.30057900 -0.94902200  0.13604600
C  -0.43869800  2.72278300 -0.06577300
C   1.72022800  0.25310200  0.16300800
C   2.08253200 -1.24372400  0.31593700
C   0.73687300 -2.03132900  0.21882300
C   3.17290100 -1.68401800 -0.66509300
H  -4.98717900 -1.70132500 -0.04071500
H  -5.29377100  0.75576100 -0.18537300
H  -3.34655900  2.30013500 -0.17734900
H  -2.71065400 -2.69470000  0.11691100
H   0.64605100  2.88652300 -0.04198800
H  -0.84496900  3.15210100 -0.99637600
H  -0.89974500  3.24278900  0.79032300
H   0.58455900 -2.69842300  1.08408300
H   0.72306000 -2.67673600 -0.67681400
H   2.81414300 -1.61775600 -1.70578100
H   4.06052500 -1.04118200 -0.56600000
H   3.46967600 -2.72775300 -0.47544000
O   2.51330500  1.18611000  0.11849300
H   4.41440700  1.08949200 -0.03616400
O                  5.36196000    0.85482500    -0.04865800
H                  2.48315000   -1.33895000    1.34252500
H                  5.52494800    0.58881300    0.86626200

CP VI-Pre

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -1266.97145575 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.39883200 a.u.
Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
-1266.57262375 a.u.

C                  5.49509500   -1.19606800    0.87496800
C                  4.94931300   -2.25917000    0.12377300
C                  3.76357400   -2.10273900   -0.59251100
C                  3.12651300   -0.85561900   -0.54273700
C                  3.66853400    0.24274400    0.21391700
C                  4.86937700    0.04592200    0.92534100
N                  1.94657600   -0.45001800   -1.15533800
C                  1.75467300    0.86628800   -0.80647000
C                  2.76026900    1.32922000    0.01498500
C                  1.10802500   -1.26719200   -2.01151800
C                  0.75856200    1.90714800   -0.80666400
C                  1.13339600    3.02691100   -0.31984100
C                  2.46104800    2.75515100    0.38761500
C                  0.47670500    4.37397700   -0.34257600
H                  6.42660100   -1.35385100    1.42452400
H                  5.46508400   -3.22244800    0.10242100
H                  3.34676700   -2.92895100   -1.17267400
H                  5.30466600    0.86141400    1.50869000
H                  0.22946500   -0.68322300   -2.30987800
H                  1.65386100   -1.58012300   -2.91751300
H                  0.76211500   -2.16815500   -1.47988800
H                  2.38319300    2.90937800    1.48030000
H                  3.23707700    3.46100500    0.03664500
H                  1.13019800    5.13297900   -0.81027700
H                 -0.46722400    4.36928300   -0.91217800
TS VI

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -1266.93973705 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.39742600 a.u.

S72
Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]:
\(-1266.54231105\) a.u.

<table>
<thead>
<tr>
<th>Atom</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-5.73785400</td>
<td>-1.84820600</td>
<td>-0.93288100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-5.32115600</td>
<td>-2.73773900</td>
<td>0.08648500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-4.22637700</td>
<td>-2.45972100</td>
<td>0.89759900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-3.53474300</td>
<td>-1.25834600</td>
<td>0.67104400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-3.94760600</td>
<td>-0.33805200</td>
<td>-0.35638300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-5.06412200</td>
<td>-0.65700000</td>
<td>-1.15952600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.42110000</td>
<td>-0.76002300</td>
<td>1.31948100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.14052200</td>
<td>0.45976800</td>
<td>0.73800300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-3.04210900</td>
<td>0.75868500</td>
<td>-0.27751200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.69126200</td>
<td>-1.40899800</td>
<td>2.39268200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.11159100</td>
<td>1.44283100</td>
<td>0.77952700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.34224000</td>
<td>2.44559200</td>
<td>-0.23738700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.65794700</td>
<td>2.04152200</td>
<td>-0.94777500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.21181300</td>
<td>3.91809400</td>
<td>0.16088500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-6.60341900</td>
<td>-2.10860800</td>
<td>-1.54635800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-5.87409800</td>
<td>-3.66801500</td>
<td>0.23899400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-3.91602800</td>
<td>-3.15622500</td>
<td>1.67879000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-5.39041700</td>
<td>0.02779300</td>
<td>-1.94590800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.81549100</td>
<td>-0.79903100</td>
<td>2.64427800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.32087600</td>
<td>-1.51972000</td>
<td>3.29106000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.34509600</td>
<td>-2.40908000</td>
<td>2.07940900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.51957400</td>
<td>1.91242800</td>
<td>-2.03573600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-3.42913600</td>
<td>2.82211800</td>
<td>-0.82481400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-2.09597000</td>
<td>4.25844000</td>
<td>0.72878200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.32354400</td>
<td>4.09743400</td>
<td>0.77980000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-1.11434700</td>
<td>4.55174400</td>
<td>-0.73374700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>-0.08015000</td>
<td>1.35953000</td>
<td>1.58074000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.70511700</td>
<td>1.90416600</td>
<td>1.22371600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.79720800</td>
<td>-3.15301400</td>
<td>0.77451900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.11831400</td>
<td>-3.75354000</td>
<td>-0.30721500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.22461000</td>
<td>-3.02465600</td>
<td>-1.09192900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.01701800</td>
<td>-1.67637600</td>
<td>-0.77251800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.70396900</td>
<td>-1.04231600</td>
<td>0.32444000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.59949300</td>
<td>-1.81204700</td>
<td>1.09339100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.18767700</td>
<td>-0.74651800</td>
<td>-1.38179300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.34672600</td>
<td>0.44057100</td>
<td>-0.70181400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.25566000</td>
<td>0.31670300</td>
<td>0.32384000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.34904700</td>
<td>-0.96551900</td>
<td>-2.54084800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.76840700</td>
<td>1.79225200</td>
<td>-0.75980600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.32560500</td>
<td>2.50508000</td>
<td>0.31237900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.35778400</td>
<td>1.63427100</td>
<td>1.04094100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

S73
CP VI-Post

SCF energy[B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -1267.02183702 a.u.
Thermal correction to Gibbs free energy at 298 K: 0.39992700 a.u.

Gibbs free energy at 298 K [B3LYP-D3BJ/DEF2TZVP/SMD(1,2-dichloroethane)]: -1266.62191002 a.u.
<table>
<thead>
<tr>
<th></th>
<th>X1</th>
<th>Y1</th>
<th>Z1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>2.11127200</td>
<td>3.68957700</td>
<td>0.09548700</td>
</tr>
<tr>
<td>H</td>
<td>7.42122600</td>
<td>-2.28746500</td>
<td>1.72444500</td>
</tr>
<tr>
<td>H</td>
<td>6.94024400</td>
<td>-3.65359600</td>
<td>-0.28965600</td>
</tr>
<tr>
<td>H</td>
<td>5.06775600</td>
<td>-3.07631600</td>
<td>-1.81950800</td>
</tr>
<tr>
<td>H</td>
<td>6.03688800</td>
<td>-0.29293100</td>
<td>2.27217100</td>
</tr>
<tr>
<td>H</td>
<td>1.97837300</td>
<td>-0.66759300</td>
<td>-2.80534500</td>
</tr>
<tr>
<td>H</td>
<td>3.54633000</td>
<td>-1.34109100</td>
<td>-3.35000200</td>
</tr>
<tr>
<td>H</td>
<td>2.42698900</td>
<td>-0.66759300</td>
<td>-2.80534500</td>
</tr>
<tr>
<td>H</td>
<td>3.08171300</td>
<td>1.48073400</td>
<td>2.33510800</td>
</tr>
<tr>
<td>H</td>
<td>4.11476200</td>
<td>2.48604100</td>
<td>1.31310100</td>
</tr>
<tr>
<td>O</td>
<td>1.09632900</td>
<td>1.39337100</td>
<td>-1.61843400</td>
</tr>
<tr>
<td>H</td>
<td>-1.16117000</td>
<td>2.03855900</td>
<td>-1.09181900</td>
</tr>
<tr>
<td>C</td>
<td>-6.59128600</td>
<td>-2.00334200</td>
<td>-1.07355800</td>
</tr>
<tr>
<td>C</td>
<td>-6.31557700</td>
<td>-2.78316700</td>
<td>0.07359800</td>
</tr>
<tr>
<td>C</td>
<td>-5.26889800</td>
<td>-2.46841400</td>
<td>0.93461300</td>
</tr>
<tr>
<td>C</td>
<td>-4.48631900</td>
<td>-1.34301400</td>
<td>0.62864800</td>
</tr>
<tr>
<td>C</td>
<td>-4.75106200</td>
<td>-0.53777700</td>
<td>-0.53395000</td>
</tr>
<tr>
<td>C</td>
<td>-5.82127000</td>
<td>-0.88895900</td>
<td>-1.38206500</td>
</tr>
<tr>
<td>N</td>
<td>-3.40394700</td>
<td>-0.81837300</td>
<td>1.30721500</td>
</tr>
<tr>
<td>C</td>
<td>-2.98641000</td>
<td>0.28925500</td>
<td>0.59626900</td>
</tr>
<tr>
<td>C</td>
<td>-3.76771800</td>
<td>0.50073200</td>
<td>-0.51634400</td>
</tr>
<tr>
<td>C</td>
<td>-2.80875000</td>
<td>-1.32962600</td>
<td>2.52572400</td>
</tr>
<tr>
<td>C</td>
<td>-1.93384700</td>
<td>1.28683300</td>
<td>0.73469900</td>
</tr>
<tr>
<td>C</td>
<td>-2.07445100</td>
<td>2.21320200</td>
<td>-0.49499400</td>
</tr>
<tr>
<td>C</td>
<td>-3.32723800</td>
<td>1.71536700</td>
<td>-1.28328100</td>
</tr>
<tr>
<td>C</td>
<td>-2.11147500</td>
<td>3.68955200</td>
<td>-0.09270500</td>
</tr>
<tr>
<td>H</td>
<td>-7.42304700</td>
<td>-2.28585200</td>
<td>-1.72341500</td>
</tr>
<tr>
<td>H</td>
<td>-6.94004000</td>
<td>-3.65417300</td>
<td>0.28870400</td>
</tr>
<tr>
<td>H</td>
<td>-5.06618500</td>
<td>-3.07836000</td>
<td>1.81746800</td>
</tr>
<tr>
<td>H</td>
<td>-6.03947400</td>
<td>-0.29054600</td>
<td>-2.27020600</td>
</tr>
<tr>
<td>H</td>
<td>-1.97440000</td>
<td>0.67213900</td>
<td>2.80159900</td>
</tr>
<tr>
<td>H</td>
<td>-3.54240200</td>
<td>-1.34326600</td>
<td>3.34889800</td>
</tr>
<tr>
<td>H</td>
<td>-2.42670100</td>
<td>-2.35413300</td>
<td>2.38161000</td>
</tr>
<tr>
<td>H</td>
<td>-3.08454300</td>
<td>1.48337100</td>
<td>-2.33406600</td>
</tr>
<tr>
<td>H</td>
<td>-4.11614300</td>
<td>2.48777700</td>
<td>-1.30966800</td>
</tr>
<tr>
<td>H</td>
<td>-3.01936100</td>
<td>3.92333400</td>
<td>0.48871900</td>
</tr>
<tr>
<td>H</td>
<td>-1.23883640</td>
<td>3.93895400</td>
<td>0.52952500</td>
</tr>
<tr>
<td>H</td>
<td>-2.09883800</td>
<td>4.34186100</td>
<td>-0.98020400</td>
</tr>
<tr>
<td>O</td>
<td>-1.09484100</td>
<td>1.39111300</td>
<td>1.61725400</td>
</tr>
<tr>
<td>H</td>
<td>1.15974800</td>
<td>2.03730200</td>
<td>1.09135500</td>
</tr>
</tbody>
</table>
References


