Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

DFT Studies on Metal Catalyzed Cycloisomerization of *trans* 1,5-enynes to Cyclopropane Sesquiterpenoids.

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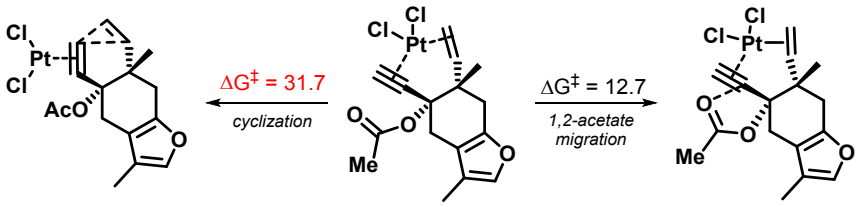
Computational methods

All structures were initially optimized using density functional theory (DFT) by using the M06[1] functional as implemented in Gaussian 09.[2] Optimizations were carried out in a solvent model (IEFPCM, solvent = toluene)[3] by using the 6-311G** basis set for non-metallic atoms and SDD[4] basis set for platinum and gold. Final energies were obtained with the basis set Def2TZVPP[5] and the functionals M06, ωB97X-D[6] and B3PW91[7], adding the D3 version of Grimme's dispersion[8] for the latter. The stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies.

Alternative mechanism

Figure S1. Alternative mechanism for the synthesis of **2**.[9]



The cyclopropanation of the substrate prior to the migration of the acetate was considered. However, this mechanism was discarded due to its high activation barrier ($\Delta G^{\ddagger}$ = 31.7 kcal).

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[4] (a) M. Dolg, U. Wedig, H. Stoll, and H. Preuss, *J. Chem. Phys*. 1987, **86**, 866. (b) D. Andrae, U. Haussermann, M. Dolg, H. Stoll and H. Preuss, *Theor. Chim. Acta* 1990, **77**, 123

[5] (a) F. Furche and R. Ahlrichs, *J. Chem. Phys*. 2003, **119**, 12753; (b) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297.

[6] J.-D. Chai and H. Head-Gordon, *Phys. Chem. Chem. Phys.* 2008, **10**, 6615

[7] J. P. Perdew in Electronic Structure of solids '91, 1991, Edited by P. Ziesche and H. Eschig (Akademic Verlag, Berlin), 11

[8] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*. 2010, **132**, 154104

[9] E. Soriano and J. Marco-Contelles, *J. Acc. Chem. Res.,* 2009, **42**, 1026.

Kinetic simulations with COPASI

The kinetic simulations shown in Table 1 were performed with the version 4.24 of COPASI (COmplex PAthway SImulator) [10], available at http://copasi.org/.

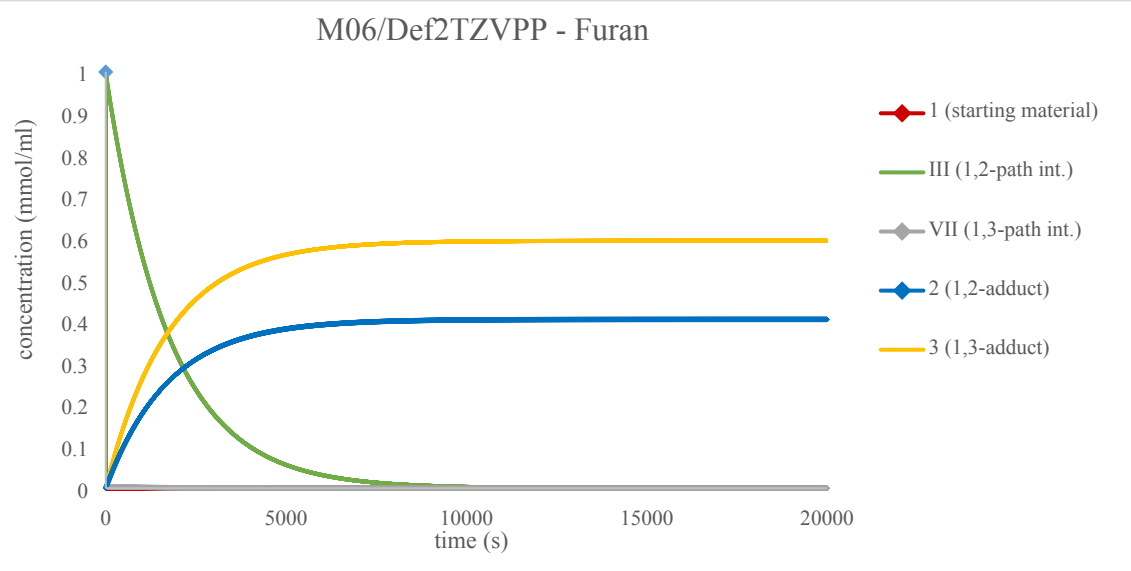
This software was used to calculate the concentration of the species during the reaction curse. A simple mass action law was selected, where the forward and backward rate constants were calculated from the free energies obtained by the DFT Gaussian calculations utilizing the Eyring equation:

$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

Where k = reaction rate (k_f if forward, k_b if backwards), k_B = Boltzmann constant, T = temperature, h = Planck's constant, R = gas constant and $\Delta G^{\ddagger} = G_{TS} - G_{SM}$ for k_f and $G_{TS} - G_{prod}$ for k_b. The temperature chosen for the simulations was 110°C, in accordance with the experimental conditions. The plotted simulations (S2-S7) were obtained performing a Time Course calculation, which simulates a time span starting from a set of initial concentrations.

This are the results of the performed Time Course simulations for each functional, with toluene as solvent.

Figure S2. Time course results for the furan, using M06/Def2TZVPP as level of theory, in toluene



[10] S. Hoops, S. Sahle, R. Gauges, C. Lee, J. Pahle, N. Simus, M. Singhal, L. Xu, P. Mendes and U. Kummer, *Bioinformatics,* 2006, **22**, 3067.

Figure S3. Time course results for the lactone, using M06/Def2TZVPP as level of theory, in toluene

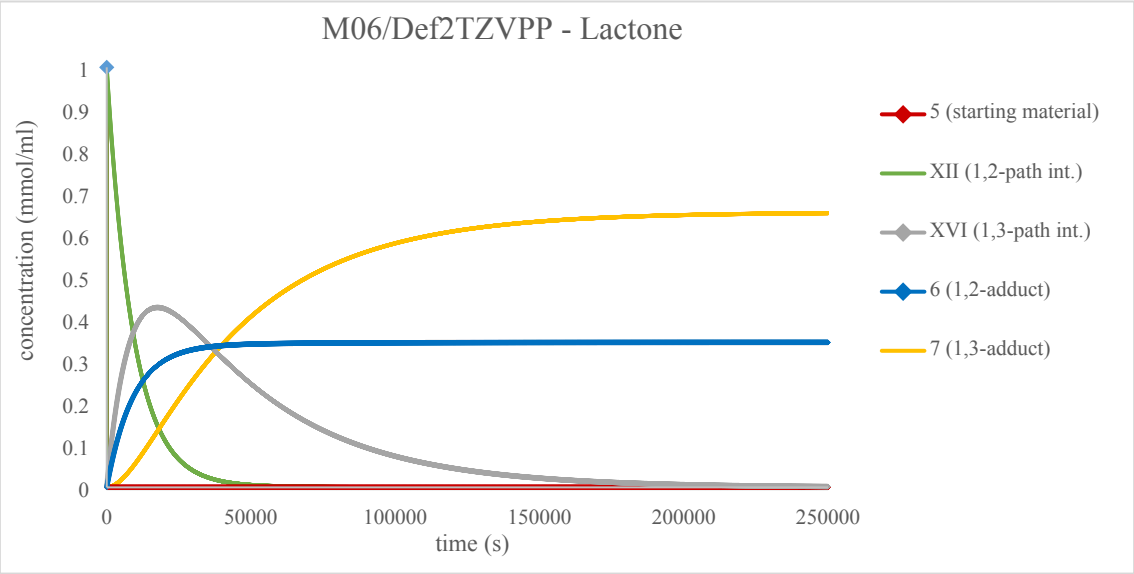


Figure S4. Time course results for the furan, using wB97XD/Def2TZVPP as level of theory, in toluene

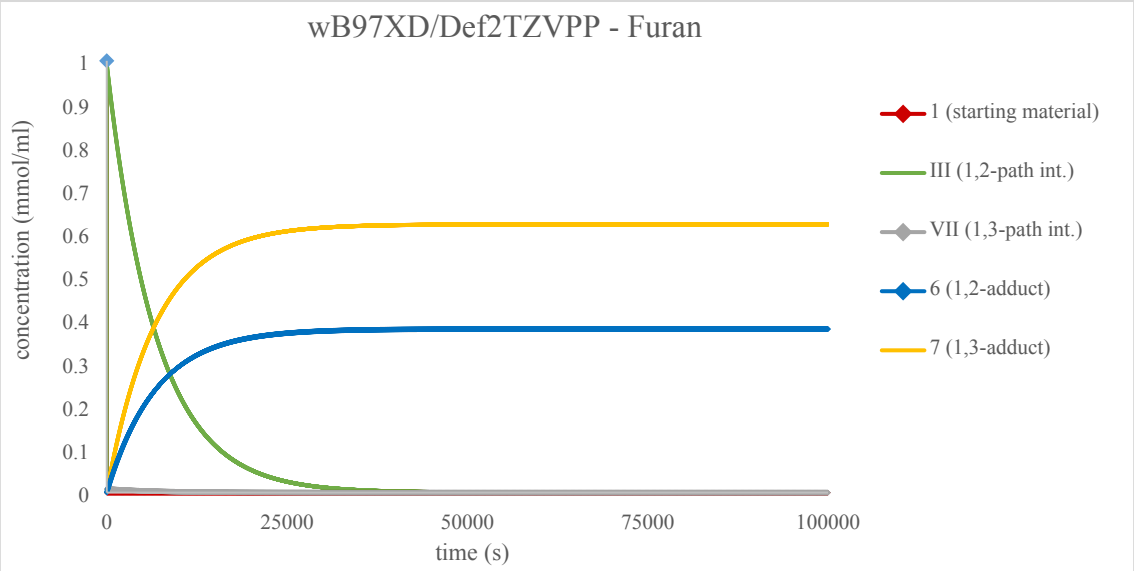


Figure S5. Time course results for the lactone, using wB97XD/Def2TZVPP as level of theory, in toluene

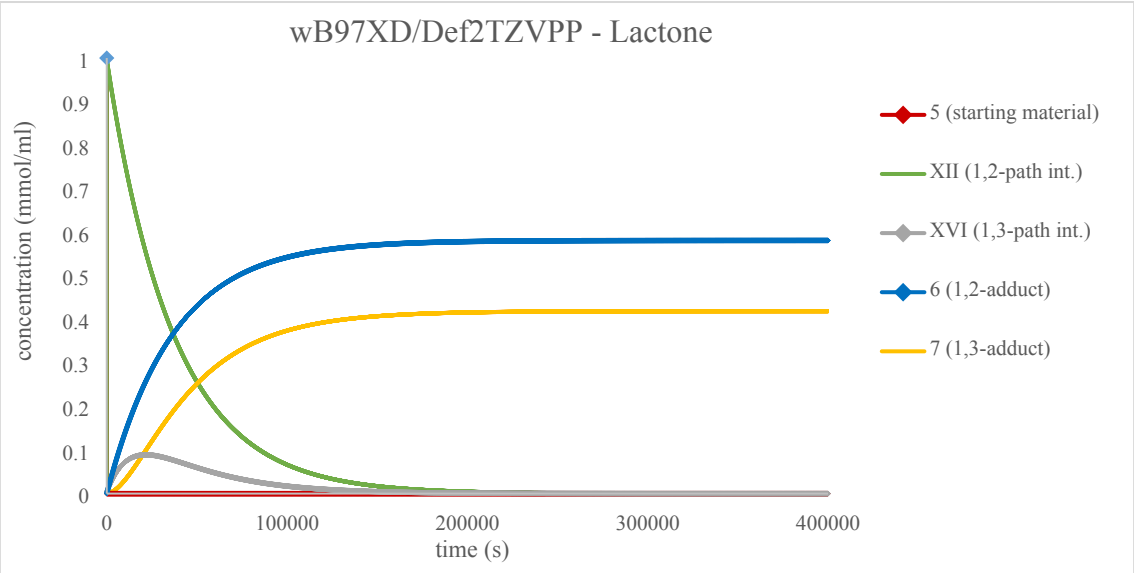


Figure S6. Time course results for the furan, using B3PW91/Def2TZVPP as level of theory, in toluene

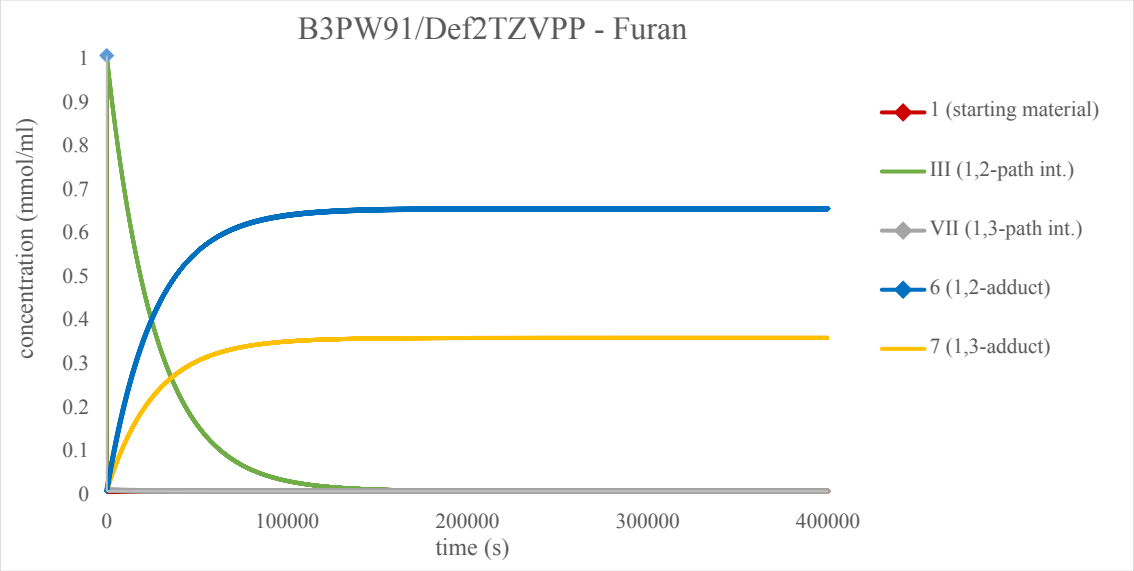
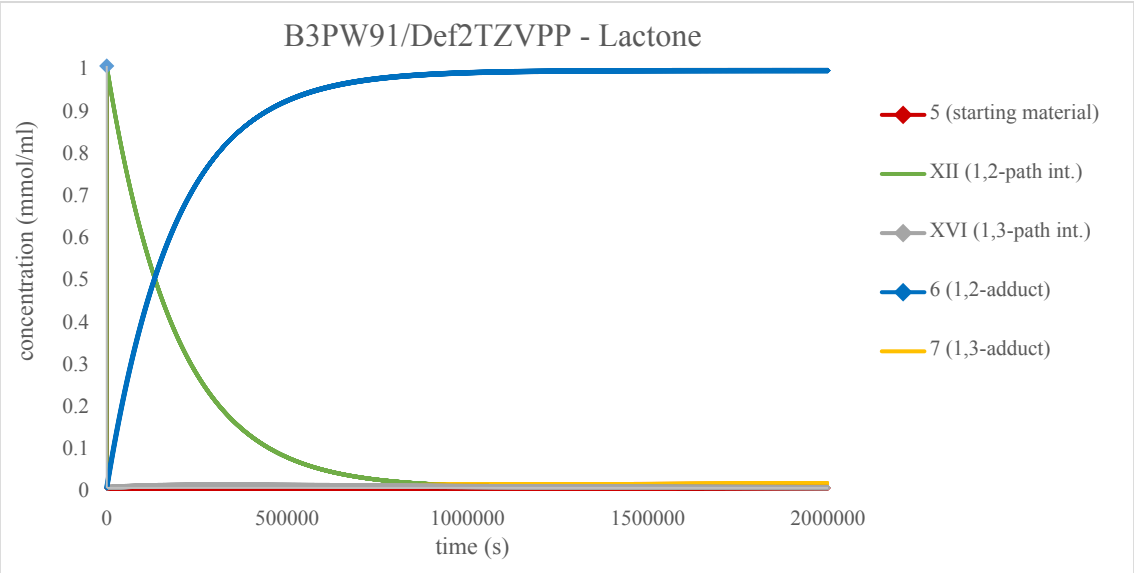


Figure S7. Time course results for the lactone, using B3PW91/Def2TZVPP as level of theory, in toluene



Structure 1

- **Thermal correction to Gibbs Free Energy = 0.253571 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -845.871045987 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.681000	-0.480000	-0.131000
2	6	0	-6.836000	0.999000	-0.533000
3	6	0	-5.716000	1.902000	0.098000
4	6	0	-4.338000	1.440000	-0.408000
5	6	0	-4.248000	-0.031000	-0.355000
6	1	0	-3.557000	1.904000	0.210000
7	1	0	-4.179000	1.787000	-1.437000
8	6	0	-5.266000	-0.913000	-0.258000
9	1	0	-7.361000	-1.076000	-0.747000
10	1	0	-7.042000	-0.586000	0.902000
11	6	0	-4.679000	-2.221000	-0.296000
12	6	0	-3.346000	-2.006000	-0.416000
13	8	0	-3.062000	-0.673000	-0.455000
14	1	0	-2.499000	-2.673000	-0.480000
15	6	0	-5.397000	-3.520000	-0.220000
16	1	0	-6.117000	-3.626000	-1.039000
17	1	0	-5.962000	-3.610000	0.715000
18	1	0	-4.702000	-4.363000	-0.274000
19	6	0	-5.764000	1.789000	1.627000
20	1	0	-5.496000	0.785000	1.970000
21	1	0	-6.757000	2.036000	2.014000
22	1	0	-5.049000	2.495000	2.059000
23	6	0	-5.978000	3.345000	-0.250000
24	6	0	-5.128000	4.207000	-0.787000
25	1	0	-6.969000	3.699000	0.036000
26	1	0	-4.120000	3.936000	-1.089000

27	1	0	-5.414000	5.241000	-0.947000
28	8	0	-6.626000	1.170000	-1.956000
29	6	0	-8.168000	1.470000	-0.153000
30	6	0	-9.245000	1.850000	0.210000
31	1	0	-10.210000	2.179000	0.516000
32	6	0	-7.459000	0.611000	-2.855000
33	6	0	-7.022000	0.973000	-4.239000
34	1	0	-6.984000	2.060000	-4.344000
35	1	0	-7.714000	0.548000	-4.965000
36	1	0	-6.013000	0.593000	-4.419000
37	8	0	-8.404000	-0.073000	-2.576000

Structure I

- **Thermal correction to Gibbs Free Energy = 0.254289 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.74778452 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.73455709 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.09630073 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1886.01647289 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.13315663 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.12065287 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.852000	-0.211000	-0.140000
2	6	0	-6.818000	1.251000	-0.602000
3	6	0	-5.639000	2.020000	0.058000
4	6	0	-4.303000	1.470000	-0.482000
5	6	0	-4.377000	-0.009000	-0.443000
6	1	0	-3.483000	1.841000	0.147000
7	1	0	-4.120000	1.831000	-1.502000

8	6	0	-5.483000	-0.779000	-0.302000
9	1	0	-7.600000	-0.754000	-0.723000
10	1	0	-7.190000	-0.246000	0.904000
11	6	0	-5.037000	-2.141000	-0.340000
12	6	0	-3.693000	-2.069000	-0.501000
13	8	0	-3.272000	-0.773000	-0.566000
14	1	0	-2.923000	-2.820000	-0.583000
15	6	0	-5.885000	-3.356000	-0.226000
16	1	0	-6.623000	-3.405000	-1.035000
17	1	0	-6.443000	-3.366000	0.717000
18	1	0	-5.282000	-4.267000	-0.269000
19	6	0	-5.667000	1.830000	1.582000
20	1	0	-5.329000	0.830000	1.862000
21	1	0	-6.660000	1.993000	2.012000
22	1	0	-4.990000	2.554000	2.046000
23	6	0	-5.751000	3.504000	-0.225000
24	6	0	-6.352000	4.145000	-1.305000
25	8	0	-6.556000	1.307000	-2.024000
26	6	0	-8.061000	1.997000	-0.329000
27	6	0	-9.151000	2.558000	-0.349000
28	6	0	-7.458000	0.815000	-2.910000
29	6	0	-6.942000	0.995000	-4.299000
30	1	0	-6.763000	2.056000	-4.495000
31	1	0	-7.664000	0.602000	-5.013000
32	1	0	-5.985000	0.479000	-4.410000
33	8	0	-8.507000	0.328000	-2.598000
34	78	0	-7.766000	4.161000	0.359000
35	1	0	-10.194000	2.795000	-0.390000
36	17	0	-9.625000	4.570000	1.762000
37	17	0	-6.814000	6.162000	1.097000
38	1	0	-6.108000	5.186000	-1.492000
39	1	0	-6.796000	3.597000	-2.129000
40	1	0	-5.070000	4.106000	0.379000

Transition state: TS I-II

- **Thermal correction to Gibbs Free Energy = 0.255119 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.72835311 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.71018085 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.08168497 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1885.99792614 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.11478504 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.09681596 Hartree**
- **Frequency = -333.3**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.841000	-0.339000	-0.049000
2	6	0	-6.904000	1.104000	-0.571000
3	6	0	-5.764000	1.968000	0.043000
4	6	0	-4.416000	1.454000	-0.517000
5	6	0	-4.397000	-0.022000	-0.422000
6	1	0	-3.604000	1.897000	0.074000
7	1	0	-4.280000	1.792000	-1.553000
8	6	0	-5.450000	-0.846000	-0.212000
9	1	0	-7.566000	-0.956000	-0.592000
10	1	0	-7.169000	-0.348000	0.998000
11	6	0	-4.927000	-2.181000	-0.198000
12	6	0	-3.595000	-2.038000	-0.403000
13	8	0	-3.253000	-0.726000	-0.541000
14	1	0	-2.784000	-2.748000	-0.471000
15	6	0	-5.697000	-3.436000	0.006000
16	1	0	-6.456000	-3.572000	-0.773000
17	1	0	-6.222000	-3.428000	0.967000
18	1	0	-5.042000	-4.311000	-0.011000

19	6	0	-5.760000	1.793000	1.572000
20	1	0	-5.378000	0.813000	1.868000
21	1	0	-6.753000	1.934000	2.009000
22	1	0	-5.106000	2.552000	2.012000
23	6	0	-5.865000	3.453000	-0.233000
24	6	0	-6.507000	4.141000	-1.260000
25	8	0	-6.720000	1.005000	-2.034000
26	6	0	-8.210000	1.754000	-0.441000
27	6	0	-8.889000	2.802000	-0.183000
28	6	0	-7.877000	0.725000	-2.597000
29	6	0	-7.830000	0.405000	-4.038000
30	1	0	-7.208000	1.137000	-4.558000
31	1	0	-8.836000	0.385000	-4.452000
32	1	0	-7.358000	-0.574000	-4.166000
33	8	0	-8.900000	0.743000	-1.914000
34	78	0	-7.701000	4.326000	0.534000
35	1	0	-9.931000	3.005000	-0.399000
36	17	0	-9.467000	4.884000	1.993000
37	17	0	-6.432000	6.214000	1.238000
38	1	0	-6.170000	5.145000	-1.499000
39	1	0	-7.082000	3.641000	-2.032000
40	1	0	-5.070000	4.001000	0.277000

Structure II

- **Thermal correction to Gibbs Free Energy = 0.25734 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.73895252 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.872000	-0.266000	-0.040000
2	6	0	-6.927000	1.189000	-0.521000

3	6	0	-5.781000	2.023000	0.075000
4	6	0	-4.444000	1.507000	-0.510000
5	6	0	-4.435000	0.029000	-0.447000
6	1	0	-3.618000	1.932000	0.075000
7	1	0	-4.321000	1.863000	-1.542000
8	6	0	-5.492000	-0.791000	-0.238000
9	1	0	-7.617000	-0.869000	-0.575000
10	1	0	-7.182000	-0.286000	1.013000
11	6	0	-4.982000	-2.130000	-0.262000
12	6	0	-3.652000	-1.995000	-0.486000
13	8	0	-3.301000	-0.683000	-0.601000
14	1	0	-2.849000	-2.710000	-0.583000
15	6	0	-5.759000	-3.383000	-0.076000
16	1	0	-6.530000	-3.496000	-0.847000
17	1	0	-6.271000	-3.394000	0.893000
18	1	0	-5.113000	-4.263000	-0.122000
19	6	0	-5.766000	1.809000	1.603000
20	1	0	-5.392000	0.819000	1.875000
21	1	0	-6.755000	1.954000	2.045000
22	1	0	-5.101000	2.553000	2.052000
23	6	0	-5.855000	3.518000	-0.147000
24	6	0	-6.471000	4.253000	-1.159000
25	8	0	-6.775000	1.026000	-2.055000
26	6	0	-8.276000	1.797000	-0.537000
27	6	0	-8.776000	2.949000	-0.132000
28	6	0	-7.963000	0.857000	-2.495000
29	6	0	-8.212000	0.400000	-3.863000
30	1	0	-7.479000	0.849000	-4.536000
31	1	0	-9.229000	0.638000	-4.168000
32	1	0	-8.068000	-0.685000	-3.898000
33	8	0	-8.917000	1.099000	-1.682000
34	78	0	-7.654000	4.416000	0.640000
35	1	0	-9.801000	3.186000	-0.419000
36	17	0	-9.421000	4.965000	2.109000
37	17	0	-6.295000	6.270000	1.396000

38	1	0	-6.104000	5.253000	-1.369000
39	1	0	-7.051000	3.788000	-1.950000
40	1	0	-5.047000	4.030000	0.379000

Transition state: TS II-III

- **Thermal correction to Gibbs Free Energy = 0.255122 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.73402325 Hartree**
- **Frequency = -302.3**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.908000	-0.269000	-0.048000
2	6	0	-6.997000	1.201000	-0.400000
3	6	0	-5.822000	2.027000	0.087000
4	6	0	-4.519000	1.516000	-0.581000
5	6	0	-4.493000	0.040000	-0.534000
6	1	0	-3.666000	1.945000	-0.042000
7	1	0	-4.468000	1.885000	-1.614000
8	6	0	-5.536000	-0.786000	-0.296000
9	1	0	-7.676000	-0.849000	-0.568000
10	1	0	-7.182000	-0.332000	1.018000
11	6	0	-5.021000	-2.123000	-0.344000
12	6	0	-3.701000	-1.978000	-0.611000
13	8	0	-3.361000	-0.663000	-0.729000
14	1	0	-2.898000	-2.687000	-0.740000
15	6	0	-5.786000	-3.380000	-0.138000
16	1	0	-6.577000	-3.496000	-0.888000
17	1	0	-6.271000	-3.395000	0.845000
18	1	0	-5.136000	-4.256000	-0.203000
19	6	0	-5.729000	1.803000	1.616000
20	1	0	-5.382000	0.798000	1.865000

21	1	0	-6.689000	1.990000	2.106000
22	1	0	-5.010000	2.521000	2.021000
23	6	0	-5.892000	3.523000	-0.127000
24	6	0	-6.473000	4.245000	-1.168000
25	8	0	-6.916000	0.947000	-2.257000
26	6	0	-8.309000	1.781000	-0.544000
27	6	0	-8.786000	2.969000	-0.167000
28	6	0	-8.121000	0.786000	-2.506000
29	6	0	-8.643000	0.352000	-3.813000
30	1	0	-7.842000	-0.046000	-4.432000
31	1	0	-9.098000	1.215000	-4.309000
32	1	0	-9.430000	-0.390000	-3.664000
33	8	0	-9.002000	1.026000	-1.562000
34	78	0	-7.695000	4.434000	0.604000
35	1	0	-9.822000	3.185000	-0.435000
36	17	0	-9.501000	5.001000	2.016000
37	17	0	-6.345000	6.279000	1.404000
38	1	0	-6.096000	5.240000	-1.384000
39	1	0	-7.033000	3.765000	-1.965000
40	1	0	-5.091000	4.032000	0.411000

Structure III

- **Thermal correction to Gibbs Free Energy = 0.250772 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.76033637 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.74331208 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.11650527 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1886.03791902 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.14915603 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.13248851 Hartree**

Cartesian Coordinates of the computed structure:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-6.830000	-0.307000	-0.756000
2	6	0	-7.026000	1.153000	-0.459000
3	6	0	-5.910000	1.961000	0.165000
4	6	0	-4.504000	1.500000	-0.318000
5	6	0	-4.424000	0.032000	-0.308000
6	1	0	-3.748000	1.949000	0.338000
7	1	0	-4.320000	1.896000	-1.328000
8	6	0	-5.460000	-0.807000	-0.505000
9	1	0	-7.130000	-0.471000	-1.805000
10	1	0	-7.587000	-0.867000	-0.184000
11	6	0	-4.930000	-2.137000	-0.436000
12	6	0	-3.605000	-1.970000	-0.199000
13	8	0	-3.278000	-0.647000	-0.115000
14	1	0	-2.792000	-2.666000	-0.065000
15	6	0	-5.682000	-3.409000	-0.593000
16	1	0	-6.176000	-3.461000	-1.570000
17	1	0	-6.463000	-3.508000	0.169000
18	1	0	-5.020000	-4.274000	-0.507000
19	6	0	-6.023000	1.725000	1.685000
20	1	0	-5.938000	0.663000	1.933000
21	1	0	-6.974000	2.104000	2.067000
22	1	0	-5.211000	2.260000	2.189000
23	6	0	-5.921000	3.443000	-0.128000
24	6	0	-6.292000	4.017000	-1.341000
25	8	0	-9.158000	1.714000	-3.097000
26	6	0	-8.295000	1.643000	-0.630000
27	6	0	-8.761000	2.920000	-0.306000
28	6	0	-9.627000	0.874000	-2.388000
29	6	0	-10.646000	-0.149000	-2.748000
30	1	0	-10.941000	-0.025000	-3.788000
31	1	0	-11.516000	-0.051000	-2.094000
32	1	0	-10.234000	-1.150000	-2.591000
33	8	0	-9.254000	0.732000	-1.078000

34	78	0	-7.778000	4.501000	0.163000
35	1	0	-9.852000	3.009000	-0.340000
36	17	0	-9.738000	5.340000	1.174000
37	17	0	-6.551000	6.487000	0.725000
38	1	0	-5.879000	4.977000	-1.634000
39	1	0	-6.744000	3.421000	-2.131000
40	1	0	-5.213000	3.996000	0.493000

Transition state: TS III-IV

- **Thermal correction to Gibbs Free Energy = 0.250134 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.71367522 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.69481023 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.06710947 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1885.98630401 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.10076739 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.08228425 Hartree**
- **Frequency = -220.5**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.739000	0.055000	0.382000
2	6	0	-6.593000	1.516000	0.087000
3	6	0	-5.175000	2.054000	-0.031000
4	6	0	-4.412000	1.317000	-1.150000
5	6	0	-4.692000	-0.129000	-1.037000
6	1	0	-3.338000	1.523000	-1.042000
7	1	0	-4.713000	1.715000	-2.129000
8	6	0	-5.700000	-0.720000	-0.357000
9	1	0	-7.750000	-0.272000	0.115000
10	1	0	-6.656000	-0.096000	1.474000
11	6	0	-5.544000	-2.133000	-0.533000

12	6	0	-4.443000	-2.268000	-1.311000
13	8	0	-3.908000	-1.054000	-1.626000
14	1	0	-3.930000	-3.129000	-1.711000
15	6	0	-6.415000	-3.200000	0.024000
16	1	0	-7.441000	-3.116000	-0.352000
17	1	0	-6.467000	-3.142000	1.117000
18	1	0	-6.045000	-4.194000	-0.240000
19	6	0	-4.495000	1.794000	1.331000
20	1	0	-4.315000	0.730000	1.501000
21	1	0	-5.105000	2.179000	2.156000
22	1	0	-3.528000	2.308000	1.353000
23	6	0	-5.130000	3.548000	-0.280000
24	78	0	-6.496000	4.281000	-1.708000
25	8	0	-8.508000	2.439000	2.497000
26	6	0	-7.684000	2.316000	0.055000
27	6	0	-7.660000	3.712000	-0.249000
28	6	0	-9.246000	1.913000	1.713000
29	6	0	-10.577000	1.309000	1.985000
30	1	0	-10.844000	1.459000	3.029000
31	1	0	-10.546000	0.240000	1.757000
32	1	0	-11.328000	1.757000	1.330000
33	8	0	-8.929000	1.797000	0.387000
34	6	0	-6.083000	4.402000	0.412000
35	1	0	-4.132000	3.951000	-0.450000
36	17	0	-8.414000	5.310000	-2.833000
37	17	0	-5.311000	4.076000	-3.720000
38	1	0	-8.562000	4.290000	-0.031000
39	1	0	-5.903000	5.475000	0.469000
40	1	0	-6.570000	4.077000	1.346000

Transition state: TS III-IV anti

- **Thermal correction to Gibbs Free Energy = 0.250437 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.71248859 Hartree**

- **Frequency = -302.8**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.568767	0.291261	0.906443
2	6	0	-1.226275	0.240855	0.234445
3	6	0	-0.708093	-1.120834	-0.215659
4	6	0	-1.753246	-1.804049	-1.144090
5	6	0	-3.096648	-1.654688	-0.553093
6	1	0	-1.485905	-2.862620	-1.258612
7	1	0	-1.716112	-1.355570	-2.148307
8	6	0	-3.490834	-0.737940	0.355855
9	1	0	-2.995785	1.297678	0.820789
10	1	0	-2.417978	0.136750	1.989056
11	6	0	-4.875712	-0.995988	0.620765
12	6	0	-5.192520	-2.054355	-0.164292
13	8	0	-4.116045	-2.473288	-0.888636
14	1	0	-6.107008	-2.607608	-0.313681
15	6	0	-5.754920	-0.250396	1.558957
16	1	0	-6.768600	-0.658809	1.564379
17	1	0	-5.822007	0.808967	1.285386
18	1	0	-5.370682	-0.293293	2.584511
19	6	0	-0.446649	-2.007127	1.007340
20	1	0	-1.385039	-2.274922	1.500741
21	1	0	0.199433	-1.500224	1.730322
22	1	0	0.056597	-2.930075	0.699050
23	6	0	0.549758	-1.026983	-1.044556
24	6	0	0.823868	0.142792	-1.857888
25	8	0	-1.480989	3.015714	-1.702357
26	6	0	-0.503471	1.355459	0.043401
27	6	0	0.811565	1.393258	-0.570369
28	6	0	-1.502648	3.364066	-0.556461
29	6	0	-2.053908	4.632876	-0.008870

30	1	0	-1.292235	5.146929	0.581893
31	1	0	-2.885048	4.405544	0.664746
32	1	0	-2.398043	5.268996	-0.822159
33	8	0	-1.003473	2.588115	0.449519
34	78	0	2.123272	-0.005927	-0.096500
35	1	0	1.137969	2.362663	-0.948696
36	17	0	3.502222	-2.029163	-0.185845
37	17	0	2.957020	0.442069	2.026043
38	1	0	1.609247	0.084871	-2.612131
39	1	0	-0.009608	0.743305	-2.246472
40	1	0	0.963538	-1.983279	-1.366955

Structure IV

- **Thermal correction to Gibbs Free Energy = 0.255446 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.77496257 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.964000	0.103000	-0.073000
2	6	0	-6.639000	1.575000	-0.055000
3	6	0	-5.177000	2.063000	-0.045000
4	6	0	-4.286000	1.265000	-1.016000
5	6	0	-4.640000	-0.164000	-0.948000
6	1	0	-3.235000	1.425000	-0.741000
7	1	0	-4.414000	1.631000	-2.043000
8	6	0	-5.815000	-0.702000	-0.559000
9	1	0	-7.861000	-0.072000	-0.683000
10	1	0	-7.233000	-0.205000	0.952000
11	6	0	-5.685000	-2.122000	-0.709000
12	6	0	-4.431000	-2.312000	-1.183000
13	8	0	-3.775000	-1.126000	-1.334000

14	1	0	-3.875000	-3.197000	-1.452000
15	6	0	-6.720000	-3.143000	-0.406000
16	1	0	-6.356000	-4.153000	-0.614000
17	1	0	-7.623000	-2.983000	-1.007000
18	1	0	-7.022000	-3.106000	0.647000
19	6	0	-4.597000	1.980000	1.369000
20	1	0	-4.383000	0.934000	1.613000
21	1	0	-5.291000	2.363000	2.122000
22	1	0	-3.657000	2.540000	1.433000
23	6	0	-5.380000	3.474000	-0.566000
24	78	0	-7.174000	3.064000	-1.595000
25	8	0	-8.209000	1.902000	2.905000
26	6	0	-7.602000	2.482000	0.466000
27	6	0	-7.412000	3.885000	0.393000
28	6	0	-9.062000	1.721000	2.090000
29	6	0	-10.426000	1.170000	2.296000
30	1	0	-11.173000	1.842000	1.870000
31	1	0	-10.605000	1.024000	3.360000
32	1	0	-10.512000	0.214000	1.771000
33	8	0	-8.861000	2.007000	0.758000
34	6	0	-6.007000	4.444000	0.393000
35	1	0	-4.670000	3.849000	-1.305000
36	17	0	-7.458000	5.113000	-2.801000
37	17	0	-6.688000	1.829000	-3.581000
38	1	0	-8.265000	4.519000	0.619000
39	1	0	-6.019000	5.452000	-0.026000
40	1	0	-5.539000	4.475000	1.386000

Structure IV anti

- **Thermal correction to Gibbs Free Energy = 0.255521 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.76781880 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.260000	0.089000	1.010000
2	6	0	-6.290000	1.537000	0.633000
3	6	0	-5.014000	2.058000	-0.058000
4	6	0	-4.969000	1.441000	-1.474000
5	6	0	-5.306000	0.003000	-1.314000
6	1	0	-3.971000	1.561000	-1.913000
7	1	0	-5.682000	1.929000	-2.152000
8	6	0	-5.862000	-0.628000	-0.247000
9	1	0	-7.231000	-0.250000	1.380000
10	1	0	-5.534000	-0.078000	1.816000
11	6	0	-5.950000	-2.016000	-0.596000
12	6	0	-5.439000	-2.100000	-1.848000
13	8	0	-5.040000	-0.878000	-2.302000
14	1	0	-5.294000	-2.927000	-2.526000
15	6	0	-6.488000	-3.111000	0.252000
16	1	0	-6.411000	-4.078000	-0.252000
17	1	0	-7.543000	-2.945000	0.497000
18	1	0	-5.946000	-3.182000	1.201000
19	6	0	-3.739000	1.675000	0.690000
20	1	0	-3.554000	0.599000	0.646000
21	1	0	-3.773000	1.982000	1.738000
22	1	0	-2.891000	2.175000	0.210000
23	6	0	-5.250000	3.550000	0.073000
24	6	0	-6.331000	4.137000	-0.787000
25	8	0	-9.616000	2.900000	1.918000
26	6	0	-7.519000	2.167000	0.277000
27	6	0	-7.529000	3.551000	-0.068000
28	6	0	-9.694000	1.905000	1.271000
29	6	0	-10.828000	0.946000	1.198000
30	1	0	-10.503000	-0.032000	1.563000
31	1	0	-11.143000	0.818000	0.160000
32	1	0	-11.655000	1.312000	1.804000

33	8	0	-8.663000	1.452000	0.468000
34	78	0	-6.468000	3.392000	1.792000
35	1	0	-8.482000	4.070000	-0.094000
36	17	0	-6.492000	5.719000	2.343000
37	17	0	-5.244000	2.783000	3.770000
38	1	0	-6.355000	5.224000	-0.687000
39	1	0	-6.271000	3.880000	-1.853000
40	1	0	-4.400000	4.174000	0.349000

Transition state: TS IV-V

- **Thermal correction to Gibbs Free Energy = 0.255238 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.75472797 Hartree**
- **Frequency = -166.3**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.648000	-0.086000	0.391000
2	6	0	-6.476000	1.397000	0.328000
3	6	0	-5.083000	1.999000	0.105000
4	6	0	-4.391000	1.384000	-1.130000
5	6	0	-4.691000	-0.062000	-1.171000
6	1	0	-3.309000	1.559000	-1.055000
7	1	0	-4.725000	1.871000	-2.056000
8	6	0	-5.675000	-0.735000	-0.531000
9	1	0	-7.682000	-0.351000	0.137000
10	1	0	-6.491000	-0.416000	1.433000
11	6	0	-5.573000	-2.102000	-0.948000
12	6	0	-4.524000	-2.133000	-1.804000
13	8	0	-3.970000	-0.896000	-1.951000
14	1	0	-4.066000	-2.927000	-2.374000
15	6	0	-6.463000	-3.219000	-0.538000

16	1	0	-6.157000	-4.162000	-0.997000
17	1	0	-7.500000	-3.022000	-0.835000
18	1	0	-6.459000	-3.357000	0.550000
19	6	0	-4.195000	1.758000	1.330000
20	1	0	-3.843000	0.722000	1.327000
21	1	0	-4.722000	1.922000	2.275000
22	1	0	-3.317000	2.413000	1.302000
23	6	0	-5.441000	3.470000	-0.138000
24	78	0	-7.353000	2.623000	-1.241000
25	8	0	-9.908000	3.497000	0.914000
26	6	0	-7.432000	2.302000	0.845000
27	6	0	-7.082000	3.727000	0.688000
28	6	0	-9.757000	2.424000	1.406000
29	6	0	-10.789000	1.546000	2.014000
30	1	0	-10.946000	0.686000	1.355000
31	1	0	-11.722000	2.097000	2.121000
32	1	0	-10.451000	1.164000	2.979000
33	8	0	-8.528000	1.791000	1.469000
34	6	0	-5.745000	4.256000	1.077000
35	1	0	-5.083000	3.994000	-1.022000
36	17	0	-7.454000	4.077000	-3.098000
37	17	0	-8.638000	0.979000	-2.326000
38	1	0	-7.889000	4.435000	0.529000
39	1	0	-5.677000	5.334000	0.966000
40	1	0	-5.326000	3.902000	2.015000

Transition state: TS IV-V anti

- **Thermal correction to Gibbs Free Energy = 0.254742 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.74553379 Hartree**
- **Frequency = -148.2**

Cartesian Coordinates of the computed structure:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-6.214000	-0.029000	1.025000
2	6	0	-6.248000	1.452000	0.732000
3	6	0	-5.113000	2.067000	-0.128000
4	6	0	-5.117000	1.377000	-1.533000
5	6	0	-5.298000	-0.090000	-1.322000
6	1	0	-4.174000	1.585000	-2.051000
7	1	0	-5.917000	1.762000	-2.175000
8	6	0	-5.785000	-0.744000	-0.231000
9	1	0	-7.196000	-0.364000	1.373000
10	1	0	-5.518000	-0.222000	1.850000
11	6	0	-5.764000	-2.153000	-0.549000
12	6	0	-5.268000	-2.223000	-1.816000
13	8	0	-4.975000	-0.975000	-2.307000
14	1	0	-5.065000	-3.049000	-2.481000
15	6	0	-6.193000	-3.287000	0.332000
16	1	0	-6.081000	-4.247000	-0.180000
17	1	0	-7.243000	-3.189000	0.632000
18	1	0	-5.599000	-3.327000	1.252000
19	6	0	-3.714000	1.873000	0.495000
20	1	0	-3.456000	0.812000	0.532000
21	1	0	-3.656000	2.276000	1.507000
22	1	0	-2.966000	2.379000	-0.122000
23	6	0	-5.493000	3.563000	-0.127000
24	6	0	-6.602000	4.006000	-0.994000
25	8	0	-9.888000	3.061000	-0.254000
26	6	0	-7.456000	2.210000	0.696000
27	6	0	-7.283000	3.624000	0.294000
28	6	0	-9.846000	2.143000	0.523000
29	6	0	-10.998000	1.377000	1.100000
30	1	0	-10.871000	0.307000	0.914000
31	1	0	-11.926000	1.732000	0.655000
32	1	0	-11.023000	1.520000	2.185000
33	8	0	-8.651000	1.628000	1.018000

34	78	0	-6.239000	3.034000	2.247000
35	1	0	-7.893000	4.390000	0.758000
36	17	0	-5.701000	5.022000	3.470000
37	17	0	-6.105000	1.686000	4.181000
38	1	0	-6.653000	5.073000	-1.190000
39	1	0	-6.858000	3.405000	-1.862000
40	1	0	-4.793000	4.302000	0.249000

Structure V

- **Thermal correction to Gibbs Free Energy = 0.258728 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.77628699 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.76150975 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.13037168 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1886.0469756 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.16612988 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.1521579 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.322000	-1.769000	1.117000
2	6	0	0.579000	-0.290000	1.069000
3	6	0	2.041000	0.125000	1.225000
4	6	0	2.893000	-0.377000	0.051000
5	6	0	2.419000	-1.745000	-0.270000
6	1	0	3.954000	-0.392000	0.339000
7	1	0	2.797000	0.281000	-0.819000
8	6	0	1.312000	-2.391000	0.180000
9	1	0	-0.702000	-2.035000	0.839000
10	1	0	0.466000	-2.134000	2.148000
11	6	0	1.318000	-3.688000	-0.429000
12	6	0	2.436000	-3.715000	-1.193000

13	8	0	3.121000	-2.540000	-1.105000
14	1	0	2.863000	-4.466000	-1.840000
15	6	0	0.296000	-4.754000	-0.260000
16	1	0	0.554000	-5.645000	-0.839000
17	1	0	-0.691000	-4.415000	-0.595000
18	1	0	0.196000	-5.054000	0.790000
19	6	0	2.597000	-0.541000	2.502000
20	1	0	2.838000	-1.594000	2.334000
21	1	0	1.905000	-0.484000	3.347000
22	1	0	3.517000	-0.020000	2.787000
23	6	0	1.959000	1.647000	1.419000
24	78	0	-0.617000	0.433000	-0.740000
25	8	0	-2.355000	-0.373000	0.251000
26	6	0	-0.247000	0.819000	1.316000
27	6	0	0.516000	2.069000	1.519000
28	6	0	-2.456000	0.020000	1.413000
29	6	0	-3.652000	-0.214000	2.249000
30	1	0	-3.369000	-0.768000	3.148000
31	1	0	-4.400000	-0.764000	1.683000
32	1	0	-4.056000	0.749000	2.572000
33	8	0	-1.494000	0.693000	2.005000
34	6	0	1.412000	2.154000	2.717000
35	1	0	2.655000	2.271000	0.868000
36	17	0	-1.793000	0.381000	-2.758000
37	17	0	1.012000	1.678000	-1.810000
38	1	0	0.152000	2.975000	1.047000
39	1	0	1.701000	3.156000	3.017000
40	1	0	1.252000	1.472000	3.545000

Structure V anti

- **Thermal correction to Gibbs Free Energy = 0.257434 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.76333946 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.430000	-2.788000	1.951000
2	6	0	1.526000	-1.290000	1.963000
3	6	0	2.805000	-0.528000	1.536000
4	6	0	3.322000	-1.141000	0.202000
5	6	0	3.222000	-2.612000	0.226000
6	6	0	2.375000	-3.365000	0.957000
7	1	0	0.390000	-3.091000	1.762000
8	1	0	1.680000	-3.170000	2.951000
9	6	0	2.631000	-4.731000	0.605000
10	6	0	3.617000	-4.676000	-0.324000
11	8	0	3.992000	-3.388000	-0.569000
12	6	0	1.957000	-5.930000	1.166000
13	1	0	0.876000	-5.901000	0.987000
14	1	0	2.099000	-5.992000	2.251000
15	1	0	2.346000	-6.851000	0.723000
16	6	0	3.954000	-0.530000	2.535000
17	1	0	4.275000	-1.544000	2.788000
18	1	0	3.680000	-0.025000	3.462000
19	1	0	4.803000	0.001000	2.089000
20	6	0	2.306000	0.907000	1.315000
21	6	0	1.324000	1.186000	0.222000
22	8	0	-1.498000	-0.040000	3.538000
23	6	0	0.463000	-0.408000	1.952000
24	6	0	0.839000	0.987000	1.625000
25	6	0	-1.791000	-0.414000	2.407000
26	6	0	-3.169000	-0.476000	1.882000
27	1	0	-3.379000	-1.496000	1.551000
28	1	0	-3.256000	0.174000	1.008000
29	1	0	-3.876000	-0.177000	2.652000
30	8	0	-0.849000	-0.813000	1.573000

31	78	0	0.493000	-0.652000	4.137000
32	1	0	0.396000	1.805000	2.183000
33	17	0	2.365000	-1.652000	5.079000
34	17	0	-0.283000	-0.368000	6.309000
35	1	0	1.289000	2.198000	-0.166000
36	1	0	1.094000	0.414000	-0.508000
37	1	0	2.962000	1.712000	1.630000
38	1	0	2.762000	-0.743000	-0.652000
39	1	0	4.362000	-0.822000	0.060000
40	1	0	4.146000	-5.437000	-0.876000

Structure 2

- **Thermal correction to Gibbs Free Energy = 0.258353 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -845.925185362 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.117000	-3.181000	0.810000
2	6	0	1.183000	-1.728000	0.479000
3	6	0	2.519000	-1.086000	0.151000
4	6	0	3.071000	-1.781000	-1.111000
5	6	0	2.888000	-3.244000	-0.957000
6	1	0	4.131000	-1.530000	-1.258000
7	1	0	2.528000	-1.413000	-1.995000
8	6	0	2.041000	-3.897000	-0.124000
9	1	0	0.086000	-3.546000	0.718000
10	1	0	1.416000	-3.363000	1.856000
11	6	0	2.247000	-5.297000	-0.351000
12	6	0	3.204000	-5.367000	-1.308000
13	8	0	3.610000	-4.123000	-1.689000
14	1	0	3.687000	-6.196000	-1.803000

15	6	0	1.545000	-6.417000	0.330000
16	1	0	1.898000	-7.388000	-0.028000
17	1	0	0.463000	-6.370000	0.161000
18	1	0	1.700000	-6.383000	1.415000
19	6	0	3.528000	-1.206000	1.291000
20	1	0	3.823000	-2.247000	1.459000
21	1	0	3.115000	-0.815000	2.226000
22	1	0	4.432000	-0.634000	1.054000
23	6	0	2.153000	0.365000	-0.145000
24	6	0	1.491000	1.190000	0.910000
25	8	0	-1.471000	0.177000	2.086000
26	6	0	0.194000	-0.864000	0.274000
27	6	0	0.649000	0.490000	-0.117000
28	6	0	-1.913000	-0.572000	1.266000
29	6	0	-3.342000	-0.970000	1.103000
30	1	0	-3.704000	-0.648000	0.123000
31	1	0	-3.944000	-0.515000	1.888000
32	1	0	-3.434000	-2.058000	1.139000
33	8	0	-1.147000	-1.196000	0.332000
34	1	0	0.082000	1.058000	-0.848000
35	1	0	1.595000	2.266000	0.822000
36	1	0	1.425000	0.816000	1.928000
37	1	0	2.733000	0.885000	-0.903000

Structure 2 anti

- **Thermal correction to Gibbs Free Energy = 0.257888 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -845.925685775 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.844000	-2.763000	1.714000

2	6	0	0.809000	-1.283000	1.505000
3	6	0	2.075000	-0.496000	1.206000
4	6	0	2.859000	-1.126000	0.039000
5	6	0	2.802000	-2.600000	0.162000
6	1	0	3.900000	-0.776000	0.047000
7	1	0	2.428000	-0.806000	-0.919000
8	6	0	1.929000	-3.351000	0.874000
9	1	0	-0.132000	-3.206000	1.478000
10	1	0	1.025000	-2.994000	2.778000
11	6	0	2.290000	-4.720000	0.648000
12	6	0	3.354000	-4.675000	-0.189000
13	8	0	3.684000	-3.389000	-0.497000
14	1	0	3.967000	-5.442000	-0.637000
15	6	0	1.620000	-5.917000	1.221000
16	1	0	1.633000	-5.893000	2.317000
17	1	0	2.108000	-6.841000	0.900000
18	1	0	0.568000	-5.969000	0.916000
19	6	0	2.951000	-0.449000	2.458000
20	1	0	3.308000	-1.446000	2.737000
21	1	0	2.387000	-0.037000	3.302000
22	1	0	3.828000	0.188000	2.287000
23	6	0	1.554000	0.906000	0.901000
24	6	0	0.577000	1.121000	-0.206000
25	8	0	-2.375000	-0.344000	-0.071000
26	6	0	-0.240000	-0.467000	1.547000
27	6	0	0.072000	0.936000	1.195000
28	6	0	-2.526000	-0.714000	1.055000
29	6	0	-3.820000	-1.079000	1.707000
30	1	0	-4.021000	-0.392000	2.533000
31	1	0	-3.756000	-2.084000	2.131000
32	1	0	-4.627000	-1.028000	0.978000
33	8	0	-1.504000	-0.868000	1.939000
34	1	0	-0.416000	1.751000	1.719000
35	1	0	0.529000	2.121000	-0.626000
36	1	0	0.367000	0.317000	-0.906000

37	1	0	2.180000	1.746000	1.193000

Transition state: TS I-VI

- **Thermal correction to Gibbs Free Energy = 0.250984 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.72108631 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.70420647 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.07450298 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1885.99043054 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.10773639 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.09126842 Hartree**
- **Frequency = -265.8**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.037000	-0.296000	0.279000
2	6	0	-6.837000	1.197000	0.019000
3	6	0	-5.449000	1.669000	0.509000
4	6	0	-4.356000	1.058000	-0.388000
5	6	0	-4.668000	-0.385000	-0.530000
6	1	0	-3.373000	1.204000	0.079000
7	1	0	-4.328000	1.561000	-1.364000
8	6	0	-5.835000	-1.014000	-0.245000
9	1	0	-7.964000	-0.635000	-0.196000
10	1	0	-7.178000	-0.458000	1.355000
11	6	0	-5.629000	-2.404000	-0.531000
12	6	0	-4.348000	-2.489000	-0.967000
13	8	0	-3.747000	-1.266000	-0.972000
14	1	0	-3.740000	-3.318000	-1.296000
15	6	0	-6.617000	-3.503000	-0.370000
16	1	0	-7.507000	-3.335000	-0.988000
17	1	0	-6.959000	-3.583000	0.668000

18	1	0	-6.189000	-4.467000	-0.657000
19	6	0	-5.221000	1.183000	1.953000
20	1	0	-5.020000	0.111000	1.996000
21	1	0	-6.068000	1.411000	2.607000
22	1	0	-4.349000	1.702000	2.362000
23	6	0	-5.394000	3.185000	0.564000
24	6	0	-6.045000	4.089000	-0.272000
25	8	0	-6.877000	1.364000	-1.443000
26	6	0	-7.890000	2.105000	0.582000
27	6	0	-9.071000	2.223000	0.145000
28	6	0	-8.025000	1.245000	-2.082000
29	6	0	-7.865000	1.258000	-3.558000
30	1	0	-8.834000	1.139000	-4.039000
31	1	0	-7.185000	0.460000	-3.863000
32	1	0	-7.411000	2.207000	-3.860000
33	8	0	-9.116000	1.155000	-1.526000
34	78	0	-7.246000	3.830000	1.519000
35	17	0	-9.042000	3.942000	3.037000
36	17	0	-6.197000	5.734000	2.467000
37	1	0	-5.716000	5.124000	-0.281000
38	1	0	-4.575000	3.575000	1.169000
39	1	0	-6.629000	3.770000	-1.128000
40	1	0	-10.075000	2.594000	0.068000

Structure VI

- **Thermal correction to Gibbs Free Energy = 0.257511 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.73995171 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.952000	-0.109000	0.184000

2	6	0	-7.011000	1.381000	-0.141000
3	6	0	-5.728000	2.098000	0.323000
4	6	0	-4.540000	1.646000	-0.547000
5	6	0	-4.606000	0.166000	-0.642000
6	1	0	-3.601000	1.971000	-0.082000
7	1	0	-4.585000	2.112000	-1.540000
8	6	0	-5.651000	-0.640000	-0.327000
9	1	0	-7.812000	-0.636000	-0.249000
10	1	0	-7.061000	-0.231000	1.269000
11	6	0	-5.227000	-1.982000	-0.599000
12	6	0	-3.956000	-1.866000	-1.053000
13	8	0	-3.561000	-0.561000	-1.085000
14	1	0	-3.224000	-2.590000	-1.377000
15	6	0	-6.024000	-3.223000	-0.411000
16	1	0	-6.935000	-3.212000	-1.021000
17	1	0	-6.339000	-3.341000	0.632000
18	1	0	-5.450000	-4.110000	-0.689000
19	6	0	-5.434000	1.703000	1.785000
20	1	0	-5.050000	0.685000	1.874000
21	1	0	-6.312000	1.812000	2.427000
22	1	0	-4.666000	2.380000	2.171000
23	6	0	-5.946000	3.600000	0.343000
24	6	0	-6.703000	4.345000	-0.559000
25	8	0	-7.029000	1.378000	-1.686000
26	6	0	-8.240000	2.142000	0.245000
27	6	0	-9.335000	1.859000	-0.442000
28	6	0	-8.114000	1.001000	-2.228000
29	6	0	-8.079000	0.525000	-3.617000
30	1	0	-7.403000	1.156000	-4.199000
31	1	0	-9.077000	0.509000	-4.051000
32	1	0	-7.656000	-0.486000	-3.620000
33	8	0	-9.237000	1.012000	-1.611000
34	78	0	-7.922000	3.901000	1.173000
35	17	0	-9.847000	3.690000	2.517000
36	17	0	-7.357000	6.066000	2.082000

37	1	0	-10.332000	2.269000	-0.379000
38	1	0	-6.569000	5.422000	-0.591000
39	1	0	-5.237000	4.146000	0.966000
40	1	0	-7.163000	3.902000	-1.437000

Transition state: TS VI-VII

- **Thermal correction to Gibbs Free Energy = 0.255869 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.73562647 Hartree**
- **Frequency = -298.9**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.676000	-0.227000	0.504000
2	6	0	-6.763000	1.217000	0.086000
3	6	0	-5.459000	1.988000	0.220000
4	6	0	-4.368000	1.396000	-0.692000
5	6	0	-4.414000	-0.079000	-0.547000
6	1	0	-3.391000	1.791000	-0.385000
7	1	0	-4.528000	1.704000	-1.733000
8	6	0	-5.415000	-0.827000	-0.022000
9	1	0	-7.575000	-0.777000	0.207000
10	1	0	-6.702000	-0.226000	1.605000
11	6	0	-4.984000	-2.191000	-0.085000
12	6	0	-3.752000	-2.145000	-0.648000
13	8	0	-3.389000	-0.863000	-0.935000
14	1	0	-3.032000	-2.909000	-0.898000
15	6	0	-5.736000	-3.387000	0.380000
16	1	0	-6.687000	-3.496000	-0.156000
17	1	0	-5.976000	-3.318000	1.447000
18	1	0	-5.161000	-4.303000	0.225000
19	6	0	-5.000000	1.827000	1.691000

20	1	0	-4.636000	0.820000	1.901000
21	1	0	-5.793000	2.080000	2.400000
22	1	0	-4.175000	2.526000	1.858000
23	6	0	-5.696000	3.474000	0.017000
24	6	0	-6.529000	4.052000	-0.940000
25	8	0	-6.962000	0.895000	-1.727000
26	6	0	-7.959000	1.999000	0.339000
27	6	0	-9.100000	1.648000	-0.243000
28	6	0	-8.104000	0.558000	-2.056000
29	6	0	-8.409000	0.011000	-3.393000
30	1	0	-9.108000	-0.822000	-3.290000
31	1	0	-7.498000	-0.303000	-3.898000
32	1	0	-8.911000	0.785000	-3.981000
33	8	0	-9.150000	0.668000	-1.263000
34	78	0	-7.595000	3.907000	0.935000
35	17	0	-9.363000	3.892000	2.493000
36	17	0	-7.001000	6.191000	1.423000
37	1	0	-10.059000	2.142000	-0.155000
38	1	0	-6.414000	5.107000	-1.168000
39	1	0	-4.945000	4.113000	0.481000
40	1	0	-7.042000	3.456000	-1.689000

Structure VII

- **Thermal correction to Gibbs Free Energy = 0.251601 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.75445536 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.73339689 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.10985307 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1886.02952484 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.14447953 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.12363976 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.749000	0.110000	-0.681000
2	6	0	-6.746000	1.479000	-0.075000
3	6	0	-5.570000	1.904000	0.769000
4	6	0	-4.196000	1.475000	0.209000
5	6	0	-4.289000	0.094000	-0.296000
6	1	0	-3.446000	1.564000	1.005000
7	1	0	-3.889000	2.165000	-0.589000
8	6	0	-5.413000	-0.536000	-0.696000
9	1	0	-7.180000	0.165000	-1.691000
10	1	0	-7.487000	-0.496000	-0.126000
11	6	0	-5.018000	-1.846000	-1.125000
12	6	0	-3.676000	-1.884000	-0.942000
13	8	0	-3.213000	-0.706000	-0.434000
14	1	0	-2.935000	-2.649000	-1.113000
15	6	0	-5.907000	-2.914000	-1.651000
16	1	0	-6.433000	-2.585000	-2.556000
17	1	0	-6.671000	-3.195000	-0.918000
18	1	0	-5.341000	-3.814000	-1.905000
19	6	0	-5.813000	1.217000	2.134000
20	1	0	-5.800000	0.127000	2.049000
21	1	0	-6.768000	1.535000	2.562000
22	1	0	-5.013000	1.517000	2.819000
23	6	0	-5.567000	3.409000	0.970000
24	6	0	-5.644000	4.309000	-0.099000
25	1	0	-5.124000	3.749000	1.907000
26	1	0	-5.715000	3.953000	-1.125000
27	1	0	-5.296000	5.329000	0.028000
28	8	0	-11.120000	1.855000	-2.390000
29	6	0	-7.799000	2.384000	-0.126000
30	6	0	-8.974000	2.144000	-0.824000
31	6	0	-10.490000	0.893000	-2.138000
32	6	0	-10.705000	-0.527000	-2.488000

33	1	0	-10.862000	-1.103000	-1.572000
34	1	0	-9.814000	-0.928000	-2.978000
35	1	0	-11.573000	-0.617000	-3.139000
36	8	0	-9.275000	0.985000	-1.364000
37	78	0	-7.547000	4.143000	0.858000
38	1	0	-9.721000	2.930000	-0.949000
39	17	0	-7.084000	6.173000	2.085000
40	17	0	-9.874000	4.277000	1.312000

Structure 4

- **Thermal correction to Gibbs Free Energy = 0.251669 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -845.875572363 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.593000	-0.391000	0.768000
2	6	0	-6.684000	1.082000	0.424000
3	6	0	-5.383000	1.888000	0.515000
4	6	0	-4.373000	1.291000	-0.484000
5	6	0	-4.393000	-0.184000	-0.379000
6	1	0	-3.369000	1.685000	-0.278000
7	1	0	-4.637000	1.602000	-1.505000
8	6	0	-5.358000	-0.963000	0.161000
9	1	0	-7.494000	-0.906000	0.416000
10	1	0	-6.579000	-0.513000	1.864000
11	6	0	-4.919000	-2.319000	0.010000
12	6	0	-3.719000	-2.236000	-0.616000
13	8	0	-3.380000	-0.938000	-0.861000
14	1	0	-3.009000	-2.981000	-0.942000
15	6	0	-5.643000	-3.541000	0.450000
16	1	0	-6.622000	-3.619000	-0.036000

17	1	0	-5.822000	-3.530000	1.531000
18	1	0	-5.078000	-4.446000	0.213000
19	6	0	-4.829000	1.779000	1.945000
20	1	0	-4.555000	0.752000	2.202000
21	1	0	-5.570000	2.131000	2.672000
22	1	0	-3.935000	2.404000	2.041000
23	6	0	-5.646000	3.346000	0.260000
24	6	0	-5.046000	4.129000	-0.623000
25	1	0	-6.393000	3.781000	0.927000
26	1	0	-4.291000	3.768000	-1.315000
27	1	0	-5.292000	5.184000	-0.689000
28	8	0	-11.268000	3.219000	-1.078000
29	6	0	-7.811000	1.612000	0.037000
30	6	0	-8.954000	2.134000	-0.298000
31	6	0	-10.541000	2.754000	-1.909000
32	6	0	-10.789000	2.714000	-3.380000
33	1	0	-11.756000	3.161000	-3.603000
34	1	0	-10.761000	1.680000	-3.733000
35	1	0	-9.996000	3.255000	-3.902000
36	8	0	-9.346000	2.177000	-1.628000
37	1	0	-9.666000	2.564000	0.398000

Transition state: TS VII-VIII

- **Thermal correction to Gibbs Free Energy = 0.249897 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.71403384 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.69254228 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.06618129 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1885.98202377 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.10135076 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.08046621 Hartree**
- **Frequency = -289.6**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.533000	-0.176000	0.998000
2	6	0	-6.685000	1.148000	0.299000
3	6	0	-5.396000	1.823000	-0.234000
4	6	0	-4.613000	0.855000	-1.151000
5	6	0	-4.580000	-0.480000	-0.525000
6	1	0	-3.597000	1.241000	-1.308000
7	1	0	-5.095000	0.809000	-2.139000
8	6	0	-5.410000	-0.965000	0.423000
9	1	0	-7.483000	-0.719000	0.924000
10	1	0	-6.379000	0.004000	2.075000
11	6	0	-4.974000	-2.303000	0.698000
12	6	0	-3.911000	-2.504000	-0.118000
13	8	0	-3.651000	-1.399000	-0.873000
14	1	0	-3.255000	-3.347000	-0.273000
15	6	0	-5.580000	-3.244000	1.674000
16	1	0	-6.628000	-3.451000	1.427000
17	1	0	-5.568000	-2.828000	2.688000
18	1	0	-5.046000	-4.197000	1.695000
19	6	0	-4.535000	2.234000	0.968000
20	1	0	-4.115000	1.350000	1.454000
21	1	0	-5.122000	2.776000	1.716000
22	1	0	-3.702000	2.867000	0.644000
23	6	0	-5.849000	2.997000	-1.021000
24	6	0	-6.357000	4.131000	-0.470000
25	1	0	-5.928000	2.870000	-2.102000
26	1	0	-6.229000	4.343000	0.589000
27	1	0	-6.670000	4.963000	-1.093000
28	8	0	-9.625000	5.068000	-1.298000
29	6	0	-7.833000	1.808000	0.237000
30	6	0	-8.093000	3.097000	-0.377000
31	6	0	-9.531000	4.078000	-1.949000
32	6	0	-10.293000	3.662000	-3.148000

33	1	0	-10.950000	4.467000	-3.471000
34	1	0	-10.876000	2.772000	-2.886000
35	1	0	-9.610000	3.372000	-3.949000
36	8	0	-8.620000	3.068000	-1.618000
37	78	0	-9.539000	1.386000	1.107000
38	1	0	-8.489000	3.897000	0.257000
39	17	0	-8.762000	2.520000	3.021000
40	17	0	-10.402000	0.234000	-0.752000

Structure VIII

- **Thermal correction to Gibbs Free Energy = 0.255028 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.76638283 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.601000	-0.257000	0.461000
2	6	0	-6.452000	1.110000	-0.188000
3	6	0	-5.010000	1.786000	-0.347000
4	6	0	-3.835000	0.911000	0.082000
5	6	0	-4.163000	-0.524000	0.111000
6	1	0	-3.492000	1.253000	1.069000
7	1	0	-3.009000	1.110000	-0.617000
8	6	0	-5.379000	-1.077000	0.293000
9	1	0	-7.478000	-0.756000	0.027000
10	1	0	-6.835000	-0.109000	1.525000
11	6	0	-5.185000	-2.498000	0.286000
12	6	0	-3.853000	-2.670000	0.102000
13	8	0	-3.210000	-1.472000	-0.012000
14	1	0	-3.232000	-3.549000	0.024000
15	6	0	-6.234000	-3.537000	0.451000
16	1	0	-6.999000	-3.458000	-0.329000

17	1	0	-6.747000	-3.436000	1.413000
18	1	0	-5.808000	-4.543000	0.402000
19	6	0	-4.766000	3.217000	0.055000
20	1	0	-4.795000	3.316000	1.144000
21	1	0	-5.465000	3.939000	-0.365000
22	1	0	-3.764000	3.502000	-0.284000
23	6	0	-5.746000	1.390000	-1.550000
24	6	0	-6.548000	2.434000	-2.296000
25	1	0	-5.393000	0.515000	-2.090000
26	8	0	-9.303000	4.987000	-0.871000
27	6	0	-7.553000	2.010000	-0.148000
28	6	0	-7.566000	2.988000	-1.301000
29	6	0	-9.659000	4.074000	-1.559000
30	6	0	-11.018000	3.864000	-2.130000
31	1	0	-11.606000	4.775000	-2.035000
32	1	0	-11.495000	3.054000	-1.566000
33	1	0	-10.958000	3.544000	-3.172000
34	8	0	-8.844000	3.043000	-1.909000
35	78	0	-8.905000	1.962000	1.119000
36	17	0	-7.665000	3.199000	2.682000
37	17	0	-10.428000	0.647000	-0.080000
38	1	0	-7.331000	3.987000	-0.905000
39	1	0	-7.102000	1.958000	-3.111000
40	1	0	-5.917000	3.217000	-2.728000

Transition state: TS VIII-IX

- **Thermal correction to Gibbs Free Energy = 0.251472 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.72587685 Hartree**
- **Frequency = -522.0**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-6.548000	-0.349000	0.551000
2	6	0	-6.532000	1.041000	-0.051000
3	6	0	-5.239000	1.772000	-0.411000
4	6	0	-3.929000	1.000000	-0.272000
5	6	0	-4.151000	-0.448000	-0.112000
6	1	0	-3.384000	1.400000	0.596000
7	1	0	-3.300000	1.207000	-1.149000
8	6	0	-5.287000	-1.072000	0.262000
9	1	0	-7.418000	-0.902000	0.171000
10	1	0	-6.714000	-0.261000	1.635000
11	6	0	-4.984000	-2.474000	0.309000
12	6	0	-3.679000	-2.566000	-0.042000
13	8	0	-3.151000	-1.337000	-0.307000
14	1	0	-3.006000	-3.403000	-0.151000
15	6	0	-5.922000	-3.568000	0.673000
16	1	0	-6.773000	-3.609000	-0.016000
17	1	0	-6.335000	-3.419000	1.677000
18	1	0	-5.426000	-4.542000	0.653000
19	6	0	-5.007000	3.238000	-0.131000
20	1	0	-4.838000	3.405000	0.938000
21	1	0	-5.801000	3.918000	-0.452000
22	1	0	-4.106000	3.560000	-0.667000
23	6	0	-6.158000	1.308000	-1.505000
24	6	0	-7.171000	2.266000	-2.099000
25	1	0	-5.824000	0.477000	-2.120000
26	8	0	-8.006000	5.157000	-1.611000
27	6	0	-7.751000	1.886000	0.211000
28	6	0	-8.102000	2.559000	-0.968000
29	6	0	-9.070000	4.665000	-1.424000
30	6	0	-10.411000	5.290000	-1.439000
31	1	0	-10.344000	6.298000	-1.841000
32	1	0	-10.779000	5.326000	-0.408000
33	1	0	-11.113000	4.682000	-2.014000

34	8	0	-9.196000	3.317000	-1.059000
35	78	0	-8.828000	1.918000	1.824000
36	17	0	-8.030000	4.104000	2.225000
37	17	0	-9.868000	-0.150000	1.470000
38	1	0	-7.774000	1.784000	-2.879000
39	1	0	-6.749000	3.177000	-2.535000
40	1	0	-7.346000	3.075000	0.144000

Structure IX

- **Thermal correction to Gibbs Free Energy = 0.25619 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1885.77724469 Hartree**
- **Electronic energy (M06/Def2TZVPP,gas) = -1885.75908818 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1886.13175909 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,gas) = -1886.04605606 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1886.16565814 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,gas) = -1886.14784938 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.261000	-1.788000	0.080000
2	6	0	1.130000	-0.484000	-0.676000
3	6	0	2.320000	0.188000	-1.382000
4	6	0	3.637000	-0.578000	-1.432000
5	6	0	3.478000	-1.988000	-1.035000
6	1	0	4.361000	-0.077000	-0.771000
7	1	0	4.053000	-0.503000	-2.448000
8	6	0	2.455000	-2.551000	-0.357000
9	1	0	0.347000	-2.376000	-0.079000
10	1	0	1.303000	-1.573000	1.160000
11	6	0	2.786000	-3.938000	-0.203000
12	6	0	3.993000	-4.084000	-0.800000

13	8	0	4.434000	-2.902000	-1.319000
14	1	0	4.642000	-4.935000	-0.944000
15	6	0	1.958000	-4.978000	0.463000
16	1	0	0.982000	-5.078000	-0.026000
17	1	0	1.766000	-4.725000	1.512000
18	1	0	2.448000	-5.954000	0.437000
19	6	0	2.568000	1.673000	-1.289000
20	1	0	3.102000	1.911000	-0.362000
21	1	0	1.669000	2.292000	-1.312000
22	1	0	3.205000	1.990000	-2.124000
23	6	0	1.186000	-0.375000	-2.189000
24	6	0	0.112000	0.577000	-2.672000
25	1	0	1.376000	-1.280000	-2.760000
26	8	0	-2.467000	2.067000	-2.918000
27	6	0	0.095000	0.476000	-0.240000
28	6	0	-0.508000	1.089000	-1.388000
29	6	0	-1.958000	2.795000	-2.123000
30	6	0	-2.310000	4.203000	-1.809000
31	1	0	-3.025000	4.578000	-2.540000
32	1	0	-1.415000	4.828000	-1.787000
33	1	0	-2.752000	4.232000	-0.808000
34	8	0	-0.933000	2.382000	-1.297000
35	78	0	-1.887000	-0.243000	-0.443000
36	17	0	-2.524000	1.306000	1.203000
37	17	0	-1.695000	-2.058000	-1.901000
38	1	0	-0.617000	0.099000	-3.325000
39	1	0	0.517000	1.441000	-3.218000
40	1	0	0.137000	0.991000	0.718000

Structure 3

- **Thermal correction to Gibbs Free Energy = 0.258174 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -845.923587983 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.623000	-0.590000	0.297000
2	6	0	-6.629000	0.822000	-0.250000
3	6	0	-5.368000	1.679000	-0.345000
4	6	0	-4.030000	1.029000	-0.009000
5	6	0	-4.143000	-0.435000	0.127000
6	1	0	-3.655000	1.463000	0.930000
7	1	0	-3.290000	1.293000	-0.780000
8	6	0	-5.260000	-1.179000	0.282000
9	1	0	-7.321000	-1.206000	-0.291000
10	1	0	-7.028000	-0.580000	1.321000
11	6	0	-4.826000	-2.541000	0.407000
12	6	0	-3.475000	-2.495000	0.320000
13	8	0	-3.037000	-1.216000	0.147000
14	1	0	-2.712000	-3.257000	0.355000
15	6	0	-5.694000	-3.734000	0.590000
16	1	0	-6.388000	-3.856000	-0.250000
17	1	0	-6.304000	-3.648000	1.497000
18	1	0	-5.102000	-4.650000	0.670000
19	6	0	-5.367000	3.144000	0.004000
20	1	0	-5.216000	3.280000	1.081000
21	1	0	-6.284000	3.664000	-0.277000
22	1	0	-4.532000	3.641000	-0.508000
23	6	0	-6.032000	1.181000	-1.602000
24	6	0	-7.023000	2.059000	-2.342000
25	1	0	-5.500000	0.414000	-2.159000
26	8	0	-8.181000	4.877000	-1.417000
27	6	0	-7.924000	1.546000	-0.211000
28	6	0	-8.133000	2.201000	-1.346000
29	6	0	-9.181000	4.276000	-1.681000
30	6	0	-10.488000	4.868000	-2.092000

31	1	0	-10.424000	5.955000	-2.074000
32	1	0	-11.280000	4.525000	-1.422000
33	1	0	-10.746000	4.527000	-3.098000
34	8	0	-9.275000	2.924000	-1.642000
35	1	0	-7.381000	1.588000	-3.266000
36	1	0	-6.609000	3.037000	-2.621000
37	1	0	-8.605000	1.527000	0.634000

Structure 5

- **Thermal correction to Gibbs Free Energy = 0.234176 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -919.906122588 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.701000	-0.460000	0.015000
2	6	0	-6.859000	1.009000	-0.414000
3	6	0	-5.772000	1.931000	0.250000
4	6	0	-4.399000	1.355000	0.014000
5	6	0	-4.238000	0.052000	-0.185000
6	6	0	-5.310000	-0.917000	-0.224000
7	1	0	-7.436000	-1.068000	-0.516000
8	1	0	-6.943000	-0.534000	1.083000
9	6	0	-4.768000	-2.123000	-0.455000
10	6	0	-3.311000	-1.929000	-0.559000
11	8	0	-3.043000	-0.582000	-0.381000
12	6	0	-5.373000	-3.468000	-0.580000
13	1	0	-6.464000	-3.425000	-0.566000
14	1	0	-5.043000	-4.119000	0.238000
15	1	0	-5.051000	-3.950000	-1.508000
16	6	0	-5.989000	2.026000	1.769000
17	1	0	-5.904000	1.049000	2.253000

18	1	0	-6.966000	2.456000	2.007000
19	1	0	-5.217000	2.674000	2.196000
20	6	0	-5.908000	3.326000	-0.315000
21	6	0	-5.086000	3.917000	-1.168000
22	1	0	-6.781000	3.871000	0.046000
23	1	0	-4.213000	3.415000	-1.577000
24	1	0	-5.263000	4.934000	-1.502000
25	8	0	-6.588000	1.130000	-1.828000
26	6	0	-8.202000	1.488000	-0.100000
27	6	0	-9.290000	1.887000	0.205000
28	1	0	-10.265000	2.231000	0.460000
29	6	0	-7.382000	0.531000	-2.739000
30	6	0	-6.888000	0.846000	-4.115000
31	1	0	-6.827000	1.929000	-4.249000
32	1	0	-7.557000	0.409000	-4.854000
33	1	0	-5.879000	0.447000	-4.243000
34	8	0	-8.331000	-0.151000	-2.471000
35	8	0	-2.443000	-2.724000	-0.758000
36	1	0	-3.542000	2.019000	0.073000

Structure X

- **Thermal correction to Gibbs Free Energy = 0.233652 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.77597155 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.11711941 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.15798683 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.872000	-0.204000	-0.024000
2	6	0	-6.837000	1.244000	-0.526000
3	6	0	-5.672000	2.022000	0.147000

4	6	0	-4.358000	1.373000	-0.222000
5	6	0	-4.350000	0.049000	-0.353000
6	6	0	-5.524000	-0.801000	-0.256000
7	1	0	-7.656000	-0.760000	-0.542000
8	1	0	-7.127000	-0.211000	1.042000
9	6	0	-5.125000	-2.070000	-0.435000
10	6	0	-3.665000	-2.039000	-0.655000
11	8	0	-3.251000	-0.718000	-0.601000
12	6	0	-5.869000	-3.347000	-0.440000
13	1	0	-6.947000	-3.192000	-0.371000
14	1	0	-5.556000	-3.977000	0.401000
15	1	0	-5.649000	-3.915000	-1.350000
16	6	0	-5.800000	1.967000	1.684000
17	1	0	-5.594000	0.965000	2.065000
18	1	0	-6.787000	2.288000	2.032000
19	1	0	-5.060000	2.642000	2.125000
20	6	0	-5.723000	3.487000	-0.249000
21	6	0	-6.282000	4.080000	-1.377000
22	8	0	-6.542000	1.246000	-1.940000
23	6	0	-8.078000	2.012000	-0.317000
24	6	0	-9.151000	2.599000	-0.413000
25	6	0	-7.428000	0.710000	-2.820000
26	6	0	-6.911000	0.864000	-4.210000
27	1	0	-6.825000	1.928000	-4.453000
28	1	0	-7.592000	0.381000	-4.910000
29	1	0	-5.912000	0.431000	-4.292000
30	8	0	-8.468000	0.210000	-2.497000
31	78	0	-7.741000	4.208000	0.249000
32	1	0	-10.184000	2.861000	-0.505000
33	17	0	-9.616000	4.705000	1.596000
34	17	0	-6.769000	6.215000	0.926000
35	1	0	-6.009000	5.105000	-1.608000
36	1	0	-6.718000	3.501000	-2.181000
37	1	0	-5.043000	4.106000	0.338000
38	1	0	-3.454000	1.970000	-0.291000

39	8	0	-2.903000	-2.933000	-0.859000

Transition state: TS X-XI

- **Thermal correction to Gibbs Free Energy = 0.234745 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.75564518 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.10199545 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.13892101 Hartree**
- **Frequency = -340.6**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.834000	-0.342000	0.085000
2	6	0	-6.917000	1.090000	-0.463000
3	6	0	-5.774000	1.963000	0.128000
4	6	0	-4.449000	1.359000	-0.292000
5	6	0	-4.362000	0.035000	-0.385000
6	6	0	-5.472000	-0.879000	-0.196000
7	1	0	-7.612000	-0.966000	-0.365000
8	1	0	-7.042000	-0.323000	1.160000
9	6	0	-5.009000	-2.128000	-0.356000
10	6	0	-3.568000	-2.018000	-0.661000
11	8	0	-3.233000	-0.673000	-0.671000
12	6	0	-5.675000	-3.445000	-0.279000
13	1	0	-5.520000	-4.010000	-1.204000
14	1	0	-6.747000	-3.352000	-0.096000
15	1	0	-5.240000	-4.048000	0.526000
16	6	0	-5.831000	1.916000	1.674000
17	1	0	-5.551000	0.933000	2.058000
18	1	0	-6.815000	2.194000	2.062000
19	1	0	-5.108000	2.637000	2.068000
20	6	0	-5.830000	3.427000	-0.266000

21	6	0	-6.463000	4.047000	-1.340000
22	8	0	-6.751000	0.949000	-1.924000
23	6	0	-8.221000	1.744000	-0.338000
24	6	0	-8.867000	2.828000	-0.151000
25	6	0	-7.918000	0.654000	-2.461000
26	6	0	-7.898000	0.333000	-3.902000
27	1	0	-7.533000	1.205000	-4.451000
28	1	0	-8.897000	0.069000	-4.243000
29	1	0	-7.197000	-0.485000	-4.086000
30	8	0	-8.927000	0.682000	-1.756000
31	78	0	-7.649000	4.383000	0.442000
32	1	0	-9.904000	3.041000	-0.382000
33	17	0	-9.380000	5.056000	1.890000
34	17	0	-6.362000	6.314000	0.962000
35	1	0	-6.110000	5.025000	-1.654000
36	1	0	-7.048000	3.498000	-2.070000
37	1	0	-5.023000	3.991000	0.204000
38	1	0	-3.588000	2.006000	-0.430000
39	8	0	-2.767000	-2.871000	-0.884000

Structure XI

- **Thermal correction to Gibbs Free Energy = 0.237338 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.76606245 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.891000	-0.267000	0.052000
2	6	0	-6.945000	1.179000	-0.453000
3	6	0	-5.812000	2.017000	0.159000
4	6	0	-4.483000	1.407000	-0.247000
5	6	0	-4.408000	0.083000	-0.363000

6	6	0	-5.531000	-0.821000	-0.206000
7	1	0	-7.667000	-0.878000	-0.422000
8	1	0	-7.126000	-0.263000	1.122000
9	6	0	-5.078000	-2.074000	-0.367000
10	6	0	-3.631000	-1.976000	-0.646000
11	8	0	-3.282000	-0.635000	-0.636000
12	6	0	-5.758000	-3.385000	-0.312000
13	1	0	-6.831000	-3.282000	-0.132000
14	1	0	-5.334000	-4.003000	0.486000
15	1	0	-5.606000	-3.938000	-1.244000
16	6	0	-5.905000	1.921000	1.705000
17	1	0	-5.631000	0.929000	2.069000
18	1	0	-6.901000	2.187000	2.072000
19	1	0	-5.197000	2.634000	2.136000
20	6	0	-5.827000	3.498000	-0.168000
21	6	0	-6.404000	4.187000	-1.233000
22	8	0	-6.767000	0.975000	-1.980000
23	6	0	-8.287000	1.795000	-0.509000
24	6	0	-8.762000	2.983000	-0.187000
25	6	0	-7.950000	0.797000	-2.434000
26	6	0	-8.181000	0.306000	-3.793000
27	1	0	-7.393000	0.671000	-4.454000
28	1	0	-9.168000	0.603000	-4.145000
29	1	0	-8.123000	-0.788000	-3.778000
30	8	0	-8.915000	1.059000	-1.640000
31	78	0	-7.629000	4.471000	0.526000
32	1	0	-9.774000	3.227000	-0.515000
33	17	0	-9.409000	5.100000	1.942000
34	17	0	-6.264000	6.342000	1.214000
35	1	0	-6.009000	5.165000	-1.490000
36	1	0	-6.978000	3.690000	-2.008000
37	1	0	-5.020000	4.018000	0.350000
38	1	0	-3.613000	2.046000	-0.353000
39	8	0	-2.835000	-2.836000	-0.863000

Transition state: TS XI-XII

- **Thermal correction to Gibbs Free Energy = 0.235762 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.76177585 Hartree**
- **Frequency = -316.2**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.826000	-0.301000	0.088000
2	6	0	-6.992000	1.166000	-0.253000
3	6	0	-5.815000	2.024000	0.168000
4	6	0	-4.533000	1.458000	-0.410000
5	6	0	-4.435000	0.148000	-0.612000
6	6	0	-5.503000	-0.799000	-0.377000
7	1	0	-7.651000	-0.905000	-0.297000
8	1	0	-6.903000	-0.371000	1.182000
9	6	0	-5.043000	-2.026000	-0.663000
10	6	0	-3.642000	-1.863000	-1.105000
11	8	0	-3.330000	-0.513000	-1.057000
12	6	0	-5.676000	-3.360000	-0.608000
13	1	0	-6.730000	-3.302000	-0.327000
14	1	0	-5.161000	-4.000000	0.117000
15	1	0	-5.595000	-3.864000	-1.576000
16	6	0	-5.718000	1.927000	1.719000
17	1	0	-5.412000	0.932000	2.046000
18	1	0	-6.661000	2.205000	2.200000
19	1	0	-4.954000	2.636000	2.052000
20	6	0	-5.895000	3.502000	-0.161000
21	6	0	-6.540000	4.147000	-1.213000
22	8	0	-7.036000	0.896000	-2.083000
23	6	0	-8.323000	1.715000	-0.295000
24	6	0	-8.780000	2.924000	0.040000
25	6	0	-8.254000	0.701000	-2.252000

26	6	0	-8.846000	0.254000	-3.523000
27	1	0	-9.673000	-0.429000	-3.325000
28	1	0	-8.091000	-0.208000	-4.156000
29	1	0	-9.257000	1.130000	-4.035000
30	8	0	-9.069000	0.921000	-1.251000
31	78	0	-7.660000	4.456000	0.615000
32	1	0	-9.833000	3.119000	-0.173000
33	17	0	-9.361000	5.103000	2.121000
34	17	0	-6.306000	6.389000	1.134000
35	1	0	-6.185000	5.127000	-1.516000
36	1	0	-7.140000	3.612000	-1.941000
37	1	0	-5.067000	4.046000	0.297000
38	1	0	-3.698000	2.131000	-0.577000
39	8	0	-2.855000	-2.682000	-1.463000

Structure XII

- **Thermal correction to Gibbs Free Energy = 0.232121 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.79335699 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.14256947 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.17920384 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.870000	-0.338000	-0.491000
2	6	0	-7.021000	1.150000	-0.375000
3	6	0	-6.032000	1.928000	0.472000
4	6	0	-4.658000	1.293000	0.500000
5	6	0	-4.440000	0.061000	0.055000
6	6	0	-5.465000	-0.806000	-0.464000
7	1	0	-7.397000	-0.703000	-1.376000
8	1	0	-7.416000	-0.783000	0.361000

9	6	0	-4.891000	-1.968000	-0.814000
10	6	0	-3.453000	-1.842000	-0.507000
11	8	0	-3.239000	-0.577000	0.029000
12	6	0	-5.447000	-3.212000	-1.387000
13	1	0	-6.516000	-3.123000	-1.593000
14	1	0	-5.294000	-4.055000	-0.705000
15	1	0	-4.929000	-3.469000	-2.318000
16	6	0	-6.574000	1.955000	1.919000
17	1	0	-6.722000	0.938000	2.295000
18	1	0	-7.519000	2.503000	1.976000
19	1	0	-5.845000	2.451000	2.568000
20	6	0	-5.761000	3.345000	-0.001000
21	6	0	-5.778000	3.782000	-1.321000
22	8	0	-8.862000	2.117000	-3.372000
23	6	0	-8.146000	1.719000	-0.896000
24	6	0	-8.540000	3.066000	-0.777000
25	6	0	-9.347000	1.173000	-2.822000
26	6	0	-10.309000	0.189000	-3.385000
27	1	0	-10.536000	0.447000	-4.418000
28	1	0	-11.224000	0.187000	-2.787000
29	1	0	-9.884000	-0.817000	-3.332000
30	8	0	-9.051000	0.860000	-1.519000
31	78	0	-7.501000	4.595000	-0.274000
32	1	0	-9.595000	3.245000	-1.003000
33	17	0	-9.524000	5.729000	0.155000
34	17	0	-6.208000	6.503000	0.369000
35	1	0	-5.195000	4.652000	-1.606000
36	1	0	-6.111000	3.135000	-2.129000
37	1	0	-5.153000	3.909000	0.708000
38	1	0	-3.850000	1.887000	0.919000
39	8	0	-2.566000	-2.622000	-0.654000

Transition state: TS XII-XIII

- **Thermal correction to Gibbs Free Energy = 0.229916 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.74290578 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.08994057 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.12771681 Hartree**
- **Frequency = -245.4**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.522000	0.025000	0.731000
2	6	0	-6.476000	1.477000	0.367000
3	6	0	-5.087000	2.067000	0.170000
4	6	0	-4.365000	1.253000	-0.881000
5	6	0	-4.651000	-0.042000	-0.995000
6	6	0	-5.669000	-0.735000	-0.232000
7	1	0	-7.549000	-0.346000	0.719000
8	1	0	-6.145000	-0.117000	1.755000
9	6	0	-5.665000	-2.022000	-0.610000
10	6	0	-4.615000	-2.164000	-1.638000
11	8	0	-4.037000	-0.920000	-1.835000
12	8	0	-4.263000	-3.129000	-2.241000
13	6	0	-6.485000	-3.178000	-0.190000
14	1	0	-7.264000	-2.889000	0.520000
15	1	0	-5.860000	-3.946000	0.276000
16	1	0	-6.958000	-3.648000	-1.059000
17	6	0	-4.315000	1.971000	1.506000
18	1	0	-4.162000	0.934000	1.815000
19	1	0	-4.841000	2.507000	2.305000
20	1	0	-3.327000	2.426000	1.382000
21	6	0	-5.113000	3.531000	-0.227000
22	78	0	-6.489000	4.005000	-1.744000
23	8	0	-8.892000	2.851000	2.368000
24	6	0	-7.613000	2.191000	0.216000

25	6	0	-7.667000	3.540000	-0.274000
26	6	0	-9.425000	2.047000	1.660000
27	6	0	-10.746000	1.397000	1.854000
28	1	0	-11.193000	1.742000	2.785000
29	1	0	-10.631000	0.311000	1.871000
30	1	0	-11.399000	1.639000	1.011000
31	8	0	-8.839000	1.609000	0.500000
32	6	0	-6.114000	4.402000	0.359000
33	1	0	-4.135000	3.964000	-0.436000
34	17	0	-8.444000	4.688000	-3.046000
35	17	0	-5.225000	3.644000	-3.677000
36	1	0	-8.606000	4.085000	-0.157000
37	1	0	-5.986000	5.481000	0.304000
38	1	0	-6.628000	4.146000	1.298000
39	1	0	-3.610000	1.734000	-1.496000

Structure XIII

- **Thermal correction to Gibbs Free Energy = 0.236194 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.80895490 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.844000	0.087000	0.339000
2	6	0	-6.588000	1.561000	0.213000
3	6	0	-5.142000	2.083000	0.196000
4	6	0	-4.221000	1.153000	-0.538000
5	6	0	-4.589000	-0.093000	-0.811000
6	6	0	-5.856000	-0.692000	-0.452000
7	1	0	-7.869000	-0.157000	0.037000
8	1	0	-6.753000	-0.190000	1.403000
9	6	0	-5.869000	-1.945000	-0.926000

10	6	0	-4.578000	-2.163000	-1.603000
11	8	0	-3.833000	-0.999000	-1.490000
12	8	0	-4.159000	-3.128000	-2.163000
13	6	0	-6.896000	-3.007000	-0.883000
14	1	0	-6.521000	-3.891000	-0.356000
15	1	0	-7.149000	-3.331000	-1.898000
16	1	0	-7.810000	-2.671000	-0.388000
17	6	0	-4.599000	2.314000	1.611000
18	1	0	-4.488000	1.349000	2.116000
19	1	0	-5.262000	2.936000	2.219000
20	1	0	-3.609000	2.784000	1.569000
21	6	0	-5.364000	3.353000	-0.620000
22	78	0	-7.135000	2.707000	-1.565000
23	8	0	-8.078000	1.561000	2.949000
24	6	0	-7.585000	2.517000	0.567000
25	6	0	-7.419000	3.886000	0.233000
26	6	0	-8.989000	1.588000	2.180000
27	6	0	-10.381000	1.110000	2.379000
28	1	0	-11.089000	1.908000	2.144000
29	1	0	-10.511000	0.775000	3.407000
30	1	0	-10.583000	0.286000	1.689000
31	8	0	-8.848000	2.097000	0.905000
32	6	0	-6.030000	4.478000	0.119000
33	1	0	-4.651000	3.580000	-1.413000
34	17	0	-7.476000	4.457000	-3.154000
35	17	0	-6.642000	1.110000	-3.264000
36	1	0	-8.290000	4.529000	0.328000
37	1	0	-6.073000	5.377000	-0.499000
38	1	0	-5.568000	4.730000	1.082000
39	1	0	-3.246000	1.530000	-0.832000

Transition state: TS XIII-XIV

- **Thermal correction to Gibbs Free Energy = 0.235124 Hartree**

- **Electronic energy (M06/Def2TZVPP,tol) = -1959.78699802 Hartree**
- **Frequency = -155.8881**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.520000	-0.119000	0.599000
2	6	0	-6.406000	1.367000	0.479000
3	6	0	-5.033000	1.993000	0.234000
4	6	0	-4.329000	1.269000	-0.887000
5	6	0	-4.642000	-0.002000	-1.128000
6	6	0	-5.688000	-0.756000	-0.463000
7	1	0	-7.565000	-0.431000	0.515000
8	1	0	-6.166000	-0.431000	1.595000
9	6	0	-5.731000	-1.974000	-1.020000
10	6	0	-4.676000	-2.020000	-2.048000
11	8	0	-4.042000	-0.786000	-2.066000
12	8	0	-4.349000	-2.906000	-2.774000
13	6	0	-6.634000	-3.122000	-0.794000
14	1	0	-6.063000	-4.031000	-0.577000
15	1	0	-7.216000	-3.325000	-1.700000
16	1	0	-7.328000	-2.937000	0.028000
17	6	0	-4.144000	1.922000	1.485000
18	1	0	-3.838000	0.886000	1.653000
19	1	0	-4.653000	2.270000	2.389000
20	1	0	-3.237000	2.518000	1.342000
21	6	0	-5.440000	3.419000	-0.176000
22	78	0	-7.303000	2.387000	-1.207000
23	8	0	-9.880000	3.496000	0.979000
24	6	0	-7.399000	2.281000	0.902000
25	6	0	-7.079000	3.695000	0.601000
26	6	0	-9.730000	2.418000	1.459000
27	6	0	-10.763000	1.515000	2.026000
28	1	0	-10.910000	0.685000	1.327000

29	1	0	-11.700000	2.056000	2.146000
30	1	0	-10.432000	1.093000	2.976000
31	8	0	-8.492000	1.796000	1.544000
32	6	0	-5.774000	4.321000	0.949000
33	1	0	-5.093000	3.853000	-1.111000
34	17	0	-7.532000	3.666000	-3.174000
35	17	0	-8.561000	0.608000	-2.094000
36	1	0	-7.902000	4.354000	0.343000
37	1	0	-5.751000	5.383000	0.724000
38	1	0	-5.352000	4.084000	1.921000
39	1	0	-3.537000	1.775000	-1.431000

Structure XIV

- **Thermal correction to Gibbs Free Energy = 0.238605 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.80617668 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.15411561 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.19243886 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.374000	-1.830000	1.243000
2	6	0	0.585000	-0.345000	1.182000
3	6	0	2.041000	0.102000	1.292000
4	6	0	2.838000	-0.492000	0.161000
5	6	0	2.461000	-1.703000	-0.248000
6	6	0	1.293000	-2.431000	0.218000
7	1	0	-0.660000	-2.134000	1.059000
8	1	0	0.640000	-2.201000	2.245000
9	6	0	1.234000	-3.591000	-0.455000
10	6	0	2.395000	-3.624000	-1.363000
11	8	0	3.100000	-2.448000	-1.201000

12	6	0	0.261000	-4.704000	-0.419000
13	1	0	0.746000	-5.634000	-0.103000
14	1	0	-0.144000	-4.889000	-1.419000
15	1	0	-0.570000	-4.500000	0.261000
16	6	0	2.648000	-0.465000	2.600000
17	1	0	2.842000	-1.537000	2.525000
18	1	0	2.007000	-0.291000	3.469000
19	1	0	3.605000	0.035000	2.781000
20	6	0	1.942000	1.632000	1.388000
21	78	0	-0.590000	0.282000	-0.658000
22	8	0	-2.351000	-0.453000	0.338000
23	6	0	-0.253000	0.761000	1.386000
24	6	0	0.494000	2.033000	1.503000
25	6	0	-2.471000	-0.010000	1.480000
26	6	0	-3.697000	-0.168000	2.289000
27	1	0	-3.448000	-0.526000	3.289000
28	1	0	-4.386000	-0.846000	1.790000
29	1	0	-4.166000	0.815000	2.399000
30	8	0	-1.506000	0.667000	2.063000
31	6	0	1.421000	2.216000	2.665000
32	1	0	2.608000	2.227000	0.773000
33	17	0	-1.758000	0.228000	-2.675000
34	17	0	1.161000	1.308000	-1.762000
35	1	0	0.100000	2.900000	0.982000
36	1	0	1.700000	3.242000	2.882000
37	1	0	1.297000	1.596000	3.546000
38	1	0	3.711000	0.012000	-0.240000
39	8	0	2.739000	-4.471000	-2.131000

Structure 6

- **Thermal correction to Gibbs Free Energy = 0.239634 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -919.90789191 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.118000	-3.179000	0.813000
2	6	0	1.185000	-1.726000	0.482000
3	6	0	2.521000	-1.086000	0.152000
4	6	0	3.064000	-1.780000	-1.115000
5	6	0	2.881000	-3.242000	-0.961000
6	6	0	2.038000	-3.896000	-0.124000
7	1	0	0.086000	-3.541000	0.723000
8	1	0	1.419000	-3.361000	1.858000
9	6	0	2.246000	-5.296000	-0.349000
10	6	0	3.200000	-5.366000	-1.309000
11	8	0	3.602000	-4.122000	-1.695000
12	8	0	3.734000	-6.321000	-1.909000
13	6	0	1.551000	-6.416000	0.338000
14	1	0	1.892000	-7.386000	-0.032000
15	1	0	0.466000	-6.363000	0.188000
16	1	0	1.725000	-6.389000	1.420000
17	6	0	3.533000	-1.212000	1.287000
18	1	0	3.821000	-2.255000	1.454000
19	1	0	3.126000	-0.818000	2.223000
20	1	0	4.441000	-0.647000	1.047000
21	6	0	2.155000	0.367000	-0.139000
22	6	0	1.493000	1.188000	0.918000
23	8	0	-1.479000	0.187000	2.080000
24	6	0	0.196000	-0.862000	0.277000
25	6	0	0.651000	0.492000	-0.112000
26	6	0	-1.915000	-0.568000	1.262000
27	6	0	-3.342000	-0.973000	1.092000
28	1	0	-3.700000	-0.652000	0.111000
29	1	0	-3.950000	-0.522000	1.875000
30	1	0	-3.429000	-2.062000	1.127000

31	8	0	-1.145000	-1.196000	0.334000
32	1	0	0.085000	1.062000	-0.843000
33	1	0	1.597000	2.265000	0.833000
34	1	0	1.422000	0.811000	1.934000
35	1	0	2.735000	0.889000	-0.896000
36	1	0	3.483000	-1.306000	-1.930000

Transition state: TS X-XV

- **Thermal correction to Gibbs Free Energy = 0.234244 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.74803688 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.09440785 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.1316488 Hartree**
- **Frequency = -339.0308**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.986737	0.502171	-1.194848
2	6	0	0.866123	0.335447	-0.169311
3	6	0	0.615201	-1.160956	0.122127
4	6	0	1.854517	-1.769117	0.734334
5	6	0	3.022366	-1.321893	0.276784
6	6	0	3.181208	-0.238280	-0.681482
7	1	0	2.209317	1.561607	-1.352383
8	1	0	1.656972	0.112758	-2.163763
9	6	0	4.495413	-0.075029	-0.898990
10	6	0	5.201289	-1.068587	-0.066608
11	8	0	4.252323	-1.794345	0.632988
12	6	0	5.243814	0.864914	-1.760521
13	1	0	5.776804	0.322094	-2.548943
14	1	0	6.007349	1.393364	-1.180381

15	1	0	4.587556	1.598642	-2.233778
16	6	0	0.346906	-1.909742	-1.205260
17	1	0	1.246978	-1.997559	-1.815978
18	1	0	-0.447043	-1.436288	-1.791972
19	1	0	0.019239	-2.925879	-0.967593
20	6	0	-0.651021	-1.329770	0.947676
21	6	0	-1.184988	-0.450364	1.884925
22	8	0	1.372935	0.967619	1.059172
23	6	0	-0.444563	0.994840	-0.474140
24	6	0	-0.651301	2.243727	-0.455128
25	6	0	1.463864	2.283523	1.113756
26	6	0	2.166199	2.760961	2.329428
27	1	0	1.625085	2.413201	3.214354
28	1	0	2.221106	3.847738	2.327659
29	1	0	3.167652	2.325629	2.370158
30	8	0	1.002581	3.038882	0.260943
31	78	0	-2.156240	-0.082979	-0.024620
32	17	0	-3.488218	0.933425	-1.675380
33	17	0	-3.914599	-1.528345	0.636979
34	1	0	-1.952565	-0.815630	2.560135
35	1	0	-1.036508	-2.350121	0.953456
36	1	0	-0.676442	0.456581	2.192157
37	1	0	-1.202246	3.161923	-0.521938
38	1	0	1.780367	-2.586826	1.443823
39	8	0	6.369707	-1.270438	0.055860

Structure XV

- **Thermal correction to Gibbs Free Energy = 0.236431 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.76621466 Hartree**

Cartesian Coordinates of the computed structure:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.935766	0.493721	1.163753
2	6	0	-0.816015	0.291943	0.146731
3	6	0	-0.582002	-1.208592	-0.104916
4	6	0	-1.825226	-1.825797	-0.701767
5	6	0	-2.989914	-1.362664	-0.251073
6	6	0	-3.139378	-0.252296	0.678196
7	1	0	-2.156369	1.556317	1.313489
8	1	0	-1.593959	0.127208	2.137095
9	6	0	-4.452238	-0.064995	0.884436
10	6	0	-5.167163	-1.074913	0.078580
11	8	0	-4.224973	-1.831630	-0.595096
12	6	0	-5.193901	0.910591	1.711507
13	1	0	-4.535555	1.663512	2.151029
14	1	0	-5.720638	0.401548	2.526227
15	1	0	-5.963390	1.412671	1.115940
16	6	0	-0.338118	-1.915624	1.253854
17	1	0	-1.243624	-1.970608	1.860431
18	1	0	0.461255	-1.435028	1.825994
19	1	0	-0.026199	-2.943318	1.047439
20	6	0	0.702127	-1.412178	-0.892292
21	6	0	1.231499	-0.575130	-1.872668
22	8	0	-1.432599	0.915615	-1.120603
23	6	0	0.479316	1.018539	0.329263
24	6	0	0.430525	2.328752	0.155844
25	6	0	-1.498639	2.186818	-1.136610
26	6	0	-2.448989	2.827209	-2.054785
27	1	0	-2.448521	2.291429	-3.006353
28	1	0	-2.211755	3.880392	-2.191005
29	1	0	-3.455423	2.727136	-1.630868
30	8	0	-0.778073	2.924810	-0.377569
31	78	0	2.144068	-0.086095	0.028781

32	17	0	3.390003	1.103091	1.635857
33	17	0	4.012052	-1.484037	-0.567443
34	1	0	1.208446	3.076691	0.198356
35	1	0	2.017630	-0.961146	-2.514102
36	1	0	1.097481	-2.426936	-0.838922
37	1	0	0.704671	0.296205	-2.247266
38	1	0	-1.755298	-2.659730	-1.392389
39	8	0	-6.337816	-1.263439	-0.043155

Transition state: TS XV-XVI

- **Thermal correction to Gibbs Free Energy = 0.235182 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.76184577 Hartree**
- **Frequency = -308.8412**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.958293	0.415516	-1.216688
2	6	0	0.781526	0.206705	-0.298535
3	6	0	0.581198	-1.242920	0.111574
4	6	0	1.825823	-1.803975	0.756115
5	6	0	2.995843	-1.352975	0.310174
6	6	0	3.155632	-0.292962	-0.670849
7	1	0	2.151151	1.476749	-1.398513
8	1	0	1.668448	0.006756	-2.194373
9	6	0	4.469052	-0.113922	-0.875083
10	6	0	5.176010	-1.073507	-0.003913
11	8	0	4.225891	-1.796306	0.698412
12	6	0	5.216208	0.816429	-1.748083
13	1	0	5.790883	0.261215	-2.497441
14	1	0	5.944890	1.390096	-1.165775

15	1	0	4.554457	1.511074	-2.270351
16	6	0	0.345793	-2.056556	-1.195762
17	1	0	1.240461	-2.103208	-1.818899
18	1	0	-0.494039	-1.663372	-1.776845
19	1	0	0.100637	-3.081151	-0.901284
20	6	0	-0.700358	-1.396021	0.916231
21	6	0	-1.189371	-0.507934	1.872239
22	8	0	1.535315	1.055566	1.145356
23	6	0	-0.449319	0.964765	-0.430083
24	6	0	-0.407447	2.285056	-0.278150
25	6	0	1.483257	2.289717	1.087423
26	6	0	2.239300	3.152130	2.015521
27	1	0	2.678117	3.982253	1.457162
28	1	0	3.003714	2.581893	2.538974
29	1	0	1.538369	3.584373	2.736943
30	8	0	0.746165	2.942307	0.213202
31	78	0	-2.138300	-0.098786	-0.027674
32	17	0	-3.398992	1.033412	-1.662497
33	17	0	-4.007026	-1.448271	0.657834
34	1	0	-1.238374	2.976990	-0.326245
35	1	0	-1.963357	-0.849097	2.552518
36	1	0	-1.105291	-2.408248	0.915103
37	1	0	-0.631542	0.366983	2.189109
38	1	0	1.745013	-2.604392	1.484204
39	8	0	6.344818	-1.252607	0.143125

Structure XVI

- **Thermal correction to Gibbs Free Energy = 0.232398 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.79938492 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.14556851 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.18367827 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.353480	0.368803	1.465306
2	6	0	-1.097440	-0.172475	0.844200
3	6	0	-1.107955	-1.542492	0.192713
4	6	0	-2.384836	-1.762628	-0.580392
5	6	0	-3.444217	-0.983099	-0.377614
6	6	0	-3.519649	0.096756	0.582890
7	1	0	-2.246704	1.435698	1.686459
8	1	0	-2.517093	-0.133529	2.431699
9	6	0	-4.741048	0.644807	0.494350
10	6	0	-5.473762	-0.100267	-0.545254
11	8	0	-4.633294	-1.089665	-1.036450
12	6	0	-5.377495	1.756499	1.232957
13	1	0	-4.672445	2.258766	1.899224
14	1	0	-6.218073	1.391148	1.833175
15	1	0	-5.791183	2.493269	0.536783
16	6	0	-0.946492	-2.639756	1.252689
17	1	0	-1.744705	-2.577121	1.998080
18	1	0	0.020501	-2.548139	1.758497
19	1	0	-1.002394	-3.627725	0.783510
20	6	0	0.053518	-1.616976	-0.795893
21	6	0	0.369044	-0.633175	-1.728032
22	1	0	0.453922	-2.618392	-0.956625
23	1	0	-0.222330	0.276047	-1.804875
24	1	0	0.986600	-0.887961	-2.583740
25	8	0	2.485947	3.541731	0.066177
26	6	0	0.044310	0.481205	0.849700
27	6	0	0.828700	1.582016	0.713776
28	6	0	1.468825	3.459213	-0.539718
29	6	0	0.973287	4.320554	-1.643271

30	1	0	-0.012999	4.718662	-1.393151
31	1	0	0.862409	3.722288	-2.551581
32	1	0	1.677014	5.132294	-1.817056
33	8	0	0.528906	2.460721	-0.277304
34	78	0	1.732742	-0.443887	-0.030803
35	1	0	1.604905	1.885848	1.412209
36	17	0	3.172774	-2.053772	-0.965176
37	17	0	3.412580	0.116282	1.528903
38	1	0	-2.418075	-2.580717	-1.295424
39	8	0	-6.583071	0.045479	-0.955972

Transition state: TS XVI-XVII

- **Thermal correction to Gibbs Free Energy = 0.230428 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.74864884 Hartree**
- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.09471253 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.13422642 Hartree**
- **Frequency = -311.7920**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.740605	-0.589490	-0.945375
2	6	0	-0.745594	0.521755	-0.773806
3	6	0	-1.245861	1.942463	-1.123622
4	6	0	-2.600410	2.195069	-0.500698
5	6	0	-3.363649	1.172159	-0.125821
6	6	0	-3.014804	-0.225629	-0.272047
7	1	0	-1.330682	-1.521814	-0.547776
8	1	0	-1.934127	-0.760564	-2.015747
9	6	0	-4.009125	-0.954121	0.256969
10	6	0	-5.034680	-0.007124	0.730619

11	8	0	-4.588166	1.282421	0.458752
12	6	0	-4.185295	-2.414982	0.399549
13	1	0	-3.257514	-2.954068	0.194693
14	1	0	-4.959779	-2.784898	-0.281941
15	1	0	-4.517042	-2.659428	1.413311
16	6	0	-1.334175	2.082410	-2.653179
17	1	0	-2.105614	1.413370	-3.042387
18	1	0	-0.388402	1.821565	-3.137181
19	1	0	-1.609311	3.105689	-2.928825
20	6	0	-0.242272	2.864792	-0.525270
21	6	0	1.002613	3.059922	-1.033812
22	1	0	-0.475289	3.264091	0.462070
23	1	0	1.249197	2.748116	-2.045704
24	1	0	1.699934	3.744303	-0.560008
25	8	0	3.656069	2.517166	0.968683
26	6	0	0.506895	0.337662	-0.377871
27	6	0	1.491126	1.355449	-0.046262
28	6	0	2.809169	2.161318	1.722198
29	6	0	2.813831	2.140832	3.202461
30	1	0	3.730844	2.590528	3.578085
31	1	0	2.734049	1.102420	3.538159
32	1	0	1.937999	2.667822	3.588260
33	8	0	1.585285	1.660800	1.261964
34	78	0	1.479936	-1.343378	-0.143475
35	1	0	2.445878	1.353792	-0.581848
36	17	0	2.586266	-0.963057	-2.195046
37	17	0	0.419251	-1.828288	1.887098
38	1	0	-2.944559	3.219881	-0.392054
39	8	0	-6.084109	-0.206554	1.258210

Structure XVII

- **Thermal correction to Gibbs Free Energy = 0.234722 Hartree**

- **Electronic energy (M06/Def2TZVPP,tol) = -1959.80304038 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.694109	-0.542426	-0.401037
2	6	0	0.829677	0.699238	-0.332471
3	6	0	1.421059	2.062684	0.280190
4	6	0	2.879225	2.010012	0.526444
5	6	0	3.638481	0.977014	0.167888
6	6	0	3.148960	-0.277265	-0.349058
7	1	0	1.423233	-1.115225	-1.296761
8	1	0	1.425773	-1.184863	0.450233
9	6	0	4.212274	-1.055851	-0.610426
10	6	0	5.412481	-0.288044	-0.240637
11	8	0	4.995482	0.946319	0.250298
12	8	0	6.566082	-0.579971	-0.301945
13	6	0	4.311731	-2.442018	-1.115166
14	1	0	3.345870	-2.821496	-1.456179
15	1	0	4.686050	-3.112816	-0.333620
16	1	0	5.027010	-2.499012	-1.941981
17	6	0	0.696256	2.849536	1.342175
18	1	0	0.866061	2.400994	2.324369
19	1	0	-0.380405	2.928051	1.200853
20	1	0	1.104346	3.866632	1.357030
21	6	0	1.005457	2.003896	-1.138070
22	6	0	-0.364596	2.521036	-1.517667
23	1	0	1.800097	2.025703	-1.879058
24	8	0	-3.954116	1.602917	0.002804
25	6	0	-0.577080	0.538429	-0.162281
26	6	0	-1.372233	1.697058	-0.719771
27	6	0	-3.657952	1.162226	-1.070126
28	6	0	-4.554884	0.464075	-2.030980

29	1	0	-5.590406	0.556745	-1.707842
30	1	0	-4.263569	-0.591825	-2.057882
31	1	0	-4.426036	0.862803	-3.039177
32	8	0	-2.394783	1.221144	-1.576880
33	78	0	-1.401334	-0.943090	0.579272
34	17	0	-1.251090	-0.111947	2.766759
35	17	0	-1.703282	-2.159239	-1.399057
36	1	0	-1.846153	2.231514	0.116574
37	1	0	-0.542148	2.337462	-2.581229
38	1	0	-0.467023	3.595493	-1.338525
39	1	0	3.326569	2.890168	0.980778

Transition state: TS XVII-XVIII

- **Thermal correction to Gibbs Free Energy = 0.230264 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.75841223 Hartree**
- **Frequency = -685.7293**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.620484	-0.366189	0.477406
2	6	0	-6.566503	1.037086	-0.123790
3	6	0	-5.218953	1.740405	-0.409955
4	6	0	-4.014254	0.861427	-0.315893
5	6	0	-4.122058	-0.444654	-0.037421
6	6	0	-5.351562	-1.134992	0.298360
7	1	0	-7.478553	-0.912801	0.072614
8	1	0	-6.819607	-0.267272	1.552375
9	6	0	-5.060376	-2.447068	0.467900
10	6	0	-3.606655	-2.600858	0.247333
11	8	0	-3.075718	-1.336839	-0.046718

12	8	0	-2.904771	-3.581804	0.288974
13	6	0	-5.926384	-3.604905	0.837915
14	1	0	-6.986507	-3.347489	0.778572
15	1	0	-5.715402	-3.939525	1.860479
16	1	0	-5.731103	-4.457621	0.179797
17	6	0	-4.909322	3.187042	-0.043443
18	1	0	-4.727745	3.287508	1.029909
19	1	0	-5.683445	3.907273	-0.321917
20	1	0	-4.004089	3.501203	-0.573153
21	6	0	-6.161418	1.372477	-1.557820
22	6	0	-7.129046	2.416616	-2.111509
23	1	0	-5.829292	0.591147	-2.234090
24	8	0	-8.015267	5.276301	-1.756256
25	6	0	-7.776666	1.911389	0.178691
26	6	0	-8.078152	2.682214	-0.966409
27	6	0	-9.081050	4.764807	-1.554906
28	6	0	-10.450127	5.341324	-1.716510
29	1	0	-10.372205	6.344720	-2.131919
30	1	0	-10.945118	5.374984	-0.741187
31	1	0	-11.051850	4.701112	-2.367516
32	8	0	-9.179195	3.448142	-1.047000
33	78	0	-8.885289	1.805491	1.760051
34	17	0	-7.834053	3.741401	2.646273
35	17	0	-10.132720	-0.076994	1.067021
36	1	0	-7.735006	2.004726	-2.928556
37	1	0	-6.653981	3.327190	-2.484233
38	1	0	-7.341456	3.109807	0.161777
39	1	0	-3.046617	1.300220	-0.538248

Structure XVIII

- **Thermal correction to Gibbs Free Energy = 0.236308 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1959.81646874 Hartree**

- **Electronic energy (B3PW91-D3/Def2TZVPP,tol) = -1960.16378945 Hartree**
- **Electronic energy (wB97XD/Def2TZVPP,tol) = -1960.20143237 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.936949	-0.521593	-0.501370
2	6	0	-0.969467	0.614697	-0.253631
3	6	0	-1.440374	2.069728	-0.110706
4	6	0	-2.905154	2.254392	-0.020619
5	6	0	-3.742198	1.220749	-0.078930
6	6	0	-3.359002	-0.154006	-0.290249
7	1	0	-1.660181	-1.363924	0.148479
8	1	0	-1.808015	-0.881446	-1.533030
9	6	0	-4.480913	-0.895264	-0.283509
10	6	0	-5.608997	0.021958	-0.067877
11	8	0	-5.097681	1.307247	0.048185
12	8	0	-6.780460	-0.196543	0.003447
13	6	0	-4.690203	-2.348009	-0.467262
14	1	0	-3.742161	-2.884096	-0.553569
15	1	0	-5.282452	-2.544741	-1.367986
16	1	0	-5.254060	-2.767536	0.372550
17	6	0	-0.752768	3.221759	-0.802921
18	1	0	-1.153751	3.349571	-1.813338
19	1	0	0.329900	3.113208	-0.892608
20	1	0	-0.945738	4.148771	-0.250593
21	6	0	-0.805433	1.346441	1.061199
22	6	0	0.663750	1.588851	1.331215
23	1	0	-1.457206	1.088003	1.890062
24	8	0	3.612229	1.159885	1.484265
25	6	0	0.390943	0.490151	-0.821237
26	6	0	1.344677	1.041206	0.095211

27	6	0	3.596121	1.654703	0.401169
28	6	0	4.709680	2.305589	-0.333286
29	1	0	5.567488	2.424355	0.325917
30	1	0	4.393091	3.270716	-0.734324
31	1	0	4.978723	1.670664	-1.183699
32	8	0	2.463695	1.643007	-0.392669
33	78	0	1.512639	-1.094092	0.003518
34	17	0	2.817602	-1.090889	-1.944756
35	17	0	0.427788	-1.590138	2.012604
36	1	0	1.009477	1.112761	2.248736
37	1	0	0.912313	2.656425	1.405405
38	1	0	0.574867	0.482926	-1.894542
39	1	0	-3.284296	3.264092	0.115689

Structure XIX

- **Thermal correction to Gibbs Free Energy = 0.250472 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.90464914 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.766000	-0.388000	0.056000
2	6	0	-6.799000	1.139000	-0.146000
3	6	0	-5.536000	1.846000	0.473000
4	6	0	-4.283000	1.350000	-0.277000
5	6	0	-4.343000	-0.116000	-0.438000
6	1	0	-3.397000	1.654000	0.295000
7	1	0	-4.201000	1.828000	-1.260000
8	6	0	-5.428000	-0.914000	-0.320000
9	1	0	-7.571000	-0.829000	-0.539000
10	1	0	-7.007000	-0.605000	1.106000
11	6	0	-4.992000	-2.245000	-0.628000

12	6	0	-3.671000	-2.127000	-0.907000
13	8	0	-3.257000	-0.832000	-0.798000
14	1	0	-2.915000	-2.845000	-1.186000
15	6	0	-5.826000	-3.475000	-0.635000
16	1	0	-6.648000	-3.394000	-1.355000
17	1	0	-6.277000	-3.658000	0.347000
18	1	0	-5.234000	-4.355000	-0.900000
19	6	0	-5.407000	1.490000	1.956000
20	1	0	-5.165000	0.436000	2.113000
21	1	0	-6.322000	1.727000	2.508000
22	1	0	-4.597000	2.084000	2.392000
23	6	0	-5.690000	3.348000	0.371000
24	6	0	-5.342000	4.132000	-0.639000
25	1	0	-6.149000	3.813000	1.245000
26	1	0	-4.885000	3.757000	-1.550000
27	1	0	-5.521000	5.202000	-0.593000
28	8	0	-6.727000	1.477000	-1.536000
29	6	0	-8.039000	1.667000	0.460000
30	6	0	-9.019000	1.882000	1.170000
31	6	0	-7.749000	1.207000	-2.381000
32	6	0	-7.494000	1.860000	-3.697000
33	1	0	-7.664000	2.937000	-3.580000
34	1	0	-8.179000	1.469000	-4.447000
35	1	0	-6.457000	1.722000	-4.008000
36	8	0	-8.722000	0.575000	-2.075000
37	79	0	-8.921000	3.588000	-0.219000
38	17	0	-9.308000	5.532000	-1.426000
39	1	0	-9.823000	1.846000	1.875000

Transition state: TS XIX-XX

- **Thermal correction to Gibbs Free Energy = 0.250021 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.88114099 Hartree**
- **Frequency = -311.0**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.879000	-0.460000	0.290000
2	6	0	-7.088000	0.999000	-0.127000
3	6	0	-5.808000	1.885000	0.066000
4	6	0	-4.670000	1.316000	-0.803000
5	6	0	-4.604000	-0.150000	-0.652000
6	1	0	-3.728000	1.791000	-0.500000
7	1	0	-4.825000	1.570000	-1.860000
8	6	0	-5.574000	-0.973000	-0.201000
9	1	0	-7.728000	-1.040000	-0.094000
10	1	0	-6.948000	-0.514000	1.386000
11	6	0	-5.056000	-2.306000	-0.295000
12	6	0	-3.808000	-2.164000	-0.804000
13	8	0	-3.514000	-0.851000	-1.031000
14	1	0	-3.032000	-2.872000	-1.048000
15	6	0	-5.756000	-3.559000	0.093000
16	1	0	-6.681000	-3.693000	-0.480000
17	1	0	-6.035000	-3.548000	1.152000
18	1	0	-5.127000	-4.437000	-0.079000
19	6	0	-5.370000	1.873000	1.535000
20	1	0	-5.066000	0.875000	1.861000
21	1	0	-6.164000	2.227000	2.201000
22	1	0	-4.514000	2.544000	1.653000
23	6	0	-6.134000	3.312000	-0.299000
24	6	0	-5.627000	4.027000	-1.293000
25	1	0	-6.848000	3.791000	0.371000
26	1	0	-4.893000	3.638000	-1.993000
27	1	0	-5.921000	5.062000	-1.434000
28	8	0	-7.290000	0.938000	-1.577000
29	6	0	-8.292000	1.552000	0.562000
30	6	0	-9.290000	2.168000	0.106000

31	6	0	-8.111000	1.681000	-2.297000
32	6	0	-7.812000	1.565000	-3.750000
33	1	0	-6.894000	2.127000	-3.951000
34	1	0	-8.628000	1.980000	-4.338000
35	1	0	-7.627000	0.522000	-4.016000
36	8	0	-9.011000	2.383000	-1.867000
37	79	0	-8.800000	1.410000	2.584000
38	1	0	-10.231000	2.676000	0.083000
39	17	0	-9.280000	1.169000	4.857000

Structure XX

- **Thermal correction to Gibbs Free Energy = 0.253647 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.90096505 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.860000	-0.446000	0.334000
2	6	0	-7.050000	1.019000	-0.044000
3	6	0	-5.755000	1.882000	0.099000
4	6	0	-4.638000	1.301000	-0.792000
5	6	0	-4.593000	-0.166000	-0.642000
6	1	0	-3.686000	1.760000	-0.496000
7	1	0	-4.792000	1.561000	-1.847000
8	6	0	-5.567000	-0.975000	-0.172000
9	1	0	-7.724000	-1.009000	-0.045000
10	1	0	-6.927000	-0.512000	1.429000
11	6	0	-5.065000	-2.315000	-0.260000
12	6	0	-3.822000	-2.191000	-0.787000
13	8	0	-3.516000	-0.884000	-1.029000
14	1	0	-3.056000	-2.910000	-1.034000
15	6	0	-5.772000	-3.555000	0.151000

16	1	0	-6.706000	-3.687000	-0.409000
17	1	0	-6.039000	-3.526000	1.213000
18	1	0	-5.155000	-4.442000	-0.016000
19	6	0	-5.275000	1.867000	1.557000
20	1	0	-4.977000	0.865000	1.875000
21	1	0	-6.045000	2.232000	2.242000
22	1	0	-4.403000	2.524000	1.642000
23	6	0	-6.082000	3.311000	-0.256000
24	6	0	-5.652000	4.002000	-1.303000
25	1	0	-6.733000	3.807000	0.465000
26	1	0	-4.981000	3.590000	-2.052000
27	1	0	-5.938000	5.041000	-1.436000
28	8	0	-7.235000	0.952000	-1.578000
29	6	0	-8.279000	1.602000	0.571000
30	6	0	-9.181000	2.180000	-0.202000
31	6	0	-8.083000	1.654000	-2.200000
32	6	0	-7.977000	1.716000	-3.669000
33	1	0	-7.112000	2.338000	-3.922000
34	1	0	-8.877000	2.147000	-4.103000
35	1	0	-7.790000	0.716000	-4.063000
36	8	0	-9.024000	2.295000	-1.636000
37	79	0	-8.647000	1.482000	2.591000
38	1	0	-10.120000	2.643000	0.060000
39	17	0	-9.127000	1.341000	4.890000

Structure XXI

- **Thermal correction to Gibbs Free Energy = 0.247967 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.91235827 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-6.686000	-0.286000	0.469000
2	6	0	-6.667000	1.221000	0.453000
3	6	0	-5.314000	1.892000	0.734000
4	6	0	-4.339000	1.471000	-0.382000
5	6	0	-4.470000	0.018000	-0.624000
6	1	0	-3.313000	1.730000	-0.089000
7	1	0	-4.562000	2.031000	-1.301000
8	6	0	-5.492000	-0.792000	-0.265000
9	1	0	-7.619000	-0.654000	0.025000
10	1	0	-6.685000	-0.639000	1.513000
11	6	0	-5.155000	-2.106000	-0.728000
12	6	0	-3.951000	-1.968000	-1.333000
13	8	0	-3.515000	-0.676000	-1.278000
14	1	0	-3.297000	-2.667000	-1.831000
15	6	0	-5.971000	-3.338000	-0.570000
16	1	0	-6.953000	-3.230000	-1.045000
17	1	0	-6.151000	-3.564000	0.488000
18	1	0	-5.476000	-4.204000	-1.017000
19	6	0	-4.798000	1.401000	2.097000
20	1	0	-4.587000	0.328000	2.094000
21	1	0	-5.531000	1.608000	2.885000
22	1	0	-3.873000	1.930000	2.346000
23	6	0	-5.459000	3.385000	0.838000
24	6	0	-4.844000	4.304000	0.109000
25	1	0	-6.117000	3.708000	1.647000
26	1	0	-4.167000	4.055000	-0.703000
27	1	0	-4.992000	5.361000	0.304000
28	8	0	-10.318000	4.909000	-0.364000
29	6	0	-7.722000	1.948000	0.161000
30	6	0	-8.449000	3.072000	-0.052000
31	6	0	-9.902000	4.728000	0.737000
32	6	0	-10.299000	5.424000	1.990000
33	1	0	-10.998000	6.226000	1.758000
34	1	0	-9.416000	5.821000	2.496000
35	1	0	-10.769000	4.707000	2.668000

36	8	0	-8.940000	3.779000	1.017000
37	79	0	-9.675000	1.231000	-0.429000
38	1	0	-8.496000	3.585000	-1.011000
39	17	0	-11.441000	-0.189000	-0.935000

Structure XXII

- **Thermal correction to Gibbs Free Energy = 0.247645 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.91543138 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.588000	-0.358000	0.949000
2	6	0	-6.720000	1.124000	0.660000
3	6	0	-5.413000	1.912000	0.527000
4	6	0	-4.565000	1.320000	-0.617000
5	6	0	-4.599000	-0.154000	-0.534000
6	1	0	-3.530000	1.681000	-0.546000
7	1	0	-4.958000	1.658000	-1.589000
8	6	0	-5.476000	-0.930000	0.141000
9	1	0	-7.542000	-0.853000	0.734000
10	1	0	-6.403000	-0.507000	2.025000
11	6	0	-5.086000	-2.289000	-0.100000
12	6	0	-4.001000	-2.208000	-0.908000
13	8	0	-3.685000	-0.910000	-1.182000
14	6	0	-5.751000	-3.508000	0.428000
15	1	0	-6.795000	-3.566000	0.098000
16	1	0	-5.762000	-3.513000	1.524000
17	1	0	-5.244000	-4.417000	0.094000
18	6	0	-4.639000	1.807000	1.855000
19	1	0	-4.347000	0.772000	2.055000
20	1	0	-5.251000	2.161000	2.691000

21	1	0	-3.729000	2.413000	1.809000
22	6	0	-5.681000	3.384000	0.349000
23	6	0	-4.904000	4.265000	-0.365000
24	1	0	-6.380000	3.800000	1.078000
25	1	0	-4.043000	3.934000	-0.940000
26	1	0	-4.967000	5.331000	-0.165000
27	8	0	-11.639000	2.949000	0.304000
28	6	0	-7.895000	1.678000	0.541000
29	6	0	-9.084000	2.193000	0.405000
30	6	0	-11.042000	3.092000	1.329000
31	6	0	-11.569000	3.682000	2.595000
32	1	0	-12.629000	3.903000	2.483000
33	1	0	-11.022000	4.599000	2.827000
34	1	0	-11.410000	2.990000	3.425000
35	8	0	-9.740000	2.725000	1.500000
36	1	0	-9.624000	2.258000	-0.536000
37	79	0	-6.683000	3.889000	-1.618000
38	1	0	-3.365000	-2.955000	-1.357000
39	17	0	-8.217000	3.937000	-3.361000

Transition state: TS XIX-XXIII

- **Thermal correction to Gibbs Free Energy = 0.248547 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.87837206 Hartree**
- **Frequency = -170.2**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.848000	-0.550000	0.313000
2	6	0	-6.952000	0.940000	-0.070000
3	6	0	-5.621000	1.734000	0.181000
4	6	0	-4.517000	1.131000	-0.705000

5	6	0	-4.547000	-0.340000	-0.609000
6	1	0	-3.547000	1.530000	-0.381000
7	1	0	-4.655000	1.442000	-1.749000
8	6	0	-5.566000	-1.116000	-0.180000
9	1	0	-7.719000	-1.057000	-0.120000
10	1	0	-6.940000	-0.649000	1.404000
11	6	0	-5.131000	-2.476000	-0.309000
12	6	0	-3.876000	-2.396000	-0.813000
13	8	0	-3.502000	-1.098000	-1.003000
14	1	0	-3.144000	-3.143000	-1.078000
15	6	0	-5.907000	-3.695000	0.039000
16	1	0	-6.832000	-3.759000	-0.545000
17	1	0	-6.194000	-3.697000	1.097000
18	1	0	-5.329000	-4.603000	-0.152000
19	6	0	-5.227000	1.613000	1.658000
20	1	0	-4.980000	0.585000	1.936000
21	1	0	-6.025000	1.975000	2.315000
22	1	0	-4.345000	2.233000	1.840000
23	6	0	-5.834000	3.200000	-0.101000
24	6	0	-5.198000	3.942000	-0.996000
25	1	0	-6.567000	3.681000	0.548000
26	1	0	-4.442000	3.547000	-1.668000
27	1	0	-5.407000	5.004000	-1.080000
28	8	0	-7.216000	0.971000	-1.488000
29	6	0	-8.097000	1.470000	0.682000
30	6	0	-8.877000	1.669000	1.646000
31	6	0	-8.038000	1.951000	-1.859000
32	6	0	-8.136000	2.119000	-3.327000
33	1	0	-9.028000	2.689000	-3.581000
34	1	0	-8.130000	1.150000	-3.827000
35	1	0	-7.251000	2.674000	-3.657000
36	8	0	-8.606000	2.623000	-1.024000
37	79	0	-10.192000	3.265000	1.731000
38	17	0	-11.710000	5.042000	1.920000
39	1	0	-8.915000	1.060000	2.548000

Structure XXIII

- **Thermal correction to Gibbs Free Energy = 0.253342 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.90094310 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.885000	-0.482000	0.368000
2	6	0	-6.944000	0.993000	0.004000
3	6	0	-5.592000	1.754000	0.172000
4	6	0	-4.524000	1.098000	-0.720000
5	6	0	-4.593000	-0.370000	-0.583000
6	1	0	-3.537000	1.480000	-0.432000
7	1	0	-4.675000	1.377000	-1.772000
8	6	0	-5.629000	-1.105000	-0.121000
9	1	0	-7.780000	-0.968000	-0.042000
10	1	0	-6.986000	-0.558000	1.460000
11	6	0	-5.234000	-2.480000	-0.223000
12	6	0	-3.985000	-2.448000	-0.746000
13	8	0	-3.576000	-1.166000	-0.973000
14	1	0	-3.277000	-3.222000	-1.001000
15	6	0	-6.037000	-3.667000	0.169000
16	1	0	-6.977000	-3.717000	-0.394000
17	1	0	-6.302000	-3.637000	1.232000
18	1	0	-5.490000	-4.595000	-0.013000
19	6	0	-5.166000	1.673000	1.642000
20	1	0	-4.942000	0.647000	1.947000
21	1	0	-5.935000	2.081000	2.305000
22	1	0	-4.261000	2.272000	1.780000
23	6	0	-5.793000	3.213000	-0.153000
24	6	0	-5.234000	3.903000	-1.137000

25	1	0	-6.453000	3.736000	0.541000
26	1	0	-4.546000	3.464000	-1.854000
27	1	0	-5.429000	4.965000	-1.247000
28	8	0	-7.249000	1.076000	-1.466000
29	6	0	-8.149000	1.688000	0.578000
30	6	0	-8.709000	1.792000	1.765000
31	6	0	-8.211000	1.904000	-1.628000
32	6	0	-8.629000	2.330000	-2.964000
33	1	0	-9.653000	2.700000	-2.942000
34	1	0	-8.515000	1.507000	-3.670000
35	1	0	-7.964000	3.143000	-3.278000
36	8	0	-8.767000	2.340000	-0.577000
37	79	0	-10.373000	2.847000	2.257000
38	17	0	-12.306000	4.076000	2.837000
39	1	0	-8.178000	1.234000	2.539000

Structure XXIV

- **Thermal correction to Gibbs Free Energy = 0.248793 Hartree**
- **Electronic energy (M06/Def2TZVPP,tol) = -1441.88393051 Hartree**

Cartesian Coordinates of the computed structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.432000	-0.244000	1.344000
2	6	0	-6.765000	1.113000	0.801000
3	6	0	-5.567000	1.870000	0.241000
4	6	0	-5.195000	1.153000	-1.082000
5	6	0	-5.215000	-0.305000	-0.842000
6	1	0	-4.201000	1.489000	-1.404000
7	1	0	-5.908000	1.437000	-1.867000
8	6	0	-5.746000	-0.960000	0.218000
9	1	0	-7.317000	-0.802000	1.652000

10	1	0	-5.780000	-0.164000	2.225000
11	6	0	-5.540000	-2.359000	-0.012000
12	6	0	-4.886000	-2.421000	-1.198000
13	8	0	-4.679000	-1.177000	-1.717000
14	1	0	-4.511000	-3.247000	-1.782000
15	6	0	-5.960000	-3.480000	0.868000
16	1	0	-7.049000	-3.512000	0.982000
17	1	0	-5.532000	-3.381000	1.872000
18	1	0	-5.640000	-4.443000	0.462000
19	6	0	-4.379000	1.769000	1.226000
20	1	0	-4.009000	0.747000	1.336000
21	1	0	-4.655000	2.156000	2.212000
22	1	0	-3.563000	2.387000	0.841000
23	6	0	-5.781000	3.351000	0.060000
24	6	0	-5.457000	4.070000	-1.002000
25	1	0	-6.141000	3.858000	0.957000
26	1	0	-5.082000	3.632000	-1.923000
27	1	0	-5.563000	5.150000	-0.992000
28	8	0	-8.716000	3.998000	1.485000
29	6	0	-8.073000	1.529000	0.652000
30	6	0	-9.175000	0.921000	1.258000
31	6	0	-8.778000	3.757000	0.316000
32	6	0	-9.322000	4.627000	-0.760000
33	1	0	-8.685000	4.589000	-1.646000
34	1	0	-9.427000	5.648000	-0.395000
35	1	0	-10.308000	4.242000	-1.042000
36	8	0	-8.332000	2.576000	-0.218000
37	79	0	-11.079000	1.410000	1.030000
38	17	0	-13.331000	1.954000	0.715000
39	1	0	-8.918000	0.086000	1.909000
