Supporting Information

Unexpected Regioselectivity in the Synthesis of Pyranonaphthoquinone via the Diels-Alder Reaction

Yi Cui, Hao Jiang, Zhengtao Li, Na Wu, Zhen Yang* and Junmin Quan*

Laboratory of Chemical Genomics, School of Chemical Biology and Biotechnology, Shenzhen Graduate School of Peking University, Shenzhen 518055, China, and Molecular Engineering of Ministry of Education and Beijing National Laboratory for Molecular Science (BNLMS), Peking University, Beijing 100871

quanjm@szpku.edu.cn, zyang@pku.edu.cn
# Table of contents

1. General methods ................................................................. S3

2.1: Synthesis of compound (E)-(buta-1,3-dienyloxy)trimethylsilane (7)------------------- S3

2.2: Synthesis of compound (E)-(4-methoxybuta-1,3-dien-2-yloxy)trimethyl silane (14) ------ S3

2.3: Synthesis of compound (3aS,5S,11bS)-10-methoxy-5-methyl-2,6,11-trioxo-3, 3a,5,6,11,11b-
hexahydro-2H-benzo[g]furo[3,2-c]isochroman-8-yl trifluoro methanesulfonate (11) ------ S4

2.4: Synthesis of compound (3aS,5S,11bS)-7-hydroxy-5-methyl-3,3a-dihydro-2H-benzo[g]
furo[3,2-c] isochromene-2,6,11(5H,11bH)-trione (15) ........................................ S4

2.5: Synthesis of compounds (3aS,5S,11bS)-8-hydroxy-5-methyl-3,3a-dihydro-2H-benzo[g]furo
[3,2-c] isochromene-2,6,11(5H,11bH)-trione (16) and (3aS, 5S,11bS)-9-hydroxy -5-methyl-
3,3a-dihydro-2H-benzo[g]furo[3,2-c]isochromene- 2,6,11(5H, 11bH)-trione (17) -------- S5

3.1: Proton NMR of compound 7-------------------------------------S7

3.2: Proton NMR of compound 11 ------------------------------------S8

3.3: 1H and C13 NMR of compound 15 --------------------------------S9

3.4: 1H and C13 NMR of compounds 16 and 17 --------------------------S10

3.5: 1H, C13 NMR and HMBC of compound 17’ --------------------------------S11

4: Computational Experimental Part:

4.1: Complete References ....................................................S13

4.2: Schematic Explanation of the Different Regioselectivity ..................S13

4.3: Activation Enthalpies for D-A Reactions of 7 and 6, 9 and 6 ...............S14

4.4: Molecular Geometries and Energies ......................................S15
General Information

All reactions were carried out under a nitrogen atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. All the chemicals were purchased commercially, and used without further purification. Anhydrous THF and dioxane were distilled from sodium-benzophenone, and dichloromethane was distilled from calcium hydride. Yields refer to chromatographically, unless otherwise stated.

Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm Tsingdao silica gel plates (60F-254) using UV light as visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate, and heat as developing agents. Tsingdao silica gel (60, particle size 0.040–0.063 mm) was used for flash column chromatography.

Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. NMR spectra were recorded on either a Bruker Advance 300 (1H: 300 MHz, 13C: 75.5 MHz), Bruker Advance 500 (1H: 500 MHz, 13C: 125 MHz) or Varian. Mass spectrometric data were obtained using ZAB-HS mass spectrometer. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad.

Synthesis of compound (E)-(buta-1,3-dienyloxy)trimethylsilane (7):

To a solution of triethylamine (61.2 mL, 440 mmol) was added anhydrous powder ZnCl₂ (861 mg, 6 mmol), and the reaction mixture was stirred at room temperature for 1 h. To this homogeneous solution was added a solution of crotonaldehyde (14 g, 200 mmol) in ethyl (200 mL), followed by addition of TMSCl (50.7 mL, 400 mmol) within 30 min. and the reaction mixture was reflux for 24 h. After cooling to room temperature, the reaction was quenched by addition of dry hexane (250 mL), and the formed mixture was filtered through a short alumina pad, and the filtrate was concentrate under vacuum to give diene 13 (26.7 g) in 94% yield; ¹H NMR (500 MHz, CDCl₃): δ 6.54 (d, J = 11.9 Hz, 1H), 6.22 (ddd, J = 10.3, 6.5, 4.3 Hz, 1H), 5.73 (dd, J = 11.9, 11.1 Hz, 1H), 4.99 (m, 1H), 4.83 (d, J = 10.3 Hz, 1H), 0.22 (s, 10H).

Synthesis of compound (E)-(4-methoxybuta-1,3-dienyloxy)trimethyl silane (14):
To a solution of triethylamine (12.2 mL, 88 mmol) was added anhydrous powder ZnCl₂ (163.2 mg, 1.2 mmol), and the reaction mixture was stirred at room temperature for 1 h. To this homogeneous solution was added a solution of (E)-4-methoxybut-3-en-2-one (4 g, 40 mmol) in benzene (20 mL), followed by addition of TMSCl (10.2 mL, 80 mmol) within 30 min. After the reaction mixture was stirred at 40 °C for 24 h, the reaction mixture was cooled to room temperature, and quenched by addition of dry ether (150 mL), and the formed mixture was filtered through an alumina pad. The filtrate was concentrated under vacuum to give diene 17 (6.0 g) in 87% yield; ¹H NMR (500 MHz, CDCl₃): δ 6.74 (dd, J = 9.2, 3.2 Hz, 1H), 5.27 (dd, J = 12.4, 3.2 Hz, 1H), 4.03 (d, J = 3.0 Hz, 1H), 3.99 (d, J = 3.0 Hz, 1H), 3.49 (d, J = 3.0 Hz, 1H), 0.05 (d, J = 3.0 Hz, 9H).


To a solution of hydroxytetracyclic quinine 10 (165 mg, 0.5 mmol) in a mixed solvent of THF/DCM (1:1, 150 mL) was first added pyridine (2.55 mL, 15 mmol) and a catalytic amount of DMAP (12.2 mg, 0.05 mmol) at 0 ºC, and followed by slow addition of trifluoromethane sulfonic anhydride (332 μL, 2 mmol). After addition, the mixture was first warmed to room temperature, and then stirred overnight. The reaction was worked up by mixing the reaction mixture with water (100 mL), and the formed solution was extracted with ethyl acetate (3 × 100 mL). The organic extract was sequentially washed with water, 10% of aqueous hydrochloric acid solution, water and brine, and finally dried over Na₂SO₄. The solvent was removed under vacuum, and the residue was purified by a flash chromatography on silica gel (EtOAc/hexane = 1/2) to give 11 (180 mg) in 78% yield; Rₚ = 0.52 (silica gel, EtOAc/hexane =1/1); ¹H NMR (500 MHz, CDCl₃): δ = 7.62 (d, J = 2.4 Hz, 1H), 7.18 (d, J = 2.4 Hz, 1H), 5.29 (d, J = 3.0 Hz, 1H), 5.01 (q, J = 6.9 Hz, 1H), 4.68 (dd, J = 5.1, 3.0 Hz, 1H), 4.04 (s, 3H), 2.98 (dd, J = 17.8, 5.2 Hz, 1H), 2.67 (d, J = 17.8 Hz, 1H), 1.54 (d, J = 6.9 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 181.5, 179.6, 173.8, 161.9, 153.4, 147.3, 136.1, 135.7, 120.0, 119.5, 117.4, 111.4, 111.2, 68.5, 66.6, 66.3, 57.2, 36.9, 18.4; HRMS (EI): m/z calcd for (C₁₈H₁₃F₃O₉S)⁺ 462.0232; found 462.0243.

To solution of 6 (46.8 mg, 0.2 mmol) in CH₂Cl₂ (10 mL) was added diene 7 (57 mg, 0.4 mmol) at -78 °C in a drop-wise manner, and the reaction mixture was first stirred at the same temperature for 0.5 h, then slowly warmed to room temperature, and stirred overnight. The solvent was removed under vacuum, and the residue was dissolved in acetone (10 mL). To this solution was added an aqueous solution of HCl (3%, 3 drops), followed by addition of Jone’s reagent (0.15 mL, 2.7 mol/L) at 0 °C, and the reaction mixture was then stirred at the same temperature for 40 min. The reaction was quenched by addition of 2-propanol (0.5 mL), and the formed mixture was stirred at room temperature for 5 min. The mixture was first poured into water (5 mL), and the mixture was then extracted with ethyl acetate (3 × 30 mL). The combined organic layer was sequentially washed with a saturated solution of NH₄Cl and brine, and then dried over Na₂SO₄. The solvent was removed under vacuum, and the residue was purified by a flash silica gel chromatography (EtOAc/hexane = 2/1) to give the Diels-Alder adduct 15 (46 mg) in 78% yield; Rf = 0.5 (silica gel, EtOAc/hexane = 2/1); ¹H NMR (500 MHz, CDCl₃): δ 11.83 (s, 1H), 7.72-7.66 (m, 2H), 7.30 (m, 1H), 5.27 (d, J = 3.0 Hz, 1H), 5.09 (t, J = 6.8 Hz, 1H), 4.69 (dd, J = 5.0, 3.0 Hz, 1H), 2.96 (dd, J = 17.8, 5.0 Hz, 1H), 2.69 (d, J = 17.8 Hz, 1H), 1.57 (d, J = 6.8 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 188.0, 181.5, 173.8, 162.0, 149.8, 137.2, 135.2, 131.6, 124.8, 119.7, 114.9, 71.1, 68.6, 66.5, 36.9, 18.6. HRMS (ESI): m/z calcd for C₁₆H₁₂O₆ (M + Na⁺), 323.0634; found 323.0628.

To solution of 6 (46.8 mg, 0.2 mmol) in CH2Cl2 (10 mL) was added diene 14 (69 mg, 0.4 mmol) at -78 °C (69 mg, 0.4 mmol) in a drop-wise manner, and the reaction mixture was first stirred at the same temperature for 0.5 h, then slowly warmed to room temperature, and stirred at the same temperature overnight. The solvent was removed under vacuum; the residue was dissolved in acetone (10 mL). To this solution was added an aqueous solution of HCl (3%, 3 drops), followed by addition of Jone’s reagent (0.15 mL, 2.7 mol/L) at 0 °C, and the reaction mixture was stirred at the same temperature for 40 min. The reaction was quenched by addition of 2-propanol (0.5 mL), and the formed mixture was stirred at room temperature for 5 min. The mixture was first poured into water (5 mL), then extracted with ethyl acetate (3 × 30 mL). The combined organic layer was sequentially washed with a saturated solution of NH4Cl and brine, and then dried over Na2SO4. The solvent was removed under vacuum, and the residue was purified by a flash silica gel chromatography (EtOAc/hexane = 2/1) to give the Diels-Alder adducts 16 and 17 (41 mg) in 68 % overall yield. The ratio of for 16/17 is 1:3.3 according to NMR’s ratio. 1H NMR form compound 17 (500 MHz, Actone-d6): δ 10.19 (brs, 1H), 7.95 (m, 1H), 7.45 (m, 1H), 7.25 (m, 1H), 5.34 (s, 1H), 4.80 (br, 1H), 4.50 (br, 1H), 3.15 (m, 4.5 Hz, 1H), 2.50 (m, 1H), 1.43 (br, 3H); 13C NMR (125 MHz, Actone-d6): δ 184.2, 182.7, 182.5, 181.1, 174.6, 163.0, 162.9, 150.4, 149.6, 135.2, 134.8, 134.7, 133.9, 129.0, 128.9, 125.2, 121.0, 111.8, 71.6, 71.5, 70.2, 70.1, 68.6, 68.5, 36.8, 19.8, 19.6. HRMS (ESI) calcd for C16H12O6 (M + Na+), 323.0634; found 323.0631.
The image contains two chemical structures labeled as 16 and 17, with a ratio of 16/17 = 1:3.3.
4.1: Complete References


4.2: Schematic Explanation of the Different Regioselectivity

The explanation of the different regioselectivity from Kraus’s and Zhen’s experiments is shown in the Figure S1. In Kraus’s experiment, the near addition of the butadiene induces more negative charge distribution on the quinone oxygen near to the lactone, which would cause larger electrostatic repulsion between the quinone oxygen and the vicinal lactone oxygen, the near product is therefore less favored. Whereas in Zhen’s experiment, such electrostatic repulsion is neutralized by a methyl proton of the terminal methoxyl group, which makes the near product more favored.

![Figure S1](attachment:image.png)

Figure S1: The schematic explanation of the different regioselectivity of Diels-Alder reaction for the Synthesis of Pyranonaphthoquinone from Kraus’s and Zhen’s group.
### 4.3: Activation Enthalpies for D-A Reactions of 7 and 6, 9 and 6

![Chemical Structures](image)

**Table S1.** Activation Enthalpies (kcal/mol) for D-A reaction of 7 and 6.

<table>
<thead>
<tr>
<th>Diene</th>
<th>Dienophile</th>
<th>Attacking Way</th>
<th>Activation Enthalpy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>6</td>
<td>exo-syn-near</td>
<td>21.5</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>exo-syn-dist</td>
<td>20.6</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>exo-anti-near</td>
<td>23.4</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>exo-anti-dist</td>
<td>22.7</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>endo-syn-near</td>
<td>16.6</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>endo-syn-dist</td>
<td>15.0</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>endo-anti-near</td>
<td>18.7</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>endo-anti-dist</td>
<td>18.0</td>
</tr>
</tbody>
</table>

**Table S2.** Activation Enthalpies (kcal/mol) for D-A reaction of 9 and 6.

<table>
<thead>
<tr>
<th>Diene</th>
<th>Dienophile</th>
<th>Attacking Way</th>
<th>Activation Enthalpy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>6</td>
<td>exo-syn-near</td>
<td>17.8</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>exo-syn-dist</td>
<td>17.7</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>exo-anti-near</td>
<td>22.2</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>exo-anti-dist</td>
<td>22.4</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>endo-syn-near</td>
<td>13.9</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>endo-syn-dist</td>
<td>14.9</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>endo-anti-near</td>
<td>22.4</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>endo-anti-dist</td>
<td>19.8</td>
</tr>
</tbody>
</table>
### 4.4: Molecular Geometries and Energies

*Cartesian coordinates and energies for all the relevant structures are presented below.*

Dienophile 6 (axial-like conformation)

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>E (0K)</th>
<th>E+ZPE (0K)</th>
<th>Enthalpy</th>
<th>Free Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>2.51580800</td>
<td>-2.02008900</td>
<td>-0.03539500</td>
<td>-839.387636</td>
<td>-839.182889</td>
<td>-839.168306</td>
<td>-839.223468</td>
</tr>
<tr>
<td>C</td>
<td>1.10545200</td>
<td>-1.91899200</td>
<td>0.41680900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.43154900</td>
<td>-0.59373300</td>
<td>0.29215400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.10717100</td>
<td>0.49985600</td>
<td>-0.11746300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.54453800</td>
<td>0.39597600</td>
<td>-0.51760600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.18762700</td>
<td>-0.93915200</td>
<td>-0.46049800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.96383300</td>
<td>-3.00759300</td>
<td>0.02682900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.22542000</td>
<td>-0.97537100</td>
<td>-0.77934100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>3.16978100</td>
<td>1.38036700</td>
<td>-0.89657600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>0.52910100</td>
<td>-2.88172400</td>
<td>0.90620100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.44635500</td>
<td>1.85646500</td>
<td>-0.21871700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.70976000</td>
<td>2.28698700</td>
<td>-1.19022700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.01838700</td>
<td>-0.51877800</td>
<td>0.68177300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.17364600</td>
<td>-1.05058300</td>
<td>1.62742200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.55504300</td>
<td>0.92256000</td>
<td>0.75663000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.40609100</td>
<td>1.35737600</td>
<td>1.75339900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.97486700</td>
<td>1.73641800</td>
<td>-0.25597800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-1.82297100</td>
<td>-1.17573900</td>
<td>-0.32750300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.99167800</td>
<td>-0.49100800</td>
<td>-0.53431000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-3.82669100</td>
<td>-0.86607300</td>
<td>-1.31052000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.01598800</td>
<td>0.73353900</td>
<td>0.37569000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.63643500</td>
<td>0.50871600</td>
<td>1.25164700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.43745700</td>
<td>1.59978200</td>
<td>-0.13707100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.91840500</td>
<td>2.82647400</td>
<td>0.87721700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.99234300</td>
<td>3.00454800</td>
<td>0.77979200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.39058300</td>
<td>3.78817400</td>
<td>0.76429400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.72201300</td>
<td>2.43327500</td>
<td>1.88054700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K

E (0K), E+ZPE (0K), Enthalpy, Free Energy

-839.387636, -839.182889, -839.168306, -839.223468

Dienophile 6 (equatorial-like conformation)

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>E (0K)</th>
<th>E+ZPE (0K)</th>
<th>Enthalpy</th>
<th>Free Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.81558200</td>
<td>2.43081400</td>
<td>0.07569500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.56410400</td>
<td>1.99627200</td>
<td>-0.59070300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.18623500</td>
<td>0.55264100</td>
<td>-0.48981900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.04771800</td>
<td>-0.36082300</td>
<td>0.01208000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.28734600</td>
<td>0.09821300</td>
<td>0.71682600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.62021900</td>
<td>1.54310200</td>
<td>0.67852300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.03698900</td>
<td>3.49307300</td>
<td>0.02561000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.54367500</td>
<td>1.82307400</td>
<td>1.17732800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>2.99153800</td>
<td>-0.68367100</td>
<td>1.34641200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.11029100</td>
<td>2.78215800</td>
<td>-1.24165200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.76606100</td>
<td>-1.84971900</td>
<td>-0.04066200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.63152300</td>
<td>-2.21339600</td>
<td>0.99098500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>2.99153800</td>
<td>-0.68367100</td>
<td>1.34641200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.11029100</td>
<td>2.78215800</td>
<td>-1.24165200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.76606100</td>
<td>-1.84971900</td>
<td>-0.04066200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.63152300</td>
<td>-2.21339600</td>
<td>0.99098500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.19159000</td>
<td>0.17696900</td>
<td>-0.97997000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.32020200</td>
<td>0.43521400</td>
<td>-2.03293100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.51497500</td>
<td>-1.30121300</td>
<td>-0.66352300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.24434400</td>
<td>-1.67475700</td>
<td>-1.38767700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.39779800</td>
<td>-2.14751900</td>
<td>-0.81393100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.89355800</td>
<td>-2.65331100</td>
<td>-0.69701300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.09480700</td>
<td>-2.27154700</td>
<td>-1.70304400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.80273700</td>
<td>-2.60442900</td>
<td>-0.09729900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.57130300</td>
<td>-3.69495100</td>
<td>-0.78346300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.16555100</td>
<td>-1.21535600</td>
<td>0.72415200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.94337400</td>
<td>-1.95860000</td>
<td>0.90901300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.42622700</td>
<td>-1.30056000</td>
<td>1.52965500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-2.17880000</td>
<td>0.94046800</td>
<td>-0.24431700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.74662200</td>
<td>0.19185900</td>
<td>0.75450200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-3.56979900</td>
<td>0.64727400</td>
<td>1.49989800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-839.381632, -839.176802, -839.162219, -839.217403

Diene 7
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-2.74395400</td>
<td>0.71441000</td>
<td>2.13814500</td>
</tr>
<tr>
<td>C</td>
<td>-1.78780900</td>
<td>0.24083900</td>
<td>1.88480400</td>
</tr>
<tr>
<td>Si</td>
<td>-1.60834300</td>
<td>0.05667000</td>
<td>0.01179100</td>
</tr>
<tr>
<td>H</td>
<td>-0.98888880</td>
<td>0.86078600</td>
<td>2.30750600</td>
</tr>
<tr>
<td>H</td>
<td>-1.75200800</td>
<td>-0.73387900</td>
<td>2.38350400</td>
</tr>
<tr>
<td>O</td>
<td>-0.11075200</td>
<td>-0.71092900</td>
<td>-0.34544800</td>
</tr>
<tr>
<td>C</td>
<td>-2.89554500</td>
<td>-1.11386400</td>
<td>-0.70562700</td>
</tr>
<tr>
<td>C</td>
<td>-1.66858300</td>
<td>1.75486500</td>
<td>-0.81934000</td>
</tr>
<tr>
<td>C</td>
<td>2.23861700</td>
<td>-0.92620700</td>
<td>-0.14268500</td>
</tr>
<tr>
<td>H</td>
<td>-2.75541600</td>
<td>-1.23751900</td>
<td>-1.78489300</td>
</tr>
<tr>
<td>H</td>
<td>-2.82498000</td>
<td>-2.10410700</td>
<td>-0.24276400</td>
</tr>
<tr>
<td>H</td>
<td>-3.91050700</td>
<td>-0.73497700</td>
<td>-0.53801700</td>
</tr>
<tr>
<td>H</td>
<td>-0.89710100</td>
<td>2.43097500</td>
<td>-0.43380400</td>
</tr>
<tr>
<td>H</td>
<td>-1.53047100</td>
<td>1.67217100</td>
<td>-1.90298000</td>
</tr>
<tr>
<td>H</td>
<td>-2.64031000</td>
<td>2.23053600</td>
<td>-0.63994700</td>
</tr>
<tr>
<td>C</td>
<td>3.57899500</td>
<td>-0.40080100</td>
<td>0.11958200</td>
</tr>
<tr>
<td>C</td>
<td>1.11230100</td>
<td>-0.19912900</td>
<td>-0.05110000</td>
</tr>
<tr>
<td>H</td>
<td>4.29415200</td>
<td>-1.12681100</td>
<td>0.50965200</td>
</tr>
</tbody>
</table>
C 4.00364500 0.85729100 -0.07656500
H 1.14375000 0.84360400 0.27078700
H 3.36627000 1.61859600 -0.51999600
H 5.01027500 1.16230100 0.19435100
H 2.14228700 -1.98000000 -0.39745200

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-354.285634, -354.09259, -354.078203, -354.133607

**TS-exo-syn-near for 7 + 6**

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.53148900</td>
<td>-1.68435500</td>
<td>-0.98916200</td>
</tr>
<tr>
<td>C</td>
<td>0.02227400</td>
<td>-0.36481900</td>
<td>-1.25732800</td>
</tr>
<tr>
<td>C</td>
<td>-1.34506000</td>
<td>-0.05205300</td>
<td>-0.71554300</td>
</tr>
<tr>
<td>C</td>
<td>-2.18403900</td>
<td>-1.01973000</td>
<td>-0.28909700</td>
</tr>
<tr>
<td>C</td>
<td>-1.72876800</td>
<td>-2.44167900</td>
<td>-0.24646600</td>
</tr>
<tr>
<td>C</td>
<td>-0.25750900</td>
<td>-2.68725300</td>
<td>-0.38485500</td>
</tr>
<tr>
<td>H</td>
<td>1.48119500</td>
<td>-1.93819700</td>
<td>-1.44453500</td>
</tr>
<tr>
<td>H</td>
<td>-0.03328400</td>
<td>-3.72387500</td>
<td>-0.62075800</td>
</tr>
<tr>
<td>O</td>
<td>-2.52081600</td>
<td>-3.35772800</td>
<td>-0.05183400</td>
</tr>
<tr>
<td>O</td>
<td>0.63072600</td>
<td>0.49736800</td>
<td>-1.90999500</td>
</tr>
<tr>
<td>C</td>
<td>-3.60108600</td>
<td>-0.71303900</td>
<td>0.15056400</td>
</tr>
<tr>
<td>H</td>
<td>-3.80117800</td>
<td>-1.26128900</td>
<td>1.07712000</td>
</tr>
<tr>
<td>C</td>
<td>-1.76250500</td>
<td>1.38948700</td>
<td>-0.71651400</td>
</tr>
<tr>
<td>H</td>
<td>-1.45351700</td>
<td>1.86101700</td>
<td>-1.65487800</td>
</tr>
<tr>
<td>C</td>
<td>-3.25814000</td>
<td>1.60589000</td>
<td>-0.42958500</td>
</tr>
<tr>
<td>H</td>
<td>-3.85171300</td>
<td>1.58835200</td>
<td>-1.35296100</td>
</tr>
<tr>
<td>O</td>
<td>-3.74247300</td>
<td>0.66080600</td>
<td>0.51655100</td>
</tr>
<tr>
<td>O</td>
<td>-1.06813800</td>
<td>2.07268400</td>
<td>0.36428300</td>
</tr>
<tr>
<td>C</td>
<td>-1.88988500</td>
<td>2.98577300</td>
<td>0.96406100</td>
</tr>
<tr>
<td>O</td>
<td>-1.52389400</td>
<td>3.68145300</td>
<td>1.87356500</td>
</tr>
<tr>
<td>C</td>
<td>-3.25104400</td>
<td>2.95503300</td>
<td>0.27513400</td>
</tr>
<tr>
<td>H</td>
<td>-3.30150100</td>
<td>3.78435900</td>
<td>-0.44106500</td>
</tr>
<tr>
<td>H</td>
<td>-4.06334400</td>
<td>3.06502900</td>
<td>0.99572200</td>
</tr>
<tr>
<td>C</td>
<td>-4.64540200</td>
<td>-1.14335700</td>
<td>-0.89224700</td>
</tr>
<tr>
<td>H</td>
<td>-4.59113400</td>
<td>-2.22444600</td>
<td>-1.04152100</td>
</tr>
<tr>
<td>H</td>
<td>-5.64564600</td>
<td>-0.88097800</td>
<td>-0.53300600</td>
</tr>
<tr>
<td>H</td>
<td>-4.47881700</td>
<td>-0.65219800</td>
<td>-1.85728500</td>
</tr>
<tr>
<td>H</td>
<td>4.64043000</td>
<td>2.86528000</td>
<td>-1.44763400</td>
</tr>
<tr>
<td>C</td>
<td>3.77844400</td>
<td>2.54954700</td>
<td>-0.84862700</td>
</tr>
<tr>
<td>Si</td>
<td>3.95599900</td>
<td>0.77010500</td>
<td>-0.27905800</td>
</tr>
<tr>
<td>H</td>
<td>3.68806800</td>
<td>3.23068800</td>
<td>0.00421600</td>
</tr>
<tr>
<td>H</td>
<td>2.87534200</td>
<td>2.64900800</td>
<td>-1.45948500</td>
</tr>
<tr>
<td>O</td>
<td>2.47158600</td>
<td>0.52474500</td>
<td>0.61034000</td>
</tr>
<tr>
<td></td>
<td>E (0K)</td>
<td>E+ZPE (0K)</td>
<td>Enthalpy</td>
</tr>
<tr>
<td>---</td>
<td>------------</td>
<td>--------------</td>
<td>----------</td>
</tr>
<tr>
<td></td>
<td>-1193.641121</td>
<td>-1193.239977</td>
<td>-1193.212281</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K

E (0K), E+ZPE (0K), Enthalpy, Free Energy

-1193.641121, -1193.239977, -1193.212281, -1193.297442

**TS-exo-syn-dist for 7 + 6**

<table>
<thead>
<tr>
<th></th>
<th>E (0K)</th>
<th>E+ZPE (0K)</th>
<th>Enthalpy</th>
<th>Free Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-0.07172100</td>
<td>2.01807800</td>
<td>-1.50659900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.52845200</td>
<td>1.69883700</td>
<td>-1.38823900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.87387000</td>
<td>0.34695500</td>
<td>-0.85995700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.97288500</td>
<td>-0.65942400</td>
<td>-0.87621100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.43704200</td>
<td>-0.43086700</td>
<td>-1.34878100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.83262100</td>
<td>0.93643600</td>
<td>-1.57088600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.12158500</td>
<td>2.88614800</td>
<td>-2.13062100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.82872400</td>
<td>1.08451900</td>
<td>-1.97177400</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>1.20056400</td>
<td>-1.40070300</td>
<td>-1.50006200</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-2.40015000</td>
<td>2.50074400</td>
<td>-1.69767100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.34194200</td>
<td>-2.05199800</td>
<td>-0.41737300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.53881200</td>
<td>-2.41484900</td>
<td>0.23221700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.27852100</td>
<td>0.13910400</td>
<td>-0.37513800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.98604300</td>
<td>0.59282300</td>
<td>-1.07740500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.62273900</td>
<td>-1.33441600</td>
<td>-0.09550700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.02419000</td>
<td>-1.82862600</td>
<td>-0.98982600</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-2.49910600</td>
<td>-2.03422700</td>
<td>0.42194700</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-3.44065300</td>
<td>0.81726400</td>
<td>0.90207300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.20787200</td>
<td>0.07083100</td>
<td>1.75236300</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-4.48505500</td>
<td>0.44048300</td>
<td>2.86210400</td>
<td></td>
</tr>
</tbody>
</table>
C  -4.62464900  -1.21472800   1.04429900
H  -5.64840000  -1.09255200   0.66978000
H  -4.60106700  -2.06798500   1.72448300
C  -1.48960800  -3.03780400  -1.58821000
H  -0.53606100  -3.12057100  -2.11467400
H  -1.77411700  -4.02052100  -1.19874900
H  -2.25322300  -2.70897500  -2.30171100
H   6.40159800  -0.30694400   1.58382700
C   5.38609900   0.05978400   1.77670600
Si  4.17242500  -0.72825400   0.56064100
H   5.13159600  -0.19414100   2.81146500
H   5.40943000   1.15185200   1.69405300
O  2.55401600  -0.27601800   0.00458200
C  4.48565400  -2.59838400   0.72070500
C  4.11673400   3.19402500   0.47551100
C  3.70113600  -0.58760000  -1.85936600
H  3.40232600   0.90974300  -1.32649200
H  3.46400700  -3.05088600   0.43596800
H  3.33683000  -2.99843100   0.06448100
H  5.07361600  -3.05088600   0.43596800
C  2.31393000   2.12419900   0.73960400
C  0.07393900   3.04426900   0.24659400
H  3.38741800   2.29566600   0.73789300
C  1.84149700   0.82462600   0.89631100
H  0.47809300   2.30831300   0.82707000
H  0.79035600   0.65621000   1.11349700
H  1.90779200   4.15737900   0.25404500
H  1.51316300   3.32378000  -0.02858200

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1193.642522, -1193.24141, -1193.21369, -1193.299096

TS-exo-anti-near for 7 + 6
C  -0.78905800   0.99456900   1.34039700
C  -0.08576100  -0.19221800   0.90881100
C  1.26303300   0.06807000   0.28057900
C  1.85380500   1.21981600   0.21773400
C  1.20714100   2.41235500   0.84853900
C  -0.22478300   2.86604800   1.26357200
H  -1.68507000   0.82896300   1.92627100
H  -0.50542700   3.01687000   2.01668600
<table>
<thead>
<tr>
<th>Element</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>1.83520500</td>
<td>3.45416000</td>
<td>1.00460100</td>
</tr>
<tr>
<td>O</td>
<td>-0.54836100</td>
<td>-1.33689100</td>
<td>1.00460100</td>
</tr>
<tr>
<td>C</td>
<td>3.21872700</td>
<td>1.42359100</td>
<td>-0.40298100</td>
</tr>
<tr>
<td>H</td>
<td>3.82554000</td>
<td>1.99214000</td>
<td>0.30862500</td>
</tr>
<tr>
<td>C</td>
<td>1.93890700</td>
<td>-1.20937500</td>
<td>-0.29011800</td>
</tr>
<tr>
<td>H</td>
<td>1.20941800</td>
<td>-1.79712900</td>
<td>-0.85931200</td>
</tr>
<tr>
<td>C</td>
<td>3.17547900</td>
<td>-0.87646400</td>
<td>-1.14279700</td>
</tr>
<tr>
<td>H</td>
<td>3.21872700</td>
<td>1.42359100</td>
<td>-0.40298100</td>
</tr>
<tr>
<td>C</td>
<td>4.21629500</td>
<td>-3.38737200</td>
<td>1.14033100</td>
</tr>
<tr>
<td>H</td>
<td>3.75911100</td>
<td>-2.90080200</td>
<td>-1.69950000</td>
</tr>
<tr>
<td>C</td>
<td>5.09323200</td>
<td>-1.93282900</td>
<td>-1.03141400</td>
</tr>
<tr>
<td>C</td>
<td>3.15218500</td>
<td>2.22080300</td>
<td>0.42606300</td>
</tr>
<tr>
<td>C</td>
<td>-3.89463900</td>
<td>-1.40950100</td>
<td>-0.22879600</td>
</tr>
<tr>
<td>H</td>
<td>-5.42411900</td>
<td>-1.10352900</td>
<td>-2.18871300</td>
</tr>
<tr>
<td>H</td>
<td>-5.82034600</td>
<td>0.06448300</td>
<td>-0.91759300</td>
</tr>
<tr>
<td>O</td>
<td>-2.62416400</td>
<td>-0.46068600</td>
<td>-0.97026800</td>
</tr>
<tr>
<td>C</td>
<td>-3.98184500</td>
<td>-1.06414800</td>
<td>1.62105800</td>
</tr>
<tr>
<td>C</td>
<td>-3.34088800</td>
<td>-3.16507400</td>
<td>-0.59683200</td>
</tr>
<tr>
<td>C</td>
<td>-2.41314600</td>
<td>3.13755100</td>
<td>-0.20379700</td>
</tr>
<tr>
<td>H</td>
<td>-3.01154700</td>
<td>-1.28480400</td>
<td>2.07591700</td>
</tr>
<tr>
<td>H</td>
<td>-4.25045000</td>
<td>-0.02717800</td>
<td>1.84817800</td>
</tr>
<tr>
<td>H</td>
<td>-4.73778000</td>
<td>-1.71158700</td>
<td>2.08182300</td>
</tr>
<tr>
<td>H</td>
<td>-3.26640500</td>
<td>-3.34199200</td>
<td>-1.67531500</td>
</tr>
<tr>
<td>H</td>
<td>-2.35606500</td>
<td>-3.33713900</td>
<td>-0.15053500</td>
</tr>
<tr>
<td>H</td>
<td>-4.04212900</td>
<td>-3.89820400</td>
<td>-0.18184600</td>
</tr>
<tr>
<td>C</td>
<td>-2.98648300</td>
<td>1.88350600</td>
<td>-0.42742200</td>
</tr>
<tr>
<td>C</td>
<td>-1.02804300</td>
<td>3.37031700</td>
<td>-0.26468000</td>
</tr>
<tr>
<td>C</td>
<td>-4.03903800</td>
<td>1.73137300</td>
<td>-0.20207000</td>
</tr>
<tr>
<td>C</td>
<td>-2.21849000</td>
<td>0.78640700</td>
<td>-0.81598400</td>
</tr>
<tr>
<td>H</td>
<td>-0.45264700</td>
<td>2.86616500</td>
<td>-1.03775100</td>
</tr>
<tr>
<td>H</td>
<td>-1.24064900</td>
<td>0.94572200</td>
<td>-1.26158600</td>
</tr>
<tr>
<td>H</td>
<td>-0.65549300</td>
<td>4.36703400</td>
<td>-0.04494500</td>
</tr>
<tr>
<td>H</td>
<td>-3.04815100</td>
<td>3.91105700</td>
<td>0.22367800</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
TS-exo-anti-dist for 7 + 6

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-0.05775900</td>
<td>2.22363100</td>
<td>0.78742700</td>
</tr>
<tr>
<td>C</td>
<td>-1.47875800</td>
<td>1.97946000</td>
<td>0.36727300</td>
</tr>
<tr>
<td>C</td>
<td>-1.87064400</td>
<td>0.57190900</td>
<td>0.07467800</td>
</tr>
<tr>
<td>C</td>
<td>-1.03555600</td>
<td>-0.46083700</td>
<td>0.32566000</td>
</tr>
<tr>
<td>C</td>
<td>0.29681300</td>
<td>0.94554100</td>
<td>2.22363100</td>
</tr>
<tr>
<td>C</td>
<td>-1.41523300</td>
<td>-1.88694200</td>
<td>0.00589000</td>
</tr>
<tr>
<td>C</td>
<td>-3.23483800</td>
<td>0.34493200</td>
<td>-0.51620000</td>
</tr>
<tr>
<td>C</td>
<td>-3.42710400</td>
<td>1.08338100</td>
<td>-1.30339900</td>
</tr>
<tr>
<td>C</td>
<td>-3.44012900</td>
<td>-1.08772500</td>
<td>-1.04072400</td>
</tr>
<tr>
<td>C</td>
<td>-5.26763900</td>
<td>-0.37970800</td>
<td>0.32658200</td>
</tr>
<tr>
<td>C</td>
<td>-4.94108500</td>
<td>-1.27029400</td>
<td>-0.86965100</td>
</tr>
<tr>
<td>C</td>
<td>-5.49520200</td>
<td>-0.90525200</td>
<td>-1.74315400</td>
</tr>
<tr>
<td>C</td>
<td>-5.22654400</td>
<td>-2.30679900</td>
<td>-0.61890400</td>
</tr>
<tr>
<td>C</td>
<td>-0.61019900</td>
<td>-2.44118700</td>
<td>-1.18252000</td>
</tr>
<tr>
<td>C</td>
<td>0.45956700</td>
<td>-2.40306300</td>
<td>-0.95971900</td>
</tr>
<tr>
<td>H</td>
<td>-0.89934700</td>
<td>-3.48131200</td>
<td>-1.36209200</td>
</tr>
<tr>
<td>H</td>
<td>-0.79586500</td>
<td>-1.86694900</td>
<td>-2.09749200</td>
</tr>
<tr>
<td>H</td>
<td>6.80196500</td>
<td>-0.66661300</td>
<td>-0.33915800</td>
</tr>
<tr>
<td>H</td>
<td>5.88895900</td>
<td>-0.29816200</td>
<td>-0.82248400</td>
</tr>
<tr>
<td>Si</td>
<td>4.36878700</td>
<td>-0.89857000</td>
<td>0.12762400</td>
</tr>
<tr>
<td>H</td>
<td>5.95473400</td>
<td>0.79464300</td>
<td>-0.86007400</td>
</tr>
<tr>
<td>H</td>
<td>6.88457900</td>
<td>-0.67083400</td>
<td>-1.85262600</td>
</tr>
<tr>
<td>O</td>
<td>2.94943700</td>
<td>-0.44561300</td>
<td>-0.79377700</td>
</tr>
<tr>
<td>C</td>
<td>4.24228700</td>
<td>-2.77199200</td>
<td>0.14469300</td>
</tr>
<tr>
<td>C</td>
<td>4.27265400</td>
<td>-0.16330100</td>
<td>1.85915900</td>
</tr>
<tr>
<td>C</td>
<td>2.80806500</td>
<td>1.98361500</td>
<td>-0.80197700</td>
</tr>
<tr>
<td>H</td>
<td>3.30869100</td>
<td>-3.07484200</td>
<td>0.62991200</td>
</tr>
<tr>
<td>H</td>
<td>4.24985800</td>
<td>-3.18038600</td>
<td>-0.87168200</td>
</tr>
<tr>
<td>H</td>
<td>5.07758300</td>
<td>-3.22055700</td>
<td>0.69474300</td>
</tr>
<tr>
<td>H</td>
<td>4.33669400</td>
<td>0.92974700</td>
<td>1.86064000</td>
</tr>
</tbody>
</table>
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1193.639211, -1193.237877, -1193.210324, -1193.29458

TS-endo-syn-near for 7 + 6

<table>
<thead>
<tr>
<th></th>
<th>E</th>
<th>E+ZPE</th>
<th>Enthalpy</th>
<th>Free Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.37016500</td>
<td>-2.03470400</td>
<td>-0.99517900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.14073800</td>
<td>-0.64113900</td>
<td>-1.25155600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.15868000</td>
<td>-0.07838700</td>
<td>-0.75046100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.17025100</td>
<td>-0.86139800</td>
<td>-0.31302300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.99022400</td>
<td>-2.33515900</td>
<td>-0.21926000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.59113300</td>
<td>-2.85123600</td>
<td>-0.36586700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.26634100</td>
<td>-2.47595100</td>
<td>-1.42071200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.56528300</td>
<td>-3.91948700</td>
<td>-0.57402900</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-2.93416900</td>
<td>-3.08563600</td>
<td>0.01002500</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>0.92081800</td>
<td>0.09215900</td>
<td>-1.88753800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.51555700</td>
<td>-0.28779100</td>
<td>0.08304800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.82027600</td>
<td>-0.74944400</td>
<td>1.02823000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.31878900</td>
<td>1.41384500</td>
<td>-0.82592700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.91582400</td>
<td>1.77479300</td>
<td>-1.77767800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.75893200</td>
<td>1.90035900</td>
<td>-0.59195300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.32945100</td>
<td>1.93480200</td>
<td>-1.52929700</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-3.41585500</td>
<td>1.10505700</td>
<td>0.38649900</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.53704300</td>
<td>2.02880100</td>
<td>0.23622300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.19970800</td>
<td>3.09841000</td>
<td>0.76640900</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.73635600</td>
<td>3.76713100</td>
<td>1.65239800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.53269900</td>
<td>3.26498300</td>
<td>0.04337700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.42700800</td>
<td>4.05093500</td>
<td>-0.71454300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.32692400</td>
<td>3.55066300</td>
<td>0.73531600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.60997600</td>
<td>-0.57433800</td>
<td>-0.95782400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.74943700</td>
<td>-1.65372400</td>
<td>-1.05442600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-5.55034200</td>
<td>-0.11942300</td>
<td>-0.63023500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.34902700</td>
<td>-0.17051200</td>
<td>-1.94225000</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.99836300</td>
<td>-0.96410400</td>
<td>-2.07008500</td>
<td></td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.09679100</td>
<td>-1.09625900</td>
<td>-1.45962100</td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>3.93586600</td>
<td>0.34352800</td>
<td>-0.25465800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.22775300</td>
<td>-1.11228900</td>
<td>-2.12368400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.18514700</td>
<td>-2.06650500</td>
<td>-0.95705300</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>2.52150900</td>
<td>0.13107500</td>
<td>0.75874700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.38909500</td>
<td>0.39927700</td>
<td>0.95107100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.63613900</td>
<td>1.98716500</td>
<td>-1.10612300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.16997300</td>
<td>-1.85537800</td>
<td>2.18176700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.24893200</td>
<td>1.18673600</td>
<td>1.69940600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.51268200</td>
<td>-0.55195600</td>
<td>1.48137100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>6.32430700</td>
<td>0.60649100</td>
<td>0.41704700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.71218000</td>
<td>1.92357400</td>
<td>-1.68817700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.52810100</td>
<td>2.79371800</td>
<td>-0.37305200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.46410400</td>
<td>2.24378100</td>
<td>-1.77735800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.73064200</td>
<td>-0.82325800</td>
<td>1.91853800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.13962400</td>
<td>-3.12237900</td>
<td>1.56390700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.51464000</td>
<td>0.17884100</td>
<td>2.27809500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.83980300</td>
<td>-0.94442600</td>
<td>1.08729200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.82423200</td>
<td>-3.57390600</td>
<td>1.34409500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.23699800</td>
<td>-1.91251000</td>
<td>0.79044900</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.05465900</td>
<td>-1.59685200</td>
<td>2.75991700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.89579700</td>
<td>-3.84486800</td>
<td>1.86132300</td>
<td></td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1193.648738, -1193.247588, -1193.219978, -1193.304336

**TS-endo-syn-dist for 7 + 6**

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.19872600</td>
<td>2.33598100</td>
<td>-1.42852200</td>
</tr>
<tr>
<td>C</td>
<td>-1.60534900</td>
<td>1.83427900</td>
<td>-1.31487600</td>
</tr>
<tr>
<td>C</td>
<td>-1.75774000</td>
<td>0.41554300</td>
<td>-0.90396600</td>
</tr>
<tr>
<td>C</td>
<td>-0.72874500</td>
<td>-0.45618400</td>
<td>-1.01526500</td>
</tr>
<tr>
<td>C</td>
<td>0.63528200</td>
<td>-0.01740300</td>
<td>-1.46963500</td>
</tr>
<tr>
<td>C</td>
<td>0.83232200</td>
<td>1.39553100</td>
<td>-1.62512600</td>
</tr>
<tr>
<td>H</td>
<td>-0.12927500</td>
<td>3.28555700</td>
<td>-1.95656500</td>
</tr>
<tr>
<td>H</td>
<td>1.79774000</td>
<td>1.71725300</td>
<td>-2.00531400</td>
</tr>
<tr>
<td>O</td>
<td>1.51937400</td>
<td>-0.87183900</td>
<td>-1.68651200</td>
</tr>
<tr>
<td>O</td>
<td>-2.57379400</td>
<td>2.54993400</td>
<td>-1.53910600</td>
</tr>
<tr>
<td>C</td>
<td>-0.90688200</td>
<td>-1.91959300</td>
<td>-0.68189900</td>
</tr>
<tr>
<td>H</td>
<td>-0.05136000</td>
<td>-2.22881700</td>
<td>-0.07323100</td>
</tr>
<tr>
<td>C</td>
<td>-3.11469200</td>
<td>-0.02180500</td>
<td>-0.43496600</td>
</tr>
<tr>
<td>H</td>
<td>-3.88860500</td>
<td>0.39499700</td>
<td>-1.08803000</td>
</tr>
<tr>
<td>C</td>
<td>-3.25645000</td>
<td>-1.54623000</td>
<td>-0.28690000</td>
</tr>
<tr>
<td>H</td>
<td>-3.60220400</td>
<td>-2.00916200</td>
<td>-1.22044200</td>
</tr>
</tbody>
</table>
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1193.651527, -1193.250079, -1193.222575, -1193.306234

TS-endo-anti-near for 7 + 6

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.72716300</td>
<td>1.22869900</td>
<td>-1.59089400</td>
</tr>
<tr>
<td>C</td>
<td>0.25585500</td>
<td>-0.02889800</td>
<td>-1.07411900</td>
</tr>
<tr>
<td>C</td>
<td>-1.08005600</td>
<td>-0.01556700</td>
<td>-0.39114900</td>
</tr>
<tr>
<td>C</td>
<td>-1.85636100</td>
<td>1.08977800</td>
<td>-0.32423500</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>-1.42859000</td>
<td>2.35168500</td>
<td>-0.98927000</td>
</tr>
<tr>
<td>C</td>
<td>-0.01007400</td>
<td>2.42324600</td>
<td>-1.47002200</td>
</tr>
<tr>
<td>H</td>
<td>1.62498200</td>
<td>1.20227000</td>
<td>-2.20089500</td>
</tr>
<tr>
<td>H</td>
<td>0.13113700</td>
<td>3.19092900</td>
<td>-2.22992100</td>
</tr>
<tr>
<td>O</td>
<td>-2.20442200</td>
<td>3.29116000</td>
<td>-1.13191800</td>
</tr>
<tr>
<td>O</td>
<td>-0.88474000</td>
<td>-1.09693400</td>
<td>-1.17053700</td>
</tr>
<tr>
<td>C</td>
<td>-3.22232800</td>
<td>1.08366200</td>
<td>0.32837800</td>
</tr>
<tr>
<td>H</td>
<td>-3.93067400</td>
<td>-1.50820000</td>
<td>1.12490900</td>
</tr>
<tr>
<td>C</td>
<td>-1.53163500</td>
<td>1.30607900</td>
<td>0.23590300</td>
</tr>
<tr>
<td>H</td>
<td>-0.69624600</td>
<td>-1.74601300</td>
<td>0.79291900</td>
</tr>
<tr>
<td>C</td>
<td>-2.77719500</td>
<td>-1.15082000</td>
<td>1.12490900</td>
</tr>
<tr>
<td>H</td>
<td>-2.51041400</td>
<td>-0.85638300</td>
<td>2.14915100</td>
</tr>
<tr>
<td>O</td>
<td>-3.70324600</td>
<td>-0.24195000</td>
<td>0.54569900</td>
</tr>
<tr>
<td>O</td>
<td>-1.92012800</td>
<td>-2.25694800</td>
<td>-0.78751100</td>
</tr>
<tr>
<td>C</td>
<td>-2.98924000</td>
<td>-2.99893100</td>
<td>-0.37201100</td>
</tr>
<tr>
<td>O</td>
<td>-3.46235900</td>
<td>-3.87995100</td>
<td>-1.03902500</td>
</tr>
<tr>
<td>C</td>
<td>-3.40954800</td>
<td>-2.53044700</td>
<td>1.01923700</td>
</tr>
<tr>
<td>H</td>
<td>-3.49611700</td>
<td>-2.51192800</td>
<td>1.11979700</td>
</tr>
<tr>
<td>C</td>
<td>-2.68389000</td>
<td>1.92039600</td>
<td>1.61730800</td>
</tr>
<tr>
<td>H</td>
<td>-3.03366800</td>
<td>2.96482700</td>
<td>1.39294500</td>
</tr>
<tr>
<td>C</td>
<td>-4.27459600</td>
<td>1.87209500</td>
<td>2.04494200</td>
</tr>
<tr>
<td>C</td>
<td>-2.55483300</td>
<td>1.55372100</td>
<td>2.36396200</td>
</tr>
<tr>
<td>C</td>
<td>4.96855500</td>
<td>-1.13590000</td>
<td>-2.05291200</td>
</tr>
<tr>
<td>C</td>
<td>4.17618600</td>
<td>-0.52990300</td>
<td>-1.59646700</td>
</tr>
<tr>
<td>Si</td>
<td>3.93550300</td>
<td>-1.06238200</td>
<td>0.19422200</td>
</tr>
<tr>
<td>H</td>
<td>4.47515100</td>
<td>0.52020200</td>
<td>-1.69490900</td>
</tr>
<tr>
<td>H</td>
<td>3.24921100</td>
<td>-0.69489900</td>
<td>-2.15239400</td>
</tr>
<tr>
<td>O</td>
<td>2.69372500</td>
<td>-0.08904200</td>
<td>0.96724000</td>
</tr>
<tr>
<td>C</td>
<td>3.30569600</td>
<td>-2.82035300</td>
<td>0.36833100</td>
</tr>
<tr>
<td>C</td>
<td>5.49414800</td>
<td>-0.74853900</td>
<td>1.21557400</td>
</tr>
<tr>
<td>C</td>
<td>1.30762100</td>
<td>1.72309600</td>
<td>1.49077900</td>
</tr>
<tr>
<td>H</td>
<td>3.16617700</td>
<td>-3.08691700</td>
<td>1.42187800</td>
</tr>
<tr>
<td>H</td>
<td>2.34582900</td>
<td>-2.91349400</td>
<td>-0.14791800</td>
</tr>
<tr>
<td>H</td>
<td>4.01195000</td>
<td>-3.53619100</td>
<td>-0.06857100</td>
</tr>
<tr>
<td>H</td>
<td>5.81694500</td>
<td>0.29691900</td>
<td>1.15116700</td>
</tr>
<tr>
<td>H</td>
<td>5.33161300</td>
<td>-0.98645700</td>
<td>2.27244800</td>
</tr>
<tr>
<td>H</td>
<td>6.32031300</td>
<td>-1.37334600</td>
<td>0.85523900</td>
</tr>
<tr>
<td>C</td>
<td>0.63078800</td>
<td>2.90125200</td>
<td>1.17508000</td>
</tr>
<tr>
<td>C</td>
<td>2.27030800</td>
<td>1.12680100</td>
<td>0.68332800</td>
</tr>
<tr>
<td>H</td>
<td>-0.17977900</td>
<td>3.19652000</td>
<td>1.83763700</td>
</tr>
<tr>
<td>C</td>
<td>0.76057300</td>
<td>3.58864600</td>
<td>-0.04920200</td>
</tr>
<tr>
<td>H</td>
<td>2.77704800</td>
<td>1.67293300</td>
<td>-0.10794100</td>
</tr>
<tr>
<td>H</td>
<td>1.73917200</td>
<td>3.63718200</td>
<td>-0.51948800</td>
</tr>
</tbody>
</table>
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy

-1193.645323, -1193.244245, -1193.216702, -1193.300551

| TS-endo-anti-dist for 7 + 6 | C   | 0.154690000 2.37104600 -0.94835200 |
|                            | C   | 1.527867000 2.01431300 -0.45245100 |
|                            | C   | 1.774207000 0.58568200 -0.13420700 |
|                            | C   | 0.847023000 -0.36676200 -0.38830300 |
|                            | C   | -0.447494000 -0.04694600 -1.08566800 |
|                            | C   | -0.716927000 1.34092400 -1.34440900 |
|                            | H   | 0.144131000 3.29722300 -1.51998100 |
|                            | H   | 1.527867000 2.37104600 -0.94835200 |
|                            | O   | -1.191103000 -0.97679700 -1.45304800 |
|                            | O   | 2.389645000 2.86747400 -0.28025100 |
|                            | C   | 1.095510000 -1.81855600 -0.05229100 |
|                            | H   | 0.807229000 -2.41248600 -0.92446800 |
|                            | C   | 3.106515000 0.23819100 0.47041600 |
|                            | H   | 3.356362000 0.95780600 1.25884500 |
|                            | C   | 3.182571000 -1.20704400 0.99392700 |
|                            | H   | 2.823403000 -1.28086400 2.02943000 |
|                            | O   | 2.483085000 -2.09737400 0.13608300 |
|                            | O   | 4.147498000 0.32694100 -0.53699300 |
|                            | C   | 5.073090000 -0.66202300 -0.36282900 |
|                            | O   | 3.021161000 -0.18773600 0.83155000 |
|                            | C   | 5.466184900 -1.52323200 0.82881100 |
|                            | H   | 5.242598000 -1.21211400 1.70587200 |
|                            | H   | 4.853528000 -2.58069900 0.63879500 |
|                            | C   | 0.251884000 -2.28773100 1.14524500 |
|                            | H   | -0.810570000 -2.14324400 0.93434400 |
|                            | H   | 0.440596000 -3.35069400 1.32558400 |
|                            | H   | 0.502312000 -1.73107200 2.05538100 |
|                            | H   | -5.232597000 -0.18449200 -2.40788700 |
|                            | C   | -4.388564000 0.17452700 -1.80639000 |
|                            | Si  | -4.357674000 -0.74647200 -0.16340300 |
| H                           | -3.463055000 -0.06238700 -2.35358300 |
| H                           | -4.511326000 1.25771100 -1.69190300 |
| O                           | -3.021161000 -0.18773600 0.83155000 |
| C                           | -5.904872000 -0.39086100 0.86012000 |
| C                           | -4.030737000 -2.58253200 -0.36801000 |
| C                           | -0.577954000 2.36479900 1.72084500 |
H     -5.85020600 -0.87243700  1.84247700
H     -6.04470100  0.68444400  1.01954200
H     -6.79881800 -0.76983900  0.35034400
H     -3.08108600 -2.72625500 -0.89202800
H     -3.97365100 -3.08658600  0.60299400
H     -4.82793500 -3.06096500 -0.94890000
C     -1.42186600  1.25162700  1.76582800
C     -0.55781700  3.30860400  0.67803100
H     -1.24660100  0.48145100  2.51250700
C     -2.40944700  0.98211300  0.82775200
H     -1.49342400  3.58141200  0.19754500
H     -2.77922200  1.74529700  0.14738800
H      0.14746000  4.13144900  0.75810300
H      0.23316400  2.39669300  2.44516900

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1193.646432, -1193.245412, -1193.217827, -1193.302163

Diene 9
C     -0.03581000 -0.33406600 -0.04162600
C      1.17194700  0.49328600 -0.00881700
H      0.97315300  1.55592600 -0.01217500
C     -0.11304800 -1.67906700 -0.00637500
H     -1.06310300 -2.19728700 -0.05653400
H      0.78179700 -2.27931700  0.06192900
C      2.46348700  0.09162400  0.01983200
O      2.81472000 -1.21038800  0.05059900
C      3.54670400  0.90929000  0.03203700
C      3.33236600  2.31363100 -0.01891400
C      4.32511100  2.76669500 -0.02023500
H      2.79224300  2.59441100 -0.93080400
H      2.76852400  2.65611100  0.85684600
C      4.19617200 -1.56260200 -0.04816600
H      4.77092900 -1.17034500  0.79612100
H      4.21065800 -2.65357500 -0.03163200
H      4.63614600 -1.19963100 -0.98252500
O     -1.13812000  0.49205500 -0.12266200
Si     -2.80059300  0.10933000  0.00351000
C     -3.17953300 -0.73232700  1.65599600
H     -2.63630300 -1.67491200  1.77196600
H     -2.90246200 -0.08418700  2.49495100
H     -4.25230100 -0.94568500  1.73754300
C     -3.62659600  1.80420700 -0.07987300

S27
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-583.334415, -583.074626, -583.055403, -583.123043

TS-exo-syn-near for 9 + 6

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.28202400</td>
<td>0.60548200</td>
<td>1.60454500</td>
</tr>
<tr>
<td>C</td>
<td>-0.95510400</td>
<td>-0.08016000</td>
<td>1.67049900</td>
</tr>
<tr>
<td>C</td>
<td>-2.08824400</td>
<td>0.49645600</td>
<td>0.85734500</td>
</tr>
<tr>
<td>C</td>
<td>-1.98158500</td>
<td>1.65047300</td>
<td>0.16446300</td>
</tr>
<tr>
<td>C</td>
<td>-0.68281800</td>
<td>2.38028000</td>
<td>0.13207700</td>
</tr>
<tr>
<td>C</td>
<td>0.51906300</td>
<td>1.67181900</td>
<td>0.70018400</td>
</tr>
<tr>
<td>H</td>
<td>1.07592000</td>
<td>0.26285200</td>
<td>2.26044700</td>
</tr>
<tr>
<td>H</td>
<td>1.31232800</td>
<td>2.37505100</td>
<td>0.95039400</td>
</tr>
<tr>
<td>O</td>
<td>-0.59357500</td>
<td>3.49469100</td>
<td>-0.37391400</td>
</tr>
<tr>
<td>O</td>
<td>-1.18876700</td>
<td>-1.09365600</td>
<td>2.37157600</td>
</tr>
<tr>
<td>C</td>
<td>-3.15006200</td>
<td>2.25469800</td>
<td>-0.5866200</td>
</tr>
<tr>
<td>H</td>
<td>-2.80410100</td>
<td>2.55182400</td>
<td>-1.58231900</td>
</tr>
<tr>
<td>C</td>
<td>-3.38885700</td>
<td>-0.25528700</td>
<td>0.89441300</td>
</tr>
<tr>
<td>H</td>
<td>-3.59246600</td>
<td>-0.58170700</td>
<td>1.91871500</td>
</tr>
<tr>
<td>C</td>
<td>-4.57311200</td>
<td>0.51063100</td>
<td>0.28107000</td>
</tr>
<tr>
<td>H</td>
<td>-5.07925100</td>
<td>1.13472200</td>
<td>1.02911600</td>
</tr>
<tr>
<td>O</td>
<td>-4.16184800</td>
<td>1.27589600</td>
<td>-0.84325200</td>
</tr>
<tr>
<td>O</td>
<td>-3.27164600</td>
<td>-1.46066500</td>
<td>0.08095500</td>
</tr>
<tr>
<td>C</td>
<td>-4.41408100</td>
<td>-1.68885300</td>
<td>-0.62607400</td>
</tr>
<tr>
<td>O</td>
<td>-4.52050500</td>
<td>-2.61952700</td>
<td>-1.38342500</td>
</tr>
<tr>
<td>C</td>
<td>-5.43691400</td>
<td>-0.61779700</td>
<td>-0.26804300</td>
</tr>
<tr>
<td>H</td>
<td>-6.11279100</td>
<td>-1.01838300</td>
<td>0.49770300</td>
</tr>
<tr>
<td>H</td>
<td>-6.02630800</td>
<td>-0.32134300</td>
<td>-1.13734000</td>
</tr>
<tr>
<td>C</td>
<td>-3.72496000</td>
<td>3.50093000</td>
<td>0.10678500</td>
</tr>
<tr>
<td>H</td>
<td>-2.95873200</td>
<td>4.27741800</td>
<td>0.15659200</td>
</tr>
<tr>
<td>H</td>
<td>-4.57869200</td>
<td>3.87487900</td>
<td>-0.46728500</td>
</tr>
<tr>
<td>H</td>
<td>-4.05789900</td>
<td>3.27816800</td>
<td>1.12687400</td>
</tr>
<tr>
<td>H</td>
<td>6.49738600</td>
<td>-0.35227700</td>
<td>1.76476300</td>
</tr>
<tr>
<td>C</td>
<td>5.42650800</td>
<td>-0.22394700</td>
<td>1.56423100</td>
</tr>
<tr>
<td>Si</td>
<td>5.18616400</td>
<td>0.42355600</td>
<td>-0.19796500</td>
</tr>
<tr>
<td>H</td>
<td>4.94474800</td>
<td>-1.19206800</td>
<td>1.73739100</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>5.03461600</td>
<td>0.48461100</td>
<td>2.3022600</td>
</tr>
<tr>
<td>O</td>
<td>3.55966000</td>
<td>0.97086700</td>
<td>-0.43432100</td>
</tr>
<tr>
<td>C</td>
<td>6.18564300</td>
<td>1.99514200</td>
<td>-0.46165000</td>
</tr>
<tr>
<td>C</td>
<td>5.59750000</td>
<td>-0.90063400</td>
<td>-1.47997000</td>
</tr>
<tr>
<td>C</td>
<td>2.25760400</td>
<td>-1.01340500</td>
<td>-0.15151800</td>
</tr>
<tr>
<td>H</td>
<td>6.02928300</td>
<td>2.39563600</td>
<td>-1.46889000</td>
</tr>
<tr>
<td>H</td>
<td>5.89550700</td>
<td>2.77033200</td>
<td>0.25578100</td>
</tr>
<tr>
<td>H</td>
<td>7.25786000</td>
<td>1.80424900</td>
<td>-0.33607700</td>
</tr>
<tr>
<td>H</td>
<td>4.94535900</td>
<td>-1.77511600</td>
<td>-1.39032800</td>
</tr>
<tr>
<td>H</td>
<td>5.49307800</td>
<td>-0.50792100</td>
<td>-2.49723100</td>
</tr>
<tr>
<td>H</td>
<td>6.63349500</td>
<td>-1.23796300</td>
<td>-1.35578800</td>
</tr>
<tr>
<td>C</td>
<td>2.39835200</td>
<td>0.31028300</td>
<td>-0.62304800</td>
</tr>
<tr>
<td>C</td>
<td>1.18553900</td>
<td>-1.86604900</td>
<td>-0.39752000</td>
</tr>
<tr>
<td>H</td>
<td>3.00264400</td>
<td>-1.38208000</td>
<td>0.54226500</td>
</tr>
<tr>
<td>C</td>
<td>1.30357200</td>
<td>1.12283500</td>
<td>-1.00728400</td>
</tr>
<tr>
<td>O</td>
<td>0.39838600</td>
<td>-1.69381700</td>
<td>-1.44405000</td>
</tr>
<tr>
<td>C</td>
<td>-0.74926200</td>
<td>-2.56541700</td>
<td>-1.62631200</td>
</tr>
<tr>
<td>H</td>
<td>-0.41137700</td>
<td>-3.58101400</td>
<td>-1.84291800</td>
</tr>
<tr>
<td>H</td>
<td>-1.39064400</td>
<td>-2.54610500</td>
<td>-0.74703600</td>
</tr>
<tr>
<td>H</td>
<td>-1.27474700</td>
<td>-2.14752400</td>
<td>-2.48355400</td>
</tr>
<tr>
<td>O</td>
<td>0.93809800</td>
<td>-2.98066500</td>
<td>0.27806000</td>
</tr>
<tr>
<td>C</td>
<td>1.33011400</td>
<td>-3.09925900</td>
<td>1.66326300</td>
</tr>
<tr>
<td>H</td>
<td>0.96804100</td>
<td>-4.08164300</td>
<td>1.96631300</td>
</tr>
<tr>
<td>H</td>
<td>2.41861600</td>
<td>-3.06545900</td>
<td>1.76746000</td>
</tr>
<tr>
<td>H</td>
<td>0.83110700</td>
<td>-2.31780800</td>
<td>2.24217200</td>
</tr>
<tr>
<td>H</td>
<td>0.46449700</td>
<td>0.61293100</td>
<td>-1.46311300</td>
</tr>
<tr>
<td>H</td>
<td>1.55227800</td>
<td>2.08185700</td>
<td>-1.45264500</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K

E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.695367, -1422.228484, -1422.195322, -1422.293187

**TS-exo-syn-dist for 9 + 6**

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.46789200</td>
<td>-0.61588300</td>
<td>-1.87350700</td>
</tr>
<tr>
<td>C</td>
<td>0.89976100</td>
<td>-1.24598700</td>
<td>-1.84548500</td>
</tr>
<tr>
<td>C</td>
<td>1.98054900</td>
<td>-0.44788300</td>
<td>-1.20721400</td>
</tr>
<tr>
<td>C</td>
<td>1.84335600</td>
<td>0.88677000</td>
<td>-1.04462200</td>
</tr>
<tr>
<td>C</td>
<td>0.55128200</td>
<td>1.60381800</td>
<td>-1.34132600</td>
</tr>
<tr>
<td>C</td>
<td>-0.52329900</td>
<td>0.80589500</td>
<td>-1.78971900</td>
</tr>
<tr>
<td>H</td>
<td>-1.11931000</td>
<td>-1.08787400</td>
<td>-2.60788900</td>
</tr>
<tr>
<td>H</td>
<td>-1.44766300</td>
<td>1.32309000</td>
<td>-2.03293700</td>
</tr>
<tr>
<td>O</td>
<td>0.51104700</td>
<td>2.84888900</td>
<td>-1.15255200</td>
</tr>
<tr>
<td>O</td>
<td>1.11866300</td>
<td>-2.35771200</td>
<td>-2.31083500</td>
</tr>
<tr>
<td>C</td>
<td>2.98241600</td>
<td>1.73046200</td>
<td>-0.52713300</td>
</tr>
<tr>
<td>S30</td>
<td>2.57480800</td>
<td>2.43351300</td>
<td>0.20469500</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
<td>-------------</td>
<td>-------------</td>
</tr>
<tr>
<td>H</td>
<td>3.23316900</td>
<td>-1.16412800</td>
<td>-0.80624300</td>
</tr>
<tr>
<td>C</td>
<td>3.51965800</td>
<td>-1.89760700</td>
<td>-1.56624300</td>
</tr>
<tr>
<td>H</td>
<td>4.39781800</td>
<td>-0.22792700</td>
<td>-0.44412900</td>
</tr>
<tr>
<td>C</td>
<td>5.00364300</td>
<td>0.02264000</td>
<td>-1.32440900</td>
</tr>
<tr>
<td>O</td>
<td>3.92919000</td>
<td>0.94557500</td>
<td>0.21143800</td>
</tr>
<tr>
<td>O</td>
<td>2.96518200</td>
<td>-1.90765900</td>
<td>0.42837300</td>
</tr>
<tr>
<td>C</td>
<td>4.01685000</td>
<td>-1.81472100</td>
<td>1.28693100</td>
</tr>
<tr>
<td>H</td>
<td>5.00364300</td>
<td>0.02264000</td>
<td>-1.32440900</td>
</tr>
<tr>
<td>O</td>
<td>3.92919000</td>
<td>0.94557500</td>
<td>0.21143800</td>
</tr>
<tr>
<td>O</td>
<td>5.14032000</td>
<td>-1.03654200</td>
<td>0.61148200</td>
</tr>
<tr>
<td>H</td>
<td>5.83991200</td>
<td>-1.74672200</td>
<td>0.15338700</td>
</tr>
<tr>
<td>H</td>
<td>5.68391800</td>
<td>-0.41680900</td>
<td>1.32653000</td>
</tr>
<tr>
<td>C</td>
<td>3.64584000</td>
<td>2.55129700</td>
<td>-1.64309200</td>
</tr>
<tr>
<td>H</td>
<td>2.90492200</td>
<td>3.23608500</td>
<td>-2.06299400</td>
</tr>
<tr>
<td>H</td>
<td>4.47733100</td>
<td>3.12941100</td>
<td>-1.22678800</td>
</tr>
<tr>
<td>H</td>
<td>4.07200000</td>
<td>1.91323700</td>
<td>-2.44796000</td>
</tr>
<tr>
<td>H</td>
<td>-7.18013700</td>
<td>-1.46087200</td>
<td>-0.90341200</td>
</tr>
<tr>
<td>C</td>
<td>-6.11839500</td>
<td>-1.71504100</td>
<td>-1.00275700</td>
</tr>
<tr>
<td>Si</td>
<td>-5.04194700</td>
<td>-0.49211400</td>
<td>-0.06302000</td>
</tr>
<tr>
<td>H</td>
<td>-5.97822500</td>
<td>-2.73338300</td>
<td>-0.62492900</td>
</tr>
<tr>
<td>H</td>
<td>-5.87113200</td>
<td>-1.71656400</td>
<td>-2.06979700</td>
</tr>
<tr>
<td>O</td>
<td>-3.44258600</td>
<td>-1.08081100</td>
<td>-0.38914400</td>
</tr>
<tr>
<td>C</td>
<td>-5.25136200</td>
<td>1.25429900</td>
<td>-0.75832400</td>
</tr>
<tr>
<td>C</td>
<td>-5.37644000</td>
<td>-0.54965900</td>
<td>1.79471400</td>
</tr>
<tr>
<td>C</td>
<td>-2.23827300</td>
<td>-0.80615900</td>
<td>0.14210500</td>
</tr>
<tr>
<td>H</td>
<td>-4.68956200</td>
<td>2.01202200</td>
<td>-0.20219600</td>
</tr>
<tr>
<td>H</td>
<td>-4.92858200</td>
<td>1.29971300</td>
<td>-1.80491100</td>
</tr>
<tr>
<td>H</td>
<td>-6.30974100</td>
<td>1.54062300</td>
<td>-0.72457500</td>
</tr>
<tr>
<td>H</td>
<td>-5.23840100</td>
<td>1.56336400</td>
<td>2.18639400</td>
</tr>
<tr>
<td>H</td>
<td>-4.71947200</td>
<td>0.11898100</td>
<td>2.35958100</td>
</tr>
<tr>
<td>H</td>
<td>-6.41257500</td>
<td>-0.25228300</td>
<td>1.99652500</td>
</tr>
<tr>
<td>C</td>
<td>-2.04547600</td>
<td>0.37958700</td>
<td>0.88164000</td>
</tr>
<tr>
<td>C</td>
<td>-1.16821500</td>
<td>-1.59835100</td>
<td>-0.35538100</td>
</tr>
<tr>
<td>H</td>
<td>-2.81499600</td>
<td>1.13822300</td>
<td>0.83294700</td>
</tr>
<tr>
<td>C</td>
<td>-0.88801800</td>
<td>0.72509100</td>
<td>1.57547600</td>
</tr>
<tr>
<td>H</td>
<td>-1.45718700</td>
<td>-2.53711200</td>
<td>-0.81936400</td>
</tr>
<tr>
<td>H</td>
<td>-0.29943900</td>
<td>-1.67707400</td>
<td>0.28558600</td>
</tr>
<tr>
<td>O</td>
<td>-0.02346600</td>
<td>-0.19892000</td>
<td>1.94836800</td>
</tr>
<tr>
<td>O</td>
<td>-0.60036000</td>
<td>1.94147700</td>
<td>2.01185200</td>
</tr>
<tr>
<td>C</td>
<td>1.20623400</td>
<td>0.15905700</td>
<td>2.62399600</td>
</tr>
<tr>
<td>C</td>
<td>-1.28334500</td>
<td>3.09994000</td>
<td>1.45937300</td>
</tr>
<tr>
<td>H</td>
<td>0.98644400</td>
<td>0.71937600</td>
<td>3.53455800</td>
</tr>
<tr>
<td>H</td>
<td>1.67843600</td>
<td>-0.79442400</td>
<td>2.85549800</td>
</tr>
<tr>
<td>H</td>
<td>1.85046100</td>
<td>0.73984300</td>
<td>1.96239700</td>
</tr>
</tbody>
</table>

S30
H  -0.79413500  3.94778700  1.92185400
H  -1.13812200  3.11563100  0.37609100
H  -2.33988200  3.07644700  1.74479000

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.695657, -1422.228414, -1422.195466, -1422.292005

TS-exo-anti-near for 9 + 6
C  -0.12604900  0.17818000  -1.34021100
C   1.05766300  0.83362100  -0.91501000
C   2.14371600  -0.03924300  -0.33893000
C   1.97743600  -1.36049500  -0.11389500
C    0.71182300  -2.03388000  -0.52043200
C   -0.42713800  -1.15886700  -0.97786200
H   -0.84528300  0.76284300  -1.90351400
H   -1.12638000  -1.71201600  -1.60352000
O    0.60695300  -3.25524900  -0.48059900
O    1.26039500  2.07063300  -0.97871400
C    3.07092300  -2.23541400   0.46058300
H    3.16057200  -3.12060400  -0.17676500
C    3.45067800  0.62708500  -0.00939700
H    3.25889700  1.58139100   0.49332300
C    4.40961900  -0.25471100   0.80799600
H    4.22107900  -0.16416500   1.88712600
O    4.35179500  -1.60842100   0.38216000
O    4.17195600   0.92779200  -1.23314500
C    5.51322600   0.75147400  -1.05596200
O    6.31594000   0.97533200  -1.92303500
C    5.76844100   0.27359800   0.37171400
H    6.08349100  1.13101300   0.97925400
H    6.55261800  -0.48488100   0.40238600
C    2.75818700  -2.70890900   1.88914000
H    1.83921800  -3.30180300   1.89102300
H    3.57976100  -3.33202000   2.25628700
H    2.62738800  -1.86430900   2.57563000
H   -7.23716400  -2.01404100  -1.01859000
C   -6.17838700  -2.18220900  -0.78937500
Si   -5.31140300  -0.56332700  -0.38457200
H   -6.12199300  -2.87928600   0.05342600
H   -5.71925900  -2.66822800  -1.65695000
O   -3.68294900  -1.07687800  -0.09088900
C   -5.38011000   0.61676900  -1.86156600
C   -6.01475400   0.23566500   1.17563000
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-2.60320600</td>
<td>-0.46457900</td>
<td>0.43478400</td>
</tr>
<tr>
<td>H</td>
<td>-4.96646700</td>
<td>1.60716900</td>
<td>-1.64382900</td>
</tr>
<tr>
<td>H</td>
<td>-4.83557800</td>
<td>0.20567900</td>
<td>-2.16967200</td>
</tr>
<tr>
<td>H</td>
<td>-5.97620100</td>
<td>-0.45870700</td>
<td>2.02208300</td>
</tr>
<tr>
<td>H</td>
<td>-5.47372100</td>
<td>1.14283100</td>
<td>1.46260000</td>
</tr>
<tr>
<td>H</td>
<td>-6.42317500</td>
<td>0.75931500</td>
<td>-2.16967200</td>
</tr>
<tr>
<td>H</td>
<td>-5.97620100</td>
<td>-0.45870700</td>
<td>2.02208300</td>
</tr>
<tr>
<td>C</td>
<td>-2.53673900</td>
<td>0.94624200</td>
<td>0.46773100</td>
</tr>
<tr>
<td>C</td>
<td>-1.48779700</td>
<td>-1.31003700</td>
<td>0.65665100</td>
</tr>
<tr>
<td>H</td>
<td>-3.28375500</td>
<td>1.49995100</td>
<td>-0.08718900</td>
</tr>
<tr>
<td>C</td>
<td>-1.52862100</td>
<td>1.71080400</td>
<td>1.03937100</td>
</tr>
<tr>
<td>H</td>
<td>-1.70289900</td>
<td>-2.37438700</td>
<td>0.68265400</td>
</tr>
<tr>
<td>O</td>
<td>-0.74746300</td>
<td>1.22771700</td>
<td>1.99784900</td>
</tr>
<tr>
<td>O</td>
<td>-1.35210400</td>
<td>3.00956900</td>
<td>0.82470400</td>
</tr>
<tr>
<td>C</td>
<td>0.39485500</td>
<td>2.00903500</td>
<td>2.42128100</td>
</tr>
<tr>
<td>C</td>
<td>1.12122500</td>
<td>-1.42070100</td>
<td>0.14890900</td>
</tr>
<tr>
<td>C</td>
<td>2.31286200</td>
<td>-0.54823500</td>
<td>0.02840300</td>
</tr>
<tr>
<td>C</td>
<td>2.28217000</td>
<td>0.73560600</td>
<td>0.45094300</td>
</tr>
<tr>
<td>C</td>
<td>1.06716700</td>
<td>1.33040500</td>
<td>1.12593000</td>
</tr>
<tr>
<td>C</td>
<td>0.14651300</td>
<td>-0.79569100</td>
<td>0.69442300</td>
</tr>
<tr>
<td>H</td>
<td>-0.78542700</td>
<td>1.12122500</td>
<td>-1.42070100</td>
</tr>
<tr>
<td>H</td>
<td>-0.78542700</td>
<td>1.12122500</td>
<td>-1.42070100</td>
</tr>
<tr>
<td>O</td>
<td>3.49467600</td>
<td>1.62894700</td>
<td>0.32160600</td>
</tr>
<tr>
<td>O</td>
<td>3.63840900</td>
<td>2.12922100</td>
<td>1.28385600</td>
</tr>
<tr>
<td>C</td>
<td>3.54667300</td>
<td>-1.15195100</td>
<td>0.69442300</td>
</tr>
<tr>
<td>H</td>
<td>3.28093600</td>
<td>-1.72917000</td>
<td>1.47266800</td>
</tr>
<tr>
<td>C</td>
<td>4.63939600</td>
<td>-0.11564500</td>
<td>0.89193100</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.688397, -1422.221467, -1422.188353, -1422.286173

TS-exo-anti-dist for 9 + 6
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.14651300</td>
<td>-0.79569100</td>
<td>0.69442300</td>
</tr>
<tr>
<td>C</td>
<td>1.12122500</td>
<td>-1.42070100</td>
<td>0.14890900</td>
</tr>
<tr>
<td>C</td>
<td>2.31286200</td>
<td>-0.54823500</td>
<td>0.02840300</td>
</tr>
<tr>
<td>C</td>
<td>2.28217000</td>
<td>0.73560600</td>
<td>0.45094300</td>
</tr>
<tr>
<td>C</td>
<td>1.06716700</td>
<td>1.33040500</td>
<td>1.12593000</td>
</tr>
<tr>
<td>C</td>
<td>-0.04228800</td>
<td>0.46603000</td>
<td>1.32811200</td>
</tr>
<tr>
<td>H</td>
<td>-0.78542700</td>
<td>1.12122500</td>
<td>-1.42070100</td>
</tr>
<tr>
<td>H</td>
<td>-0.84237500</td>
<td>0.83550600</td>
<td>1.96186600</td>
</tr>
<tr>
<td>O</td>
<td>1.12815700</td>
<td>2.52224600</td>
<td>1.51025600</td>
</tr>
<tr>
<td>O</td>
<td>1.15059500</td>
<td>-2.59014100</td>
<td>0.21434400</td>
</tr>
<tr>
<td>C</td>
<td>3.49467600</td>
<td>1.62894700</td>
<td>0.32160600</td>
</tr>
<tr>
<td>H</td>
<td>3.63840900</td>
<td>2.12922100</td>
<td>1.28385600</td>
</tr>
<tr>
<td>C</td>
<td>3.54667300</td>
<td>-1.15195100</td>
<td>0.69442300</td>
</tr>
<tr>
<td>H</td>
<td>3.28093600</td>
<td>-1.72917000</td>
<td>1.47266800</td>
</tr>
<tr>
<td>C</td>
<td>4.63939600</td>
<td>-0.11564500</td>
<td>0.89193100</td>
</tr>
</tbody>
</table>
H  4.50247600  0.32708500  -1.88828900
O  4.69596300  0.88221900  0.11700600
O  4.16658200 -2.07717100  0.35541300
C  5.52580200 -1.99889000  0.28234900
O  6.25210300 -2.69534600  0.94164100
C  5.90897200 -0.94274800 -0.75152400
H  6.16967100 -1.44670900 -1.69040800
H  6.76686700 -0.35534500 -0.41951300
C  3.31682400  2.71586200 -0.75166000
H  2.49514800  3.30316700 -0.82556200
H  3.09871200  2.28472800 -1.73592100
H -6.11929200 -3.94123200 -0.02626100
C -5.09052600 -3.62628000 -0.23657800
Si -4.90227600 -1.76610000 -0.04325000
H -4.42689700 -4.16065900  0.45161300
H -4.84124700 -3.94346800 -1.25468600
O -3.22227200 -1.52269600 -0.39039900
C -5.95175000 -0.81795900 -1.29591400
C -5.29306500 -1.23593900  1.73019300
C -2.93230200  0.84160800 -0.22005900
H -5.80572000  0.26489300 -1.23043800
H -5.71256100 -1.12603600 -2.31958800
H -7.01534600 -1.02399400 -1.12566100
H -4.58539800 -1.68118700  2.43773500
H -5.27182600 -0.14974600  1.87268500
H -6.29725100 -1.58156600  2.00384200
C -2.45756300 -0.43665100 -0.61308600
C -2.30704200  2.05899500 -0.42526500
H -3.83509000  0.87094200  0.37536200
C -1.12816300 -0.72535200 -0.99885000
H -0.96976500 -1.73210600 -1.37325400
H -0.57968800  0.05425500 -1.51029800
O -1.37137200  2.23475100 -1.34608900
O -2.66518200  3.19489000  0.17892200
C -0.58392000  3.45163800 -1.31275100
H  0.19400900  3.29194100 -2.05879500
H -1.20255400  4.30851600 -1.58876300
H -0.14534000  3.58496400 -0.32286800
C -3.49807500  3.15673000  1.34226300
H -3.10856400  2.43433800  2.06525700
H -3.46151100  4.16364800  1.75805600
H -4.53015200  2.90751900  1.07289800

Energies at 0K, H and G at 298.15 K

S33
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.687880, -1422.221388, -1422.188073, -1422.287646

TS-endo-syn-near for 9 + 6

C  1.51823400  -1.91391200  1.62714500
C  0.60343400  -2.31879000  0.61760300
C -0.73318200  -1.61434000  0.61230900
C -1.11978600  -0.74899400  1.57485000
C -0.18111600  -0.39727100  2.67306800
C  1.24514100  -0.83936700  2.50736400
H  2.45378600  -2.46040700  1.70250600
H  1.77407100  -0.82534800  3.45951000
O  -0.55162000   0.24579900  3.65086000
O   0.79494200  -3.22636400  -0.22189900
C  -2.49669900  -0.11991100  1.59674000
H  -2.37616500  0.95382300  1.77466300
C  -1.68193800  -1.99964900  -0.48675000
H  -1.64481900  -3.08379000  -0.63043100
C  -3.11699800  -1.48867500  -0.28778200
H  -3.71779600  -2.19598500  0.29791000
O  -3.12172500  -0.19635600  0.30707400
O  -1.25185400  -1.39374300  -1.74499100
C  -2.32312100  -1.00320700  -2.49042300
O  -2.19640000  -0.50197000  -3.57877700
C  -3.60145300  -1.31619700  -1.72201500
H  -4.03159100  -2.24515500  -2.11606800
H  -4.33703200  -0.51743200  -1.83355000
C  -3.40207800  -0.68914200  2.69939400
H  -2.95726100  -0.48110600  3.67518900
H  -4.38770800  -0.21528700  2.64456300
H  -3.52736900  -1.77327100  2.60246700
H  -1.92301000  3.08940900  -2.15985200
C  -1.32749300  2.34839900  -1.61197700
Si -0.09812500  3.23393900  -0.49236700
H  -2.01770300  1.73093700  -1.02636500
H  -0.85642700  1.69868400  -2.35638600
O  0.53429500  2.15287000  0.71306900
C  1.34109300  3.98033100  -1.46509000
C  -0.96115000  4.53281900  0.56269800
C  1.51973600  1.23525800  0.68658300
H  2.03377900  4.51165800  -0.80320100
H  1.91180500  3.22129500  -2.00940800
H  0.95922800  4.70081800  -2.19837800

S34
H  -1.75509700  4.08320100  1.16890000
H  -0.25560400  5.02001200  1.24411400
H  -1.41649300  0.55760500  -0.51973300
C   1.81408300  -0.33525000  -0.73078200
C   2.04295000  -1.26147900  -2.74193100
H   1.10877300  -1.33557000
C   1.76653900  -1.48572600  -0.05362000
C   2.85705200  -1.87113300  -2.77098300
H   1.00045200  -1.58363800  -2.23794000
H   1.75384000  -0.32185700  -3.28138000

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.701795, -1422.234351, -1422.201561, -1422.296353

TS-endo-syn-dist for 9 + 6
C   -1.20246200  -1.11676500  2.22149000
C    0.29495100  -1.02153900  2.23166800
C    0.99563500  -1.35862000  0.96554000
C    0.33309000  -1.94505800  -0.05693800
C   -1.14747100  -2.43206000  0.00818700
C   -1.81799800  -1.88107200  1.20808100
H   -1.60583300  -1.18395000  3.22996100
H   -2.85394600  -2.19265500  1.30534100
O   -1.68425900  -2.81267600  -0.97292500
O    0.91908700  -0.72142100  3.24345900
C    1.06283300  -2.37859800  -1.30869200
H    0.50090500  -2.01085500  -2.17279800
C    2.48296200  -1.15817400  0.93024200
H    2.91649500  -1.47878000  1.88336000
C    3.16025500  -1.84787700  -0.26296600
H    3.40608300  -2.89376900  -0.03936000
O    2.34413200  -1.74536500  -1.42255400
O    2.81907000  0.25503300  0.77274600
C    3.91700800  0.40191400  -0.01542900
<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>4.40059300</td>
<td>1.48112900</td>
<td>-0.25425800</td>
</tr>
<tr>
<td>C</td>
<td>4.37965700</td>
<td>-0.96806700</td>
<td>-0.49683100</td>
</tr>
<tr>
<td>H</td>
<td>5.23139800</td>
<td>-1.28931700</td>
<td>0.11498500</td>
</tr>
<tr>
<td>H</td>
<td>4.69341900</td>
<td>-0.93600300</td>
<td>-1.54193500</td>
</tr>
<tr>
<td>C</td>
<td>1.16841700</td>
<td>-3.90742600</td>
<td>-1.43385300</td>
</tr>
<tr>
<td>H</td>
<td>0.16308100</td>
<td>-4.32751300</td>
<td>-1.50202500</td>
</tr>
<tr>
<td>H</td>
<td>1.73211500</td>
<td>-4.15798800</td>
<td>-2.33839500</td>
</tr>
<tr>
<td>H</td>
<td>1.67437300</td>
<td>-4.35365100</td>
<td>-0.57068900</td>
</tr>
<tr>
<td>H</td>
<td>2.32966200</td>
<td>4.69209700</td>
<td>-0.24323300</td>
</tr>
<tr>
<td>C</td>
<td>1.94681600</td>
<td>3.87284400</td>
<td>0.37775600</td>
</tr>
<tr>
<td>Si</td>
<td>0.48768100</td>
<td>3.05062800</td>
<td>-0.46518300</td>
</tr>
<tr>
<td>H</td>
<td>2.76416300</td>
<td>3.16299700</td>
<td>0.53593100</td>
</tr>
<tr>
<td>H</td>
<td>1.64909700</td>
<td>4.29319400</td>
<td>1.34455400</td>
</tr>
<tr>
<td>O</td>
<td>-0.19979400</td>
<td>2.05376100</td>
<td>0.78966300</td>
</tr>
<tr>
<td>C</td>
<td>-0.82726600</td>
<td>4.31771400</td>
<td>-0.96719800</td>
</tr>
<tr>
<td>C</td>
<td>1.00777300</td>
<td>2.00386700</td>
<td>-1.95498700</td>
</tr>
<tr>
<td>C</td>
<td>-2.02963300</td>
<td>0.99243500</td>
<td>-0.31521600</td>
</tr>
<tr>
<td>H</td>
<td>-1.73817400</td>
<td>3.84473500</td>
<td>-1.34865200</td>
</tr>
<tr>
<td>H</td>
<td>-1.10820000</td>
<td>4.95013500</td>
<td>-0.11789300</td>
</tr>
<tr>
<td>H</td>
<td>-0.43390600</td>
<td>4.97204900</td>
<td>-1.75458200</td>
</tr>
<tr>
<td>H</td>
<td>1.42819400</td>
<td>1.04279900</td>
<td>-1.64240900</td>
</tr>
<tr>
<td>H</td>
<td>0.18055300</td>
<td>1.81158900</td>
<td>-2.64785800</td>
</tr>
<tr>
<td>H</td>
<td>1.78714200</td>
<td>2.53436700</td>
<td>-2.51499300</td>
</tr>
<tr>
<td>C</td>
<td>-1.33678000</td>
<td>1.35182200</td>
<td>0.87235000</td>
</tr>
<tr>
<td>C</td>
<td>-3.26584700</td>
<td>0.37697200</td>
<td>-0.40266800</td>
</tr>
<tr>
<td>H</td>
<td>-1.51387400</td>
<td>1.14865100</td>
<td>-1.25284800</td>
</tr>
<tr>
<td>C</td>
<td>-1.66055400</td>
<td>0.85114800</td>
<td>2.15469300</td>
</tr>
<tr>
<td>O</td>
<td>-4.11650600</td>
<td>0.35353300</td>
<td>0.62014500</td>
</tr>
<tr>
<td>O</td>
<td>-3.78930700</td>
<td>-0.12237600</td>
<td>-1.51814500</td>
</tr>
<tr>
<td>C</td>
<td>-5.28962200</td>
<td>-0.47746800</td>
<td>0.52881900</td>
</tr>
<tr>
<td>H</td>
<td>-5.97344500</td>
<td>-0.09774800</td>
<td>-0.23353100</td>
</tr>
<tr>
<td>H</td>
<td>-5.01065600</td>
<td>-1.50839800</td>
<td>0.29757400</td>
</tr>
<tr>
<td>H</td>
<td>-5.75051000</td>
<td>-0.41656000</td>
<td>1.51470400</td>
</tr>
<tr>
<td>C</td>
<td>-2.95703800</td>
<td>-0.35418500</td>
<td>-2.67070300</td>
</tr>
<tr>
<td>H</td>
<td>-2.12889500</td>
<td>-1.01066200</td>
<td>-2.40043300</td>
</tr>
<tr>
<td>H</td>
<td>-3.60834100</td>
<td>-0.85331600</td>
<td>-3.38811500</td>
</tr>
<tr>
<td>H</td>
<td>-2.61210500</td>
<td>0.59701400</td>
<td>-3.08927300</td>
</tr>
<tr>
<td>H</td>
<td>-2.70775400</td>
<td>0.68868900</td>
<td>2.36490200</td>
</tr>
<tr>
<td>H</td>
<td>-1.07106000</td>
<td>1.25003600</td>
<td>2.97515500</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.700158, -1422.232683, -1422.199981, -1422.294614
TS-endo-anti-near for 9 + 6

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.06943300</td>
<td>2.04059100</td>
<td>1.52021600</td>
</tr>
<tr>
<td>C</td>
<td>-0.96602500</td>
<td>1.83811400</td>
<td>0.43438600</td>
</tr>
<tr>
<td>C</td>
<td>-1.63467700</td>
<td>0.48706300</td>
<td>0.35871400</td>
</tr>
<tr>
<td>C</td>
<td>-1.36916600</td>
<td>-0.52064500</td>
<td>1.21840700</td>
</tr>
<tr>
<td>C</td>
<td>-0.41502700</td>
<td>-0.30957800</td>
<td>2.33873400</td>
</tr>
<tr>
<td>C</td>
<td>0.36884200</td>
<td>0.97920800</td>
<td>2.35554800</td>
</tr>
<tr>
<td>H</td>
<td>0.28244000</td>
<td>3.05326200</td>
<td>1.69170900</td>
</tr>
<tr>
<td>H</td>
<td>0.65152500</td>
<td>1.23701300</td>
<td>3.37636900</td>
</tr>
<tr>
<td>O</td>
<td>-0.28450300</td>
<td>-1.14787000</td>
<td>3.22516700</td>
</tr>
<tr>
<td>O</td>
<td>-1.25559700</td>
<td>2.69089100</td>
<td>-0.43418000</td>
</tr>
<tr>
<td>C</td>
<td>-2.09057200</td>
<td>-1.85106400</td>
<td>1.16790600</td>
</tr>
<tr>
<td>H</td>
<td>-2.45609700</td>
<td>-2.06684900</td>
<td>2.17686000</td>
</tr>
<tr>
<td>C</td>
<td>-2.65778800</td>
<td>0.30172400</td>
<td>-0.72945100</td>
</tr>
<tr>
<td>H</td>
<td>-2.26147200</td>
<td>0.70096900</td>
<td>-1.67096700</td>
</tr>
<tr>
<td>C</td>
<td>-3.13119300</td>
<td>-1.15138300</td>
<td>-0.89432600</td>
</tr>
<tr>
<td>H</td>
<td>-2.46821200</td>
<td>-1.72064700</td>
<td>-1.56137900</td>
</tr>
<tr>
<td>O</td>
<td>-3.27210400</td>
<td>-1.78844800</td>
<td>0.36667700</td>
</tr>
<tr>
<td>O</td>
<td>-3.85856500</td>
<td>1.05266800</td>
<td>-0.41823900</td>
</tr>
<tr>
<td>C</td>
<td>-4.96842700</td>
<td>0.37108900</td>
<td>-0.82291400</td>
</tr>
<tr>
<td>O</td>
<td>-6.08044000</td>
<td>0.81379200</td>
<td>-0.70414100</td>
</tr>
<tr>
<td>C</td>
<td>-4.53964000</td>
<td>-0.95945000</td>
<td>-1.43728700</td>
</tr>
<tr>
<td>H</td>
<td>-4.54232000</td>
<td>-0.86100500</td>
<td>-2.52994200</td>
</tr>
<tr>
<td>H</td>
<td>-5.22084900</td>
<td>-1.76440300</td>
<td>-1.15583600</td>
</tr>
<tr>
<td>C</td>
<td>-1.18114100</td>
<td>-3.01125900</td>
<td>0.73632100</td>
</tr>
<tr>
<td>H</td>
<td>-0.33514900</td>
<td>-3.09552300</td>
<td>1.42330600</td>
</tr>
<tr>
<td>H</td>
<td>-1.75035300</td>
<td>-3.94623300</td>
<td>0.75109500</td>
</tr>
<tr>
<td>H</td>
<td>-0.78972400</td>
<td>-2.85624900</td>
<td>-0.27557600</td>
</tr>
<tr>
<td>H</td>
<td>3.24439600</td>
<td>-4.85455000</td>
<td>-0.77959100</td>
</tr>
<tr>
<td>C</td>
<td>2.81868400</td>
<td>-4.11464800</td>
<td>-0.09173700</td>
</tr>
<tr>
<td>Si</td>
<td>2.86050300</td>
<td>-2.39159600</td>
<td>-0.84413300</td>
</tr>
<tr>
<td>H</td>
<td>1.79182700</td>
<td>-4.41841400</td>
<td>0.13798500</td>
</tr>
<tr>
<td>H</td>
<td>3.39313600</td>
<td>-4.14870400</td>
<td>0.84005500</td>
</tr>
<tr>
<td>O</td>
<td>2.12720700</td>
<td>-1.41350100</td>
<td>0.38331200</td>
</tr>
<tr>
<td>C</td>
<td>4.62301600</td>
<td>-1.77976100</td>
<td>-1.13631200</td>
</tr>
<tr>
<td>C</td>
<td>1.85365700</td>
<td>-2.33992200</td>
<td>-2.44616000</td>
</tr>
<tr>
<td>C</td>
<td>2.09957800</td>
<td>0.79721000</td>
<td>-0.50393600</td>
</tr>
<tr>
<td>H</td>
<td>4.64101300</td>
<td>-0.73842600</td>
<td>-1.47390200</td>
</tr>
<tr>
<td>H</td>
<td>5.22004400</td>
<td>-1.84589000</td>
<td>-0.22023200</td>
</tr>
<tr>
<td>H</td>
<td>5.11498300</td>
<td>-2.39067800</td>
<td>-1.90243600</td>
</tr>
<tr>
<td>H</td>
<td>0.79421100</td>
<td>-2.54391000</td>
<td>-2.25632500</td>
</tr>
<tr>
<td>H</td>
<td>1.92673200</td>
<td>-1.37840100</td>
<td>-2.96584000</td>
</tr>
<tr>
<td>H</td>
<td>2.21939900</td>
<td>-3.11090900</td>
<td>-3.13548500</td>
</tr>
<tr>
<td>C</td>
<td>2.20408100</td>
<td>-0.07933400</td>
<td>0.59672300</td>
</tr>
</tbody>
</table>
C       2.23623500  2.18095400  -0.47659900
H       1.79194900  0.36939600  -1.44936100
C       2.13742900  0.34097200   1.95243400
O       2.88451600  2.80006000   0.50494300
O       1.90900100  2.99413700  -1.47252200
C       2.81692100  4.23847700   0.57890800
H       1.77616300  4.57087800  -0.47659900
H       3.30092000  4.49130300   1.52255600
H       3.35449600  4.69155600  -0.25688600
H       3.30319200  4.49130300   1.52255600
C       1.08347000  2.52999600  -2.55885600
H       1.62823000  1.79400000  -3.16761700
H       0.14565900  2.13744100  -2.16611700
H       0.88857100  3.41890900  -3.15826100
H       2.64966800  1.26546500   2.18344700
H       2.28087300  -0.45101600   2.68303700

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.687760, -1422.221119, -1422.188023, -1422.285629

TS-endo-anti-dist for 9 + 6
C       -0.62452900  -0.09800600  -2.14469300
C        0.52426200   0.57093700  -1.42358600
C       1.36627700  -0.27717000  -0.55497200
C       1.10948800  -1.59985400  -0.40934500
C       -0.02551000  -2.29082300  -1.12921200
C       -0.73861000  -1.50508900  -2.06705300
H       -0.79599900   0.35946800  -3.11972000
H       -1.43631800  -2.02265600  -2.71857100
O       -0.21304400  -3.51451100  -0.91958900
O       0.73615100   1.77718100  -1.53951300
C       2.00001800  -2.47802000   0.43900000
H       2.23625500  -3.36553000  -0.15636600
C       2.51279600   0.38426500   0.15462400
H       2.17243500   1.30891000   0.63480500
C       3.21051700  -0.53220300   1.17502800
H       2.72792100  -0.47406600   2.16064100
O       3.26501100  -1.86960500   0.70410700
O       3.55206800   0.75426000  -0.79252900
C       4.78969100   0.55699900  -0.25546700
O       5.80302200   0.82479600  -0.84581900
C       4.63732900  -0.00359100   1.15637700
H       4.77642500   0.81307400   1.87542900
H       5.38061700  -0.77691800   1.35845300

S38
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.31754200</td>
<td>-2.95511400</td>
<td>1.73099300</td>
</tr>
<tr>
<td>H</td>
<td>0.43812400</td>
<td>-3.54545000</td>
<td>1.46381900</td>
</tr>
<tr>
<td>H</td>
<td>2.01407700</td>
<td>-3.59427000</td>
<td>2.29973000</td>
</tr>
<tr>
<td>H</td>
<td>1.01293900</td>
<td>-2.11204900</td>
<td>2.36319200</td>
</tr>
<tr>
<td>H</td>
<td>0.46700000</td>
<td>4.97903000</td>
<td>1.29454800</td>
</tr>
<tr>
<td>C</td>
<td>-1.42087500</td>
<td>3.54557400</td>
<td>0.52519600</td>
</tr>
<tr>
<td>H</td>
<td>1.05015800</td>
<td>3.48414000</td>
<td>0.53443400</td>
</tr>
<tr>
<td>H</td>
<td>0.42649000</td>
<td>3.45778500</td>
<td>2.20252800</td>
</tr>
<tr>
<td>O</td>
<td>-1.57203800</td>
<td>1.81434200</td>
<td>0.69417200</td>
</tr>
<tr>
<td>C</td>
<td>-2.79136400</td>
<td>4.23127000</td>
<td>1.63017300</td>
</tr>
<tr>
<td>C</td>
<td>-1.59615200</td>
<td>4.20589000</td>
<td>-1.23247700</td>
</tr>
<tr>
<td>C</td>
<td>-2.11384500</td>
<td>0.80325300</td>
<td>0.00256500</td>
</tr>
<tr>
<td>H</td>
<td>-3.78320400</td>
<td>3.95483800</td>
<td>1.25456000</td>
</tr>
<tr>
<td>H</td>
<td>-2.70184400</td>
<td>3.85464000</td>
<td>2.65470500</td>
</tr>
<tr>
<td>H</td>
<td>-2.74370300</td>
<td>5.32620400</td>
<td>1.66848300</td>
</tr>
<tr>
<td>H</td>
<td>-0.84739100</td>
<td>3.75789300</td>
<td>-1.89207600</td>
</tr>
<tr>
<td>H</td>
<td>-2.59452600</td>
<td>4.04665800</td>
<td>-1.65340500</td>
</tr>
<tr>
<td>H</td>
<td>-1.42160900</td>
<td>5.28928100</td>
<td>-1.20655800</td>
</tr>
<tr>
<td>C</td>
<td>-2.40917900</td>
<td>-0.32551000</td>
<td>0.81444600</td>
</tr>
<tr>
<td>C</td>
<td>-2.17261700</td>
<td>0.81977800</td>
<td>-1.41654100</td>
</tr>
<tr>
<td>H</td>
<td>-2.11681500</td>
<td>-0.22390200</td>
<td>1.85130000</td>
</tr>
<tr>
<td>C</td>
<td>-2.99919600</td>
<td>-1.51619000</td>
<td>0.43943900</td>
</tr>
<tr>
<td>H</td>
<td>-2.06430200</td>
<td>1.79197100</td>
<td>-1.88121900</td>
</tr>
<tr>
<td>H</td>
<td>-2.93398700</td>
<td>0.19397100</td>
<td>-1.86304100</td>
</tr>
<tr>
<td>O</td>
<td>-3.60989700</td>
<td>-1.69090400</td>
<td>-0.72551900</td>
</tr>
<tr>
<td>O</td>
<td>-3.11195400</td>
<td>-2.57873300</td>
<td>1.23899400</td>
</tr>
<tr>
<td>C</td>
<td>-3.74896700</td>
<td>-3.04457200</td>
<td>-1.22641400</td>
</tr>
<tr>
<td>C</td>
<td>-2.49827900</td>
<td>-2.58204900</td>
<td>2.53170400</td>
</tr>
<tr>
<td>H</td>
<td>-2.77271700</td>
<td>-3.53694100</td>
<td>-1.23165200</td>
</tr>
<tr>
<td>H</td>
<td>-4.46552500</td>
<td>-3.60253800</td>
<td>-0.62029300</td>
</tr>
<tr>
<td>H</td>
<td>-4.12776500</td>
<td>-2.92318300</td>
<td>-2.24124100</td>
</tr>
<tr>
<td>H</td>
<td>-1.43097500</td>
<td>-2.36394700</td>
<td>2.45163900</td>
</tr>
<tr>
<td>H</td>
<td>-2.98752300</td>
<td>-1.85663600</td>
<td>3.19027400</td>
</tr>
<tr>
<td>H</td>
<td>-2.64596000</td>
<td>-3.59065300</td>
<td>2.91768100</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1422.692509, -1422.224837, -1422.192209, -1422.287515

**TS-endo-syn-near for 12 + 6**

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.50303500</td>
<td>1.19662500</td>
<td>1.23941700</td>
</tr>
<tr>
<td>C</td>
<td>0.55854500</td>
<td>0.16046500</td>
<td>1.48634400</td>
</tr>
<tr>
<td>C</td>
<td>-0.77623400</td>
<td>0.30806700</td>
<td>0.79992800</td>
</tr>
</tbody>
</table>
C  -1.15995500  1.43359300  0.15728300  
C  -0.21150700  2.56847700  0.02509200  
C   1.23085900  2.28898700  0.36272500  
H   2.43403500  1.16489200  1.79732900  
H   1.75989400  3.21834400  0.57748400  
O  -0.57400900  3.66219900 -0.39676400  
O   0.73472800 -0.81668400  2.24554800  
C  -2.54976000  1.59888600 -0.42382200  
H  -2.45559300  2.02188000 -1.42964100  
C  -1.72350600 -0.84971000  0.93338300  
H  -1.67967000 -1.23766400  1.95551000  
C  -3.16208200 -0.54821900  0.48443300  
H  -3.76639800 -0.15363300  1.31150600  
O  -3.17628400  0.32886900 -0.63408800  
O  -2.34973800 -2.55806600 -0.52307600  
O  -2.21279600 -3.48667900 -1.27549500  
C  -3.63259600 -1.90358800 -0.02706400  
H  -4.05019700 -2.51794200  0.78008800  
H  -4.37277400 -1.82523600 -0.82530900  
C  -3.43286200  2.54339500  0.40623600  
H  -2.98514900  3.53982400  0.42429000  
H  -4.42711800  2.60552000 -0.04789900  
H  -3.53950200  2.19489700  1.43941900  
C   1.44031700  0.85818700 -1.88999500  
C   1.75066000 -0.41014900 -1.42222100  
C   1.94896100  2.07799100 -1.35656900  
H   1.08919100 -1.22761300 -1.68545900  
C   2.80582100 -0.73622000 -0.54978800  
H   1.62636200  2.98735200 -1.86053100  
H   2.99865900  2.09477700 -1.08562800  
O   3.87043200  0.05191000 -0.44013200  
O   2.94532100 -1.89070300  0.07215800  
C   4.85130400 -0.25145600  0.57079100  
C   1.91002300 -2.90290100  0.01776400  
H   5.35226000 -1.19641300  0.35001400  
H   5.56082500  0.57462500  0.52733700  
H   4.37799300 -0.30372200  1.55459600  
H   2.24385500 -3.67022700  0.71487200  
H   0.95316800 -2.49358500  0.33315900  
H   1.85432400 -3.31360200 -0.99478800  
H   0.57751800  0.91790600 -2.54997600  

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy

S40
### TS-endo-syn-dist for 12 + 6

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.08881800</td>
<td>-1.41224200</td>
<td>-1.68825200</td>
</tr>
<tr>
<td>C</td>
<td>0.41337500</td>
<td>-1.48251300</td>
<td>-1.64592000</td>
</tr>
<tr>
<td>C</td>
<td>1.10035700</td>
<td>-0.34385400</td>
<td>-0.99035700</td>
</tr>
<tr>
<td>C</td>
<td>0.47338900</td>
<td>0.84673800</td>
<td>-0.84399400</td>
</tr>
<tr>
<td>C</td>
<td>-0.97475200</td>
<td>1.04514400</td>
<td>-1.21170500</td>
</tr>
<tr>
<td>C</td>
<td>-1.68141000</td>
<td>-0.11500300</td>
<td>-1.63864000</td>
</tr>
<tr>
<td>H</td>
<td>-1.49634400</td>
<td>-2.09937000</td>
<td>-2.43027000</td>
</tr>
<tr>
<td>H</td>
<td>-2.70287000</td>
<td>0.03000300</td>
<td>-1.97885700</td>
</tr>
<tr>
<td>O</td>
<td>-1.46868800</td>
<td>2.19442100</td>
<td>-1.12307300</td>
</tr>
<tr>
<td>O</td>
<td>1.03527100</td>
<td>-2.43210500</td>
<td>-2.10488500</td>
</tr>
<tr>
<td>C</td>
<td>1.22182600</td>
<td>2.05024800</td>
<td>-0.31811400</td>
</tr>
<tr>
<td>H</td>
<td>0.58876300</td>
<td>2.55352900</td>
<td>0.41924900</td>
</tr>
<tr>
<td>H</td>
<td>0.58373800</td>
<td>-0.53994800</td>
<td>-0.59462400</td>
</tr>
<tr>
<td>O</td>
<td>3.06380600</td>
<td>-1.10160700</td>
<td>-1.37052000</td>
</tr>
<tr>
<td>O</td>
<td>3.26280000</td>
<td>0.76416200</td>
<td>-0.23676700</td>
</tr>
<tr>
<td>H</td>
<td>3.72450800</td>
<td>1.22228400</td>
<td>-1.12114400</td>
</tr>
<tr>
<td>O</td>
<td>0.09580700</td>
<td>1.67248900</td>
<td>0.42074800</td>
</tr>
<tr>
<td>O</td>
<td>2.58275600</td>
<td>-1.34271100</td>
<td>0.62543300</td>
</tr>
<tr>
<td>C</td>
<td>3.55847100</td>
<td>-0.88730400</td>
<td>1.46541900</td>
</tr>
<tr>
<td>C</td>
<td>2.09689400</td>
<td>3.90486000</td>
<td>-1.00430100</td>
</tr>
<tr>
<td>H</td>
<td>2.13488800</td>
<td>2.61562200</td>
<td>-2.23071100</td>
</tr>
<tr>
<td>C</td>
<td>-1.63711300</td>
<td>-0.65812800</td>
<td>1.46938000</td>
</tr>
<tr>
<td>C</td>
<td>-1.03983400</td>
<td>-1.80386900</td>
<td>0.95613400</td>
</tr>
<tr>
<td>C</td>
<td>-2.89541400</td>
<td>-0.14869300</td>
<td>1.14402000</td>
</tr>
<tr>
<td>H</td>
<td>-1.06804300</td>
<td>-0.06134700</td>
<td>2.17307100</td>
</tr>
<tr>
<td>C</td>
<td>-1.47445400</td>
<td>-2.49858100</td>
<td>-0.20896100</td>
</tr>
<tr>
<td>O</td>
<td>3.82329900</td>
<td>-0.92647000</td>
<td>0.57131700</td>
</tr>
<tr>
<td>O</td>
<td>-3.34925600</td>
<td>1.05284000</td>
<td>1.43507300</td>
</tr>
<tr>
<td>C</td>
<td>-5.02515000</td>
<td>-0.31795600</td>
<td>0.05680700</td>
</tr>
<tr>
<td>H</td>
<td>-5.61706000</td>
<td>0.11105800</td>
<td>0.86783500</td>
</tr>
<tr>
<td>H</td>
<td>-4.77366100</td>
<td>0.45686000</td>
<td>-0.67187400</td>
</tr>
<tr>
<td>H</td>
<td>-5.56797100</td>
<td>-1.13413100</td>
<td>-0.41934500</td>
</tr>
<tr>
<td>C</td>
<td>-2.46208200</td>
<td>2.06767600</td>
<td>1.95346300</td>
</tr>
<tr>
<td>H</td>
<td>-1.66911700</td>
<td>2.26159800</td>
<td>1.23213200</td>
</tr>
</tbody>
</table>
Energies at 0K, H and G at 298.15 K

E (0K), E+ZPE (0K), Enthalpy, Free Energy

-1224.413904, -1224.053855, -1224.029913, -1224.106031

TS-endo-syn-near for 13 + 6

| H   | -3.09009200 | 2.95155400 | 2.06102200 |
| H   | -2.07372500 | 1.76863800 | 2.93137400 |
| H   | -2.54407400 | -2.59450500 | -0.35687100 |
| H   | -0.92720900 | -3.40871200 | -0.44723400 |
| H   | -0.05088200 | -2.03748600 | 1.34356100 |

C    | -1.15805500 | -2.83030100 | -1.11083900 |
C    | -1.99084000 | -1.64355000 | -1.23475300 |
C    | -1.80478900 | -0.59151000 | -0.17943300 |
C    | -1.19782000 | -0.85536200 | 0.99645600 |
C    | -0.61349100 | -2.05601000 | 1.25151000 |
C    | -0.42844600 | -3.08990800 | 0.06426400 |
H    | -1.35667600 | -3.62623800 | -1.82220300 |
H    | -0.23056800 | -4.12415300 | 0.33457400 |
O    | -0.28104400 | -2.53771000 | 2.37985900 |
O    | -2.84187900 | -1.48204800 | -2.11214700 |
C    | -1.10081400 | 0.18000000 | 2.09665000 |
H    | -0.07148300 | 0.17819400 | 2.46966400 |
C    | -2.41295100 | 0.75204500 | -0.45543800 |
H    | -3.40755100 | 0.61745100 | -0.89263700 |
C    | -2.44326300 | 1.68315400 | 0.76662900 |
H    | -3.36073700 | 1.54715100 | 1.35281000 |
O    | -1.28634400 | 1.50287400 | 1.57697400 |
O    | -1.59997000 | 1.45085900 | -1.44188400 |
C    | -1.52850900 | 2.78233500 | -1.15055300 |
O    | -0.91751500 | 3.55832100 | -1.83830500 |
C    | -2.32413600 | 3.05705100 | 0.12161800 |
H    | -3.30734100 | 3.45631000 | -0.15591300 |
H    | -1.81842600 | 3.78751500 | 0.75566700 |
C    | -2.04201500 | -0.10830400 | 3.27642900 |
H    | -1.77312600 | -1.06487800 | 3.72994500 |
H    | -1.94119700 | 0.68595500 | 4.02305400 |
H    | -3.08897700 | -0.15959200 | 2.95779200 |
H    | 2.39480300 | 3.31116200 | 0.18541600 |
C    | 1.89741700 | 2.35888200 | -0.03703800 |
Si   | 3.11116600 | 0.93823600 | 0.20597000 |
H    | 1.04025700 | 2.26241300 | 0.63877000 |
H    | 1.50687400 | 2.42762800 | -1.05733000 |
O    | 2.27417000 | -0.57527400 | 0.37125900 |
C    | 4.32893700 | 0.79469100 | -1.23205200 |
C  4.00010000  1.08308100  1.85992300
C  1.77002000 -1.40811500 -2.18312000
H  5.04502400 -0.01785400 -1.06669400
H  3.81941700  0.60760200 -2.18312000
H  4.89730800  1.72636000 -1.33824100
H  3.28601700  1.09712600  2.69061100
H  4.68171400  0.24047000  2.01764200
H  4.58728400  2.00766400  1.90766800
C  1.15493600 -0.91927700 -1.74748900
C  1.63151700 -2.75730900 -0.20536000
H  1.01249200  0.15420000 -1.83869600
C  0.49780700 -1.74354000 -2.62787500
H  2.05309000 -3.06735500  0.74584700
H  1.64482400 -3.50535900 -0.98818200
H  -0.10410000 -1.32206500 -3.42645600
H  0.74176100 -2.79347600 -2.72785300

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy

**TS-endo-syn-dist for 13 + 6**

C  1.09243500 -2.30065600  1.63396900
C  1.08709100 -0.83957100  1.94413000
C  1.44217800  0.08889900  0.83397600
C  2.02808900 -0.36510000 -0.29680100
C  2.31620700 -1.83133700 -0.49770800
C  1.78043000 -2.74775100  0.49074900
H  1.13311200 -2.91397500  2.53082400
H  2.13731300 -3.77061700  0.42340200
O  3.01258900 -2.18656500 -1.45693600
O  0.83971000 -0.41375200  3.06579000
C  2.46474700  0.58573800 -1.39036300
H  2.09685600  0.19349800 -2.34410300
C  1.26736100  1.55931800  1.09196500
H  1.62210100  1.79240100  2.10161500
C  1.94110000  2.44626600  0.03303600
H  2.99061300  2.64652200  0.28200200
O  1.82022400  1.85850600 -1.25568000
O -0.14115200  1.92718900  1.04355400
C -0.29740100  3.15654200  0.47864100
O -1.37586900  3.68451000  0.37275500
C  1.06287000  3.68922600  0.04563600
H  1.40873200  4.42012100  0.78649600
H  1.00334800  4.18155300 -0.92686300
<table>
<thead>
<tr>
<th>Atoms</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>3.99269200</td>
<td>0.72750500</td>
<td>-1.49262800</td>
</tr>
<tr>
<td>H</td>
<td>4.42621100</td>
<td>-0.23866000</td>
<td>-1.75650400</td>
</tr>
<tr>
<td>H</td>
<td>4.23333800</td>
<td>1.46020600</td>
<td>-2.26948900</td>
</tr>
<tr>
<td>H</td>
<td>4.43640000</td>
<td>1.05965900</td>
<td>-0.54761600</td>
</tr>
<tr>
<td>H</td>
<td>-4.74232000</td>
<td>1.87900500</td>
<td>-0.00575600</td>
</tr>
<tr>
<td>C</td>
<td>-3.95168300</td>
<td>1.35107000</td>
<td>0.54132500</td>
</tr>
<tr>
<td>Si</td>
<td>-3.13288100</td>
<td>0.08020500</td>
<td>-0.56932100</td>
</tr>
<tr>
<td>H</td>
<td>-3.22643400</td>
<td>2.09565800</td>
<td>0.88300800</td>
</tr>
<tr>
<td>H</td>
<td>-4.40765200</td>
<td>0.87039600</td>
<td>1.41353300</td>
</tr>
<tr>
<td>O</td>
<td>-2.19110700</td>
<td>-0.87424000</td>
<td>0.54606200</td>
</tr>
<tr>
<td>C</td>
<td>-4.39828400</td>
<td>-1.08203800</td>
<td>-1.36377700</td>
</tr>
<tr>
<td>C</td>
<td>-2.04293300</td>
<td>0.87508100</td>
<td>-1.89866700</td>
</tr>
<tr>
<td>C</td>
<td>-0.98586200</td>
<td>-2.37829500</td>
<td>-0.91378100</td>
</tr>
<tr>
<td>H</td>
<td>-3.92013300</td>
<td>-1.89803600</td>
<td>-1.91675300</td>
</tr>
<tr>
<td>H</td>
<td>-5.05637500</td>
<td>-1.52630400</td>
<td>-0.60906500</td>
</tr>
<tr>
<td>H</td>
<td>-5.02726700</td>
<td>-0.52651200</td>
<td>-2.06996500</td>
</tr>
<tr>
<td>H</td>
<td>-1.05010200</td>
<td>1.12593700</td>
<td>-1.51259500</td>
</tr>
<tr>
<td>H</td>
<td>-1.91821800</td>
<td>0.23496200</td>
<td>-2.77927300</td>
</tr>
<tr>
<td>H</td>
<td>-2.50661200</td>
<td>1.81078800</td>
<td>-2.23242400</td>
</tr>
<tr>
<td>C</td>
<td>-1.45247100</td>
<td>-1.97848200</td>
<td>0.37135800</td>
</tr>
<tr>
<td>C</td>
<td>-0.13394700</td>
<td>-3.43094900</td>
<td>-1.10059300</td>
</tr>
<tr>
<td>H</td>
<td>-1.17180500</td>
<td>-1.70749500</td>
<td>-1.74774400</td>
</tr>
<tr>
<td>C</td>
<td>-0.96141800</td>
<td>-2.61248800</td>
<td>1.52713600</td>
</tr>
<tr>
<td>H</td>
<td>-0.80301100</td>
<td>-3.68346200</td>
<td>1.48674900</td>
</tr>
<tr>
<td>H</td>
<td>-1.30640000</td>
<td>-2.23050400</td>
<td>2.48323300</td>
</tr>
<tr>
<td>H</td>
<td>-0.04203900</td>
<td>-4.23631900</td>
<td>-0.38430600</td>
</tr>
<tr>
<td>H</td>
<td>0.32830800</td>
<td>-3.60473200</td>
<td>-2.06699700</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy

Diene 14 (cis)
<table>
<thead>
<tr>
<th>Atoms</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.47415500</td>
<td>-0.57527300</td>
<td>0.11045800</td>
</tr>
<tr>
<td>C</td>
<td>1.81221600</td>
<td>0.03674500</td>
<td>0.13424700</td>
</tr>
<tr>
<td>H</td>
<td>1.85178600</td>
<td>1.06035900</td>
<td>0.49296800</td>
</tr>
<tr>
<td>C</td>
<td>0.23220100</td>
<td>-1.88875700</td>
<td>0.28257500</td>
</tr>
<tr>
<td>H</td>
<td>-0.75820000</td>
<td>-2.31881100</td>
<td>0.19019400</td>
</tr>
<tr>
<td>H</td>
<td>1.04256200</td>
<td>-2.56605700</td>
<td>0.52264100</td>
</tr>
<tr>
<td>C</td>
<td>2.91218100</td>
<td>-0.59193100</td>
<td>-0.31489700</td>
</tr>
<tr>
<td>O</td>
<td>4.18827300</td>
<td>-0.13975400</td>
<td>-0.32096900</td>
</tr>
<tr>
<td>C</td>
<td>4.42481200</td>
<td>1.14758300</td>
<td>0.23093700</td>
</tr>
<tr>
<td>H</td>
<td>5.50104300</td>
<td>1.31563400</td>
<td>0.16292900</td>
</tr>
<tr>
<td>H</td>
<td>3.89424200</td>
<td>1.92402400</td>
<td>-0.33539100</td>
</tr>
<tr>
<td>H</td>
<td>4.10724500</td>
<td>1.19041400</td>
<td>1.28098200</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>O</td>
<td>-0.48709600</td>
<td>0.37807500</td>
<td>-0.10245400</td>
</tr>
<tr>
<td>Si</td>
<td>-2.19738400</td>
<td>0.24220700</td>
<td>-0.03022700</td>
</tr>
<tr>
<td>C</td>
<td>-2.75106900</td>
<td>-0.39352000</td>
<td>1.66342400</td>
</tr>
<tr>
<td>H</td>
<td>-2.36621500</td>
<td>-1.39489600</td>
<td>1.87815500</td>
</tr>
<tr>
<td>H</td>
<td>-2.40698600</td>
<td>0.27319600</td>
<td>2.46198100</td>
</tr>
<tr>
<td>H</td>
<td>-3.84608400</td>
<td>-0.43438500</td>
<td>1.71114300</td>
</tr>
<tr>
<td>C</td>
<td>-2.76948300</td>
<td>2.01965700</td>
<td>-0.29195600</td>
</tr>
<tr>
<td>H</td>
<td>-2.42202500</td>
<td>2.40692900</td>
<td>-1.25598200</td>
</tr>
<tr>
<td>H</td>
<td>-3.86368600</td>
<td>2.08837000</td>
<td>-0.27608300</td>
</tr>
<tr>
<td>H</td>
<td>-2.37987400</td>
<td>2.67706700</td>
<td>0.49297500</td>
</tr>
<tr>
<td>C</td>
<td>-2.84950600</td>
<td>-0.86556000</td>
<td>-1.41944900</td>
</tr>
<tr>
<td>H</td>
<td>-2.48501100</td>
<td>-0.52191400</td>
<td>-2.39399300</td>
</tr>
<tr>
<td>H</td>
<td>-2.54930300</td>
<td>-1.91151400</td>
<td>-1.30235000</td>
</tr>
<tr>
<td>H</td>
<td>-3.94572400</td>
<td>-0.83299600</td>
<td>-1.44307900</td>
</tr>
<tr>
<td>H</td>
<td>2.86713400</td>
<td>-1.58657600</td>
<td>-0.74856100</td>
</tr>
</tbody>
</table>

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-468.807947, -468.583268, -468.566806, -468.626415

Diene 14 (trans)
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.42411600</td>
<td>-0.38508600</td>
<td>-0.14415500</td>
</tr>
<tr>
<td>C</td>
<td>-1.67257900</td>
<td>0.34901100</td>
<td>-0.38915300</td>
</tr>
<tr>
<td>H</td>
<td>-1.58969300</td>
<td>1.31968700</td>
<td>-0.87065400</td>
</tr>
<tr>
<td>C</td>
<td>-0.32169200</td>
<td>-1.72870400</td>
<td>-0.12977800</td>
</tr>
<tr>
<td>H</td>
<td>0.59581000</td>
<td>-2.24229700</td>
<td>0.13324200</td>
</tr>
<tr>
<td>H</td>
<td>-1.17486600</td>
<td>-2.34389200</td>
<td>-0.38785700</td>
</tr>
<tr>
<td>C</td>
<td>-2.87928000</td>
<td>-0.09785700</td>
<td>-0.01234400</td>
</tr>
<tr>
<td>O</td>
<td>-4.02251600</td>
<td>0.56412500</td>
<td>-0.32847000</td>
</tr>
<tr>
<td>C</td>
<td>-5.16751800</td>
<td>0.19617600</td>
<td>0.42839600</td>
</tr>
<tr>
<td>H</td>
<td>-6.01681200</td>
<td>0.71780300</td>
<td>-0.01717900</td>
</tr>
<tr>
<td>H</td>
<td>-5.34521100</td>
<td>-0.88744200</td>
<td>0.38212100</td>
</tr>
<tr>
<td>H</td>
<td>-5.06693100</td>
<td>0.49871100</td>
<td>1.47922600</td>
</tr>
<tr>
<td>O</td>
<td>0.61726800</td>
<td>0.47967900</td>
<td>0.06753200</td>
</tr>
<tr>
<td>Si</td>
<td>2.30675100</td>
<td>0.17182600</td>
<td>0.05476800</td>
</tr>
<tr>
<td>C</td>
<td>2.81119900</td>
<td>-0.67635200</td>
<td>-1.55922100</td>
</tr>
<tr>
<td>H</td>
<td>2.30098300</td>
<td>-1.63471700</td>
<td>-1.69462100</td>
</tr>
<tr>
<td>H</td>
<td>2.57076200</td>
<td>-0.04640300</td>
<td>-2.42282700</td>
</tr>
<tr>
<td>H</td>
<td>3.89202800</td>
<td>-0.86208500</td>
<td>-1.57039700</td>
</tr>
<tr>
<td>C</td>
<td>3.05109800</td>
<td>1.89968600</td>
<td>0.17340000</td>
</tr>
<tr>
<td>H</td>
<td>2.73602300</td>
<td>2.40006700</td>
<td>1.09593200</td>
</tr>
<tr>
<td>H</td>
<td>4.14672300</td>
<td>1.85788900</td>
<td>0.17048200</td>
</tr>
<tr>
<td>H</td>
<td>2.73481200</td>
<td>2.52285600</td>
<td>-0.66975300</td>
</tr>
<tr>
<td>C</td>
<td>2.82594100</td>
<td>-0.86085000</td>
<td>1.55473800</td>
</tr>
</tbody>
</table>

S45
H  2.46014000  -0.40915100  2.48370200
H  2.44965200  -1.88789100  1.51347800
H  3.92016900  -0.90912000  1.61631200
H  -3.00443900  -1.02641300  0.54623100

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-468.803546, -468.581280, -468.564374, -468.625513

TS-endo-syn-near-cis for 14 + 6
C  0.84260800  2.83595500  1.10906300
C  1.67175400  2.06339700  0.23035000
C  1.69548000  0.57492700  0.47423600
C  1.15059300  0.00071400  1.56811600
C  0.42053000  0.83725700  2.56000500
C  0.09248800  2.23986300  2.14476000
H  0.88214800  3.91565900  0.99998500
H  -0.17799600  2.86022700  2.99737700
O  0.08006300  0.38733300  3.64948300
O  2.38809900  2.52904400  -0.67189400
C  1.26230900  -1.48386000  1.84285100
H  0.26869600  -1.85126600  2.11966700
C  2.45652900  -0.25033800  -0.52320200
H  3.38771100  0.26311800  -0.78152700
C  2.69870400  -1.70208300  -0.08159900
H  3.62641900  -1.79649100  0.49683000
O  1.58589300  -2.20732000  0.64726800
O  1.68131500  -0.36653400  -1.75513300
C  1.82136300  -1.60664800  -2.30430200
O  1.28332400  -1.91214100  -3.33751000
C  2.73017900  -2.44327600  -1.41208700
H  3.73840300  -2.45027600  -1.84409900
H  2.37586000  -3.47309400  -1.33863700
C  2.23262400  -1.81429100  2.98694200
H  1.87039000  -1.36023500  3.91201300
H  2.28703400  -2.90011400  3.11625300
H  3.24034600  -1.43342900  2.78764500
H  -1.92775400  -3.21782200  -1.61093400
C  -1.56291500  -2.25724700  -1.22603600
Si -2.92308100  -1.42863200  -0.21891700
H  -0.68151400  -2.45879100  -0.60703900
H  -1.23192400  -1.66896300  -2.08768200
O  -2.27467900  -0.17173000  0.79261900
C  -4.26583100  -0.68482300  -1.32210000

S46
C  -3.64229700  -2.61932800  1.04905200
C  -1.90621500  1.09829800  0.53339800
H  -5.06583700  -0.23232400  -0.72594600
H  -3.86916200   0.08478200  -1.99221300
H  -4.71395900  -1.46836300  -1.94470100
H  -2.86150200  -2.99695400   1.71821800
H  -4.40397700  -2.13029700  1.66555000
H  -4.10689600  -3.48131700  0.55619200
C  -1.42906600   1.47415400  -0.74715200
C  -1.83313700   1.95953800  1.65290700
H  -1.28690200   0.69694000  -1.48891700
C  -0.99697400   2.75440700  -1.02364000
H  -2.26334200  1.57358500  2.57262000
H  -2.01171500  3.01588400  1.48528500
O  -0.42244800  3.18596600  -2.13651800
C  -0.04853000  2.23843800  -3.15197400
H  -0.42244800  3.18596600  -2.13651800
H  -0.42244800  3.18596600  -2.13651800
C  -0.43933500  0.25886300   2.62239800
C  -0.43933500  0.25886300  2.62239800
C  -0.71745600  1.71475600  2.41207000
H  2.18598400   3.07610100  1.57509300
H  0.59458000  2.29394300   2.9387300
O  0.41432400  2.09173600   1.51364100
O  3.22058200  1.43283200  -0.21454300
C  0.41432400  2.09173600   1.51364100
H  0.41432400  2.09173600  1.51364100
H  0.41432400  2.09173600  1.51364100
H  0.41432400  2.09173600  1.51364100
O  0.41432400  2.09173600  1.51364100
O  0.41432400  2.09173600  1.51364100
H  0.41432400  2.09173600  1.51364100
H  0.41432400  2.09173600  1.51364100
O  0.41432400  2.09173600  1.51364100
C  -1.82338800  -2.6182300  -0.28695800
H  2.59751200  -3.13325300   0.29478900
O  0.54686200  -2.74407900   0.33091400
O  1.50243800  -0.78566400  -1.75972200

Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1308.173390, -1307.73881, -1307.708725, -1307.79756

TS-endo-syn-near-trans for 14 + 6

S47
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1308.171725, -1307.738011, -1307.707608, -1307.797713

**TS-endo-syn-dist-cis for 14 + 6**

C  -1.59764900  -0.87651900  2.35836700
C  -0.10838600  -1.01195400  2.27407300
C     0.45313600  -1.44529500   0.96741500  
C    -0.34908100  -1.93547500  -0.00546600  
C     -1.84845600  -2.02406400   0.16240300  
C     -2.39054300  -1.52604000  1.39312400  
H    -1.94656800   -0.86751000  3.38878900  
H    -3.44427600  -1.71804700  1.57194500  
O     -2.52287700  -2.54993000  -0.74705400  
O     0.61710100  -0.81372500   3.24147800  
C     0.22861900  -2.46953300  -1.29736800  
H    -0.33259900  -2.02830600  -2.12722400  
C     1.94975100  -1.46533600   0.83804100  
H     2.38892600  -1.85358600   1.76298700  
C     2.44261400  -2.23879400  -0.39393000  
H     2.55308700  -3.30964500  -0.18191700  
O     1.57391900  -2.01793300  -1.49757300  
O     2.47398100  -0.11553800   0.65826800  
C     3.52834100  -0.12067200  -0.20193800  
O     4.14489400   0.88009400  -0.47181800  
C     3.75550200  -1.53803100  -0.71318300  
H     4.59443800  -1.98258800  -0.16417000  
H     3.99552100  -1.54072600  -1.77809100  
C     0.11646800   -3.99878800  -0.44294700  
H    -0.93817100  -4.28026300  -1.42075800  
H     0.58655400  -4.32316500  -2.34863000  
H     0.60758800  -4.50946400  -0.57917300  
H     2.66355800  -4.40391500  -0.32079300  
C     2.19618600   3.64900800   0.32329100  
Si    0.59456200   3.04640100  -0.44294700  
H     2.90647300   2.82572000   0.44408100  
H     2.01127700   4.10689400   1.30098600  
O    -0.18322900   2.19497900   0.86656600  
C    -0.53930600   4.48539400  -0.92054000  
C     0.88533200   1.91024400  -1.92978000  
C    -2.15110400   1.28821200  -0.17631500  
H    -1.52244600   4.14496900  -1.26311100  
H    -0.69473600   5.16252900  -0.07357000  
H    -0.08612700   5.06607600  -1.73314200  
H     1.11729600   0.88718500  -1.61784900  
H     0.03046800   1.87729800  -2.61470800  
H     1.74778300   2.27873100  -2.49765000  
C    -1.37777100   1.60167600   0.97669400  
C    -3.37000600   0.65848700  -0.09948200  
H    -1.70829200   1.46278800  -1.14933300  
C    -1.74005500   1.15573900   2.26704300
### Energies at 0K, H and G at 298.15 K

E (0K), E+ZPE (0K), Enthalpy, Free Energy

-1308.171238, -1307.736644, -1307.706566, -1307.795333

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>-4.10710100</td>
<td>0.20485200</td>
<td>-1.10772500</td>
</tr>
<tr>
<td>C</td>
<td>-3.54234700</td>
<td>0.17055900</td>
<td>-2.42314900</td>
</tr>
<tr>
<td>H</td>
<td>-2.62152300</td>
<td>-0.41715400</td>
<td>-2.42424500</td>
</tr>
<tr>
<td>H</td>
<td>-4.29009700</td>
<td>-0.31628700</td>
<td>-3.04871800</td>
</tr>
<tr>
<td>H</td>
<td>-3.35616200</td>
<td>1.18715400</td>
<td>-2.78970200</td>
</tr>
<tr>
<td>H</td>
<td>-2.79626700</td>
<td>1.35492000</td>
<td>2.51108100</td>
</tr>
<tr>
<td>H</td>
<td>-1.09455100</td>
<td>1.47687400</td>
<td>3.07920400</td>
</tr>
<tr>
<td>H</td>
<td>-3.91600000</td>
<td>0.56669700</td>
<td>0.83019700</td>
</tr>
</tbody>
</table>

#### TS-endo-syn-dist-trans for 14 + 6

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.75551700</td>
<td>-0.23246000</td>
<td>2.32620100</td>
</tr>
<tr>
<td>C</td>
<td>-0.37988900</td>
<td>-0.81621400</td>
<td>2.25427500</td>
</tr>
<tr>
<td>C</td>
<td>0.00241400</td>
<td>-1.47363900</td>
<td>0.97597900</td>
</tr>
<tr>
<td>C</td>
<td>-0.92140900</td>
<td>-1.73883300</td>
<td>0.02337400</td>
</tr>
<tr>
<td>C</td>
<td>-2.37033700</td>
<td>-1.35539400</td>
<td>0.19365600</td>
</tr>
<tr>
<td>C</td>
<td>-2.71503900</td>
<td>-0.64891300</td>
<td>1.39267400</td>
</tr>
<tr>
<td>H</td>
<td>-2.07069500</td>
<td>-0.03968500</td>
<td>3.34882400</td>
</tr>
<tr>
<td>H</td>
<td>-3.77420700</td>
<td>-0.49389100</td>
<td>1.57998400</td>
</tr>
<tr>
<td>O</td>
<td>-3.19075500</td>
<td>-1.69294500</td>
<td>-0.68309000</td>
</tr>
<tr>
<td>O</td>
<td>0.38408000</td>
<td>-0.79718900</td>
<td>3.21220300</td>
</tr>
<tr>
<td>C</td>
<td>-0.54687400</td>
<td>-2.46076100</td>
<td>-1.25168400</td>
</tr>
<tr>
<td>H</td>
<td>-0.95518600</td>
<td>-1.88774100</td>
<td>-2.09017600</td>
</tr>
<tr>
<td>C</td>
<td>1.41617600</td>
<td>-1.96739700</td>
<td>0.85692600</td>
</tr>
<tr>
<td>H</td>
<td>1.70952200</td>
<td>-2.45172500</td>
<td>1.79455500</td>
</tr>
<tr>
<td>H</td>
<td>1.63676800</td>
<td>-2.89095600</td>
<td>-0.35117000</td>
</tr>
<tr>
<td>O</td>
<td>1.41156000</td>
<td>-3.93646300</td>
<td>-0.10548500</td>
</tr>
<tr>
<td>O</td>
<td>0.87090600</td>
<td>-2.44584900</td>
<td>-1.46248500</td>
</tr>
<tr>
<td>O</td>
<td>2.34229500</td>
<td>-0.86024000</td>
<td>0.65111400</td>
</tr>
<tr>
<td>C</td>
<td>3.34142800</td>
<td>-1.22117300</td>
<td>-0.19971300</td>
</tr>
<tr>
<td>O</td>
<td>4.24972800</td>
<td>-0.47869300</td>
<td>-0.47806000</td>
</tr>
<tr>
<td>C</td>
<td>3.10109900</td>
<td>-2.64506400</td>
<td>-0.68606500</td>
</tr>
<tr>
<td>H</td>
<td>3.76198400</td>
<td>-3.32385800</td>
<td>-0.13360900</td>
</tr>
<tr>
<td>H</td>
<td>3.31761700</td>
<td>-2.73989900</td>
<td>-1.75185200</td>
</tr>
<tr>
<td>C</td>
<td>-1.11892800</td>
<td>-3.88614000</td>
<td>-1.32849200</td>
</tr>
<tr>
<td>H</td>
<td>-2.20929900</td>
<td>-3.83517200</td>
<td>-1.32585700</td>
</tr>
<tr>
<td>H</td>
<td>-0.77859300</td>
<td>-4.35981400</td>
<td>-2.25483300</td>
</tr>
<tr>
<td>H</td>
<td>-0.79779500</td>
<td>-4.50224600</td>
<td>-0.48141100</td>
</tr>
<tr>
<td>H</td>
<td>4.04859000</td>
<td>3.31030000</td>
<td>-0.33133200</td>
</tr>
<tr>
<td>C</td>
<td>3.32989000</td>
<td>2.78837200</td>
<td>0.31219900</td>
</tr>
<tr>
<td>Si</td>
<td>1.64931000</td>
<td>2.71711400</td>
<td>-0.51746300</td>
</tr>
</tbody>
</table>
Energies at 0K, H and G at 298.15 K
E (0K), E+ZPE (0K), Enthalpy, Free Energy
-1308.173734, -1307.739462, -1307.709308, -1307.797995