Electronic Supplementary Information

Redox-Switchable Olefin Cross Metathesis (CM) Reactions and Acyclic Diene Metathesis (ADMET) Polymerizations

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1.) Determining the Volume of Ethylene Produced and the Reaction Conversion

Since the cross metathesis (CM) condensations and acyclic diene metathesis (ADMET) polymerizations described in the main text produce gaseous ethylene as a by-product, the rates of the reactions were monitored over time by recording the change in volume of a graduated burette that was connected to the reaction vessel at 20 °C (see Figure S1). Prior to running a reaction, the burette was filled with water such that the meniscus rested on a predetermined graduated mark (50 mL).

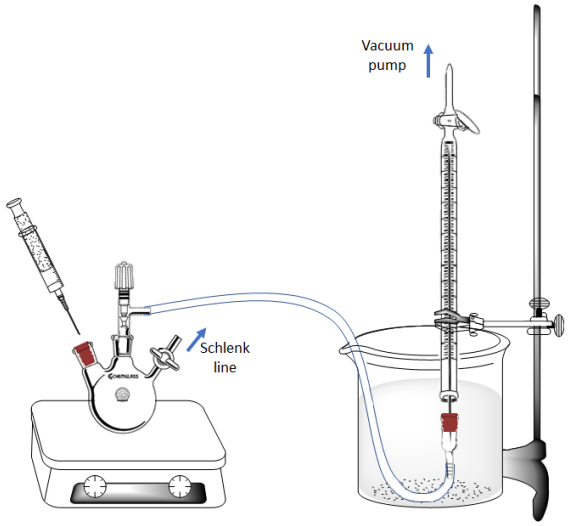

Figure S1. Illustration of the setup that was used to monitor the evolution of ethylene.

The volume of gas in the system at time t, $V_{system}(t)$, is the sum of the volume of the reaction flask, the connective tubing, the upper portion of the burette (from the 50 mL mark to the valve), and the change in the volume of the burette from its initial state. The volumes of each of these components were measured as their water volume equivalents and are as follows:

- Volume of the reaction flask = 54 mL
- Volume of the connecting (Tygon) tubing = 42 mL
- Volume of the upper portion of the burette = 3.5 mL
- Change in volume of the burette = $\{50 - V_b(t)\}$ mL, where $V_b(t)$ = the graduated value of the burette recorded at time t.

Thus,

$$V_{system}(t) = (54 + 3.5 + 42)\ \text{mL} + \{50 - V_b(t)\}\ \text{mL}$$

$$V_{system}(t) = 149.5\ \text{mL} - V_b(t)\ \text{mL}$$

The pressure of the system at time t, $P_{system}(t)$, can be determined by subtracting the vapor pressure of H_2O at 20 °C (0.0224 atm) and the pressure of the water column, $P_{column}(t)$, from 1 atm. Since the length of the burette (from 0 mL to 50 mL) was measured to be 522 mm, the height of water column at time, $h_{column}(t)$, is equal to $V_b(t) \times 10.4$ mm/mL. The height of the water column (h) can be converted to pressure (P) using the equation: $P = \rho g h_{column}(t)$, where ρ = density of water at 20 °C (0.998 g/mL) and g = acceleration of gravity (9.81 m/s^2). Thus,

$$P_{column}(t) = 9.66 \times 10^{-5} \text{ atm/mm} \times 10.4 \text{ mm/mL} \times V_b(t)$$

Therefore,

$$P_{system}(t) = 1 \text{ atm} - 0.0224 \text{ atm} - P_{column}(t)$$

Assuming that the changes in $P_{system}(t)$ and $V_{system}(t)$ originate from the generation of ethylene during the reaction, the volume and pressure of ethylene gas produced at time t, $V_{ethylene}(t)$ and $P_{ethylene}(t)$, can be expressed as:

$$V_{ethylene}(t) = V_{system}(t) - V_{system}(0)$$

$$P_{ethylene}(t) = P_{system}(t) - P_{system}(0)$$

Using the ideal gas equation, the number of moles of ethylene gas produced at time t, $N_{ethylene}(t)$, can be expressed as:

$$N_{ethylene}(t) = \triangle \{P_{system}(t) \times V_{system}(t)\} / RT$$

$$= \{P_{system}(t) \times V_{system}(t) - P_{system}(0) \times V_{system}(0)\} / RT,$$

where R = gas constant and T = temperature (20 °C)

For either CM condensations or ADMET polymerizations, the conversion of the corresponding reaction (p) at time t may be expressed as:

$$p = N_{ethylene}(t) / N_{ethylene}(\infty)$$

- Assuming that $N_{ethylene}(\infty)$ is equal to half the number of moles of substrate that were initially added, the p for CM condensations can be represented as: $p = 2N_{ethylene}(t) / N_{substrate}(0)$.
- Assuming that $N_{ethylene}(\infty)$ is equal to the number of moles of monomer that were initially added, the p for ADMET polymerizations can be represented as: $p = N_{ethylene}(t) / N_{monomer}(0)$.

2.) Kinetics of Cross Metathesis Condensations: Theory

Homo-cross metathesis reactions can be represented as:

$$2A + B \rightarrow C + D$$

where A = substrate (terminal olefin), B = catalyst, C = dimerized product, D = ethylene

Because the concentration of the catalyst is effectively constant during the catalytic cycle,

$$-d[A] / dt = k'[A]^2[B]_0 = k[A]^2$$

Solving the differential equation affords:

$$1 / [A]_t = kt + 1/[A]_0$$

where $[A]_t$ = concentration of substrate at time t, $[A]_0$ = initial concentration of substrate

Multiplying $[A]_0$ by both sides of the equation affords:

$$[A]_0 / [A]_t = k[A]_0t + 1$$

Because $[A]_0$ is constant, the equation can be re-written as:

$$[A]_0 / [A]_t = k't + 1$$

The conversion of substrate to product (p) can be expressed as the ratio of $[A]_t / [A]_0$:

$$p = 1 - ([A]_t / [A]_0)$$

which can be re-written as:

$$[A]_0 / [A]_t = 1 / (1 - p)$$

Therefore,

$$1 / (1 - p) = k't + 1$$

Plotting 1 / (1 - p) versus time affords the corresponding rate constant, *k'*. Dividing *k'* by $[A]_0$ gives *k*.

3.) Kinetics of ADMET Polymerizations: Theory

The overall rate of an ADMET polymerization is second order in monomer and can be expressed as:

$$2A + B \rightarrow C + D$$

where A = terminal olefin, B = catalyst, C = polymer, D = ethylene

Let the number of terminal olefins at time t be defined as $N_{\text{terminal olefin}}(t)$. The value can be calculated from the difference between the initial moles of terminal olefins, $N_{\text{terminal olefin}}(0)$, and the number of moles of terminal olefins that are consumed by the reaction. In other words, $N_{\text{terminal olefin}}(0)$ is equal to twice the initial moles of monomer and the number of moles of terminal olefins consumed at time t, $N_{\text{terminal olefin}}(t)$, is equal to twice that of $N_{\text{ethylene}}(t)$. Thus,

$$N_{\text{terminal olefin}}(t) = N_{\text{terminal olefin}}(0) - 2 \times N_{\text{ethylene}}(t)$$

As described in Section 2,

$$[A]_0 / [A]_t = k't + 1$$

Re-writing the equation in terms of $N_{\text{terminal\_olefin}}(t)$ gives

$$N_{\text{terminal olefin}}(0) / N_{\text{terminal olefin}}(t) = k't + 1$$

The conversion of monomer to polymer (p) can be expressed in terms of $N_{\text{terminal\_olefin}}(t)$ / $N_{\text{terminal\_olefin}}(0)$:

$$p = 1 - \{N_{\text{terminal olefin}}(t) / N_{\text{terminal olefin}}(0)\}$$

which can be re-written as:

$$N_{\text{terminal olefin}}(0) / N_{\text{terminal olefin}}(t) = 1 / (1 - p)$$

Therefore,

$$1 / (1 - p) = k't + 1$$

Plotting 1 / (1 - p) versus time affords the corresponding rate constant, *k'*. Dividing *k'* by $[A]_0$ gives *k*.

4.) Kinetics Data

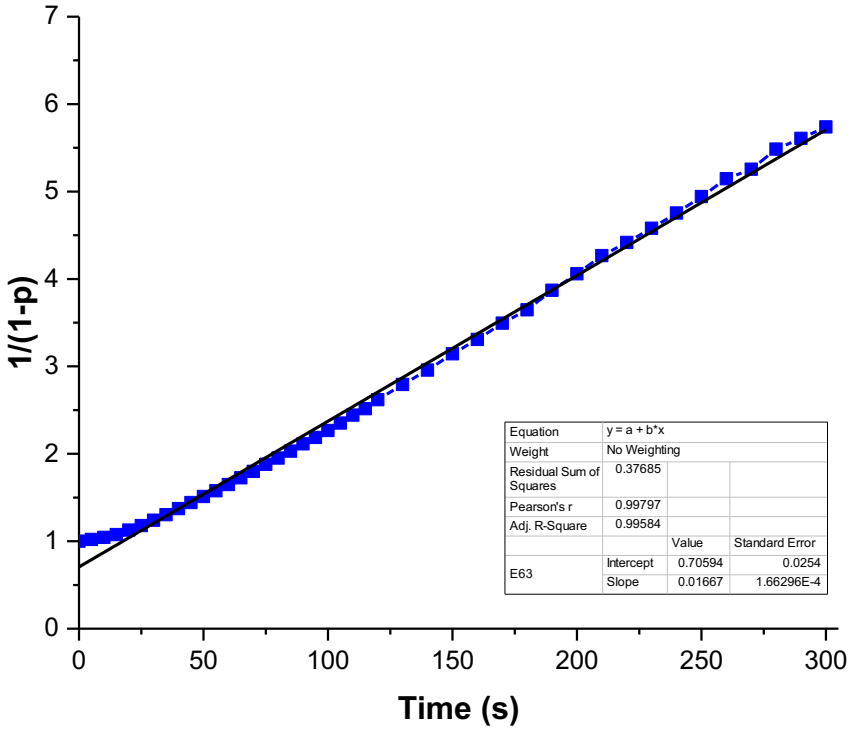

Figure S1. Plot of 1 / (1 - p) versus time for the conversion of **2** to its CM product using **1** as the initiator. Conditions: $\mathbf{2}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{2}_0/\mathbf{1}_0$ = 450, 65 °C, neat. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of **2** ($[\mathbf{2}]_0$ = 5.28 M). See also Figure 1.

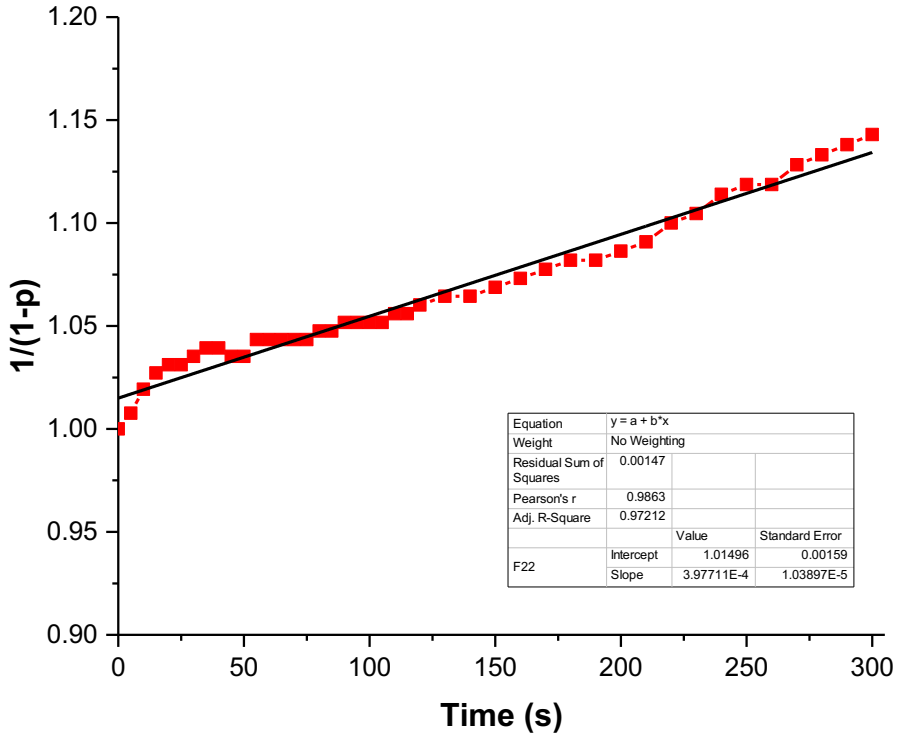

Figure S2. Plot of 1 / (1 - p) versus time for the conversion of **2** to its CM product using $\mathbf{1}_{red}$ as the initiator (prepared by using 1.0 equiv. of $CoCp_2$ rel. to **1**). Conditions: $\mathbf{2}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{2}_0/\mathbf{1}_0$ = 450, 65 °C. The reaction was conducted in bulk substrate although a concentrated solution of $CoCp_2$ in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.05 mL) was used to reduce the catalyst prior to the addition of the substrate. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of **2** ($[\mathbf{2}]_0$ = 4.45 M). See also Figure 1.

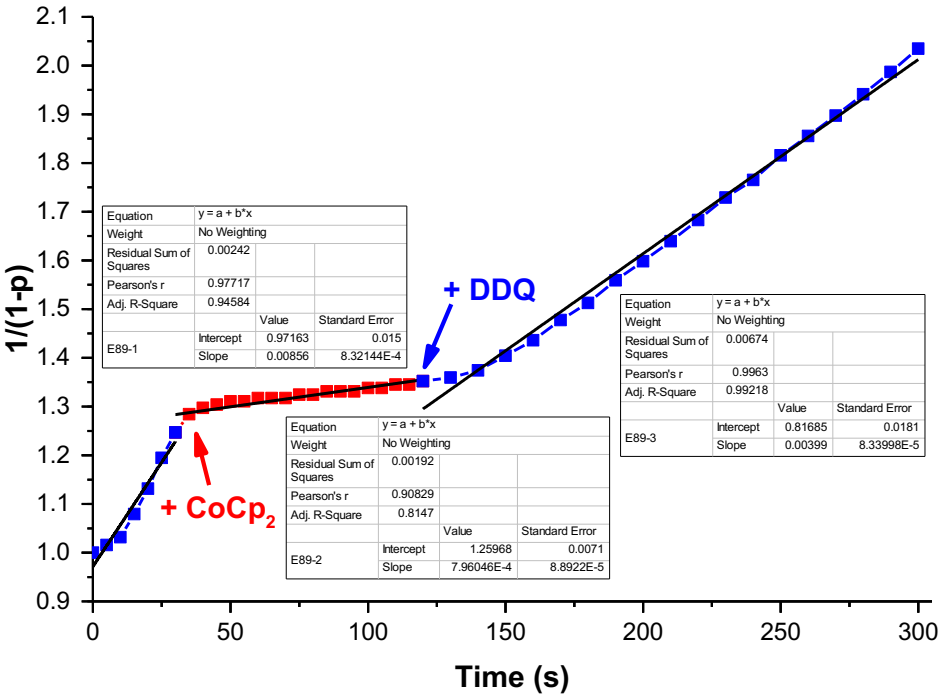

Figure S3. Plot of 1 / (1 - p) versus time for the conversion of **2** to its CM product using **1** as the initiator followed by the in situ reduction and re-oxidation of the catalyst using $CoCp_2$ (1.0 equiv. rel. to **1**) and DDQ (1.5 equiv. rel. to **1**), respectively (indicated). Conditions: $\mathbf{2}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{2}_0/\mathbf{1}_0$ = 450, 65 °C. Note: the reaction was conducted in bulk substrate although $CoCp_2$ and DDQ were added as their respective concentrated solutions in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.05 mL; $[DDQ]_0$ = 0.05 M, 0.15 mL). As noted above, the corresponding rate constants were calculated by dividing the slopes of the fitted lines by the concentrations of **2** at the indicated times ($[\mathbf{2}]_0$ = 5.28 M, $[\mathbf{2}]_{t,\ 30\ s}$ = 3.90 M, $[\mathbf{2}]_{t,\ 120\ s}$ = 2.99 M). The concentration calculations considered the volumes of **2** (d = 0.741 g/mL) and **3** (d = 0.790 g/mL; value predicted using the Advanced Chemistry Development (ACD/Labs) Software package, V11.02) as well as the added solvent. See also Figure 1.

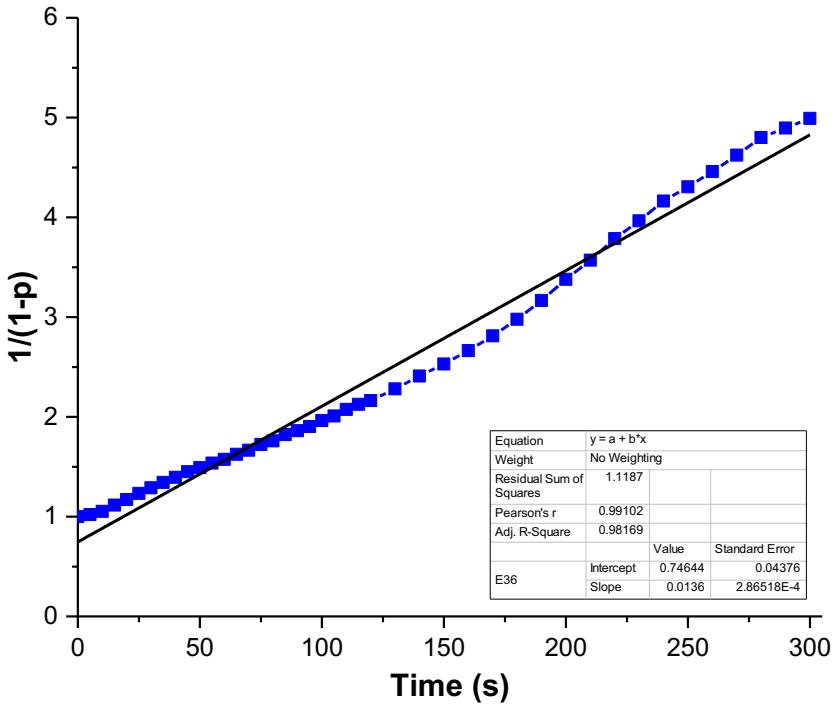

Figure S4. Plot of 1 / (1 - p) versus time for the conversion of **4** to its CM product using **1** as the initiator. Conditions: $\mathbf{4}_0 = 2.25$ mmol, $\mathbf{1}_0 = 5$ µmol, $\mathbf{4}_0/\mathbf{1}_0 = 450$, 50 °C, neat. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of **4** ($[\mathbf{4}]_0 = 7.55$ M). See also Figure 2.

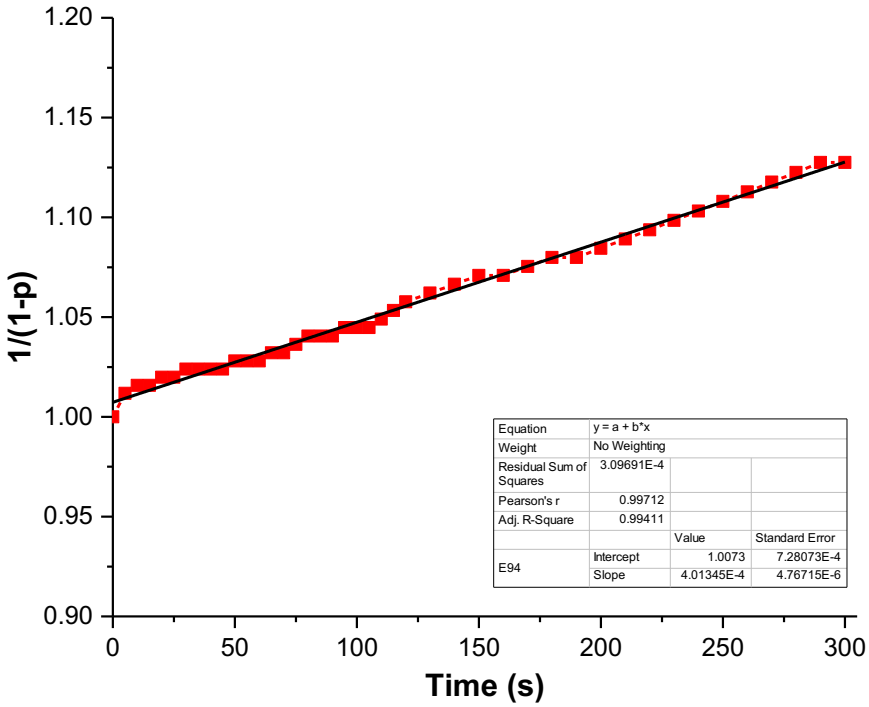

Figure S5. Plot of 1 / (1 - p) versus time for the conversion of **4** to its CM product using $\mathbf{1}_{red}$ as the initiator (prepared by using 1.0 equiv. of $CoCp_2$ rel. to **1**). Conditions: $\mathbf{4}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{4}_0/\mathbf{1}_0$ = 450, 50 °C. Note: the reaction was conducted in bulk substrate although a concentrated solution of $CoCp_2$ in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.05 mL) was used to reduce the catalyst prior to the addition of the substrate. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of **4** ($[\mathbf{4}]_0$ = 6.47 M). See also Figure 2.

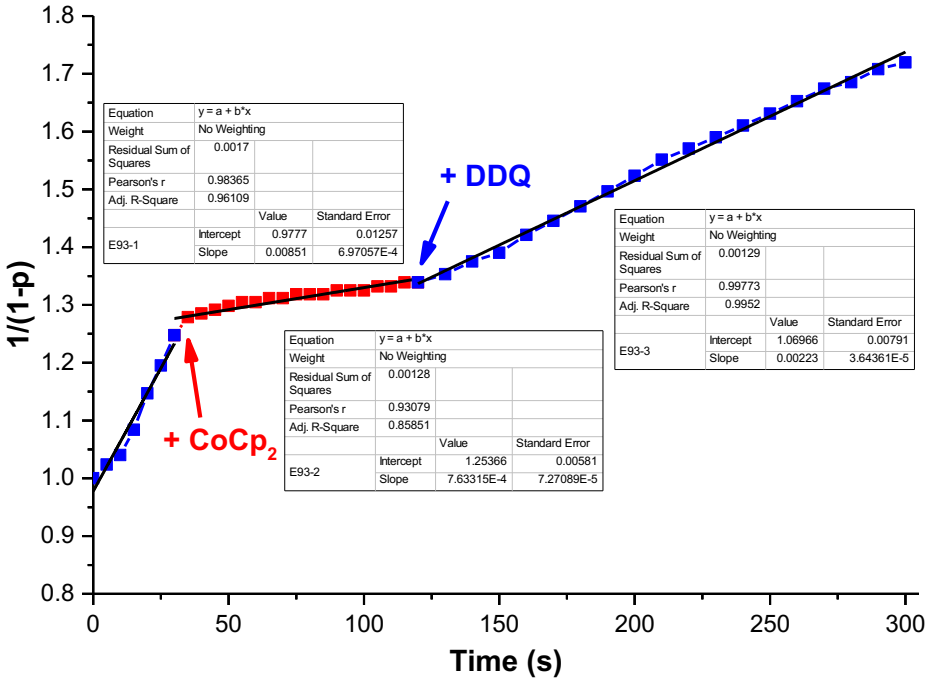

Figure S6. Plot of 1 / (1 - p) versus time for the conversion of **4** to its CM product using **1** as the initiator followed by the in situ reduction and re-oxidation of the catalyst using $CoCp_2$ (1.0 equiv. rel. to **1**) and DDQ (1.5 equiv. rel. to **1**), respectively (indicated). Conditions: $\mathbf{4}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{4}_0/\mathbf{1}_0$ = 450, 50 °C. Note: the reaction was conducted in bulk substrate although $CoCp_2$ and DDQ were added as their respective concentrated solutions in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.05 mL; $[DDQ]_0$ = 0.05 M, 0.15 mL). As noted above, the corresponding rate constants were calculated by dividing the slopes of the fitted lines by the concentrations of **4** at the indicated times ($[\mathbf{4}]_0$ = 7.55 M, $[\mathbf{4}]_{t,\ 30\ s}$ = 5.27 M, $[\mathbf{4}]_{t,\ 120\ s}$ = 3.95 M). The concentration calculations considered the volumes of **4** (d = 0.893 g/mL) and **5** (d = 0.993 g/mL; value predicted using the Advanced Chemistry Development (ACD/Labs) Software package, V11.02) as well as the added solvent. See also Figure 2.

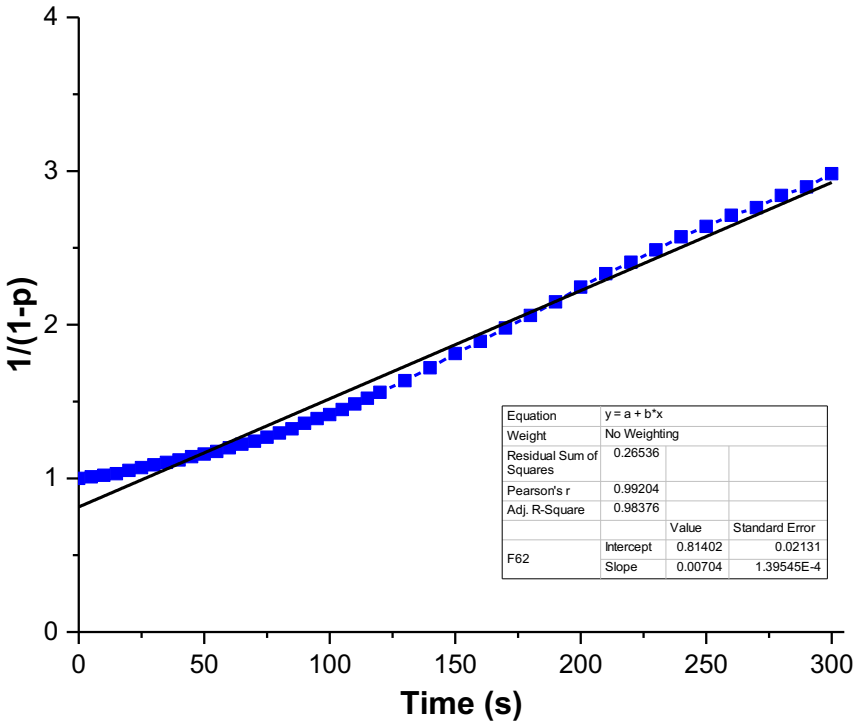

Figure S7. Plot of 1 / (1 - p) versus time for the conversion of **6** to its ADMET product using **1** as the initiator. Conditions: $\mathbf{6}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 µmol, $\mathbf{6}_0/\mathbf{1}_0$ = 450, 60 °C. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of terminal olefin ($[\text{terminal olefin}]_0$ = 4.17 M). See also Figure 3.

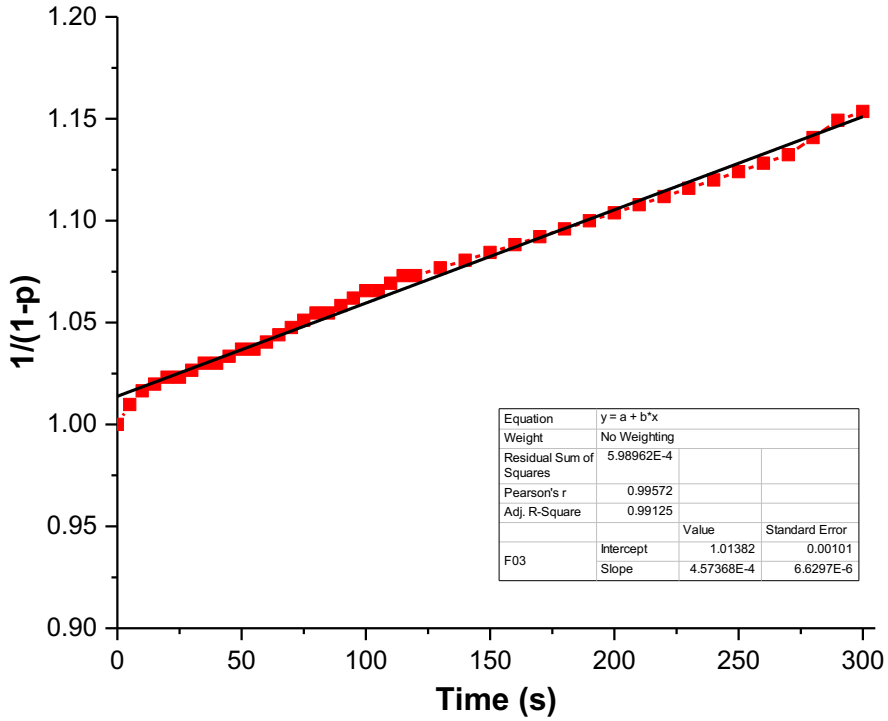

Figure S8. Plot of 1 / (1 - p) versus time for the conversion of **6** to its ADMET product using $\mathbf{1}_{red}$ as the initiator (prepared by using 1.0 equiv. of $CoCp_2$ rel. to **1**). Conditions: $\mathbf{6}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 μmol, $\mathbf{6}_0/\mathbf{1}_0$ = 450, 60 °C. Note: the reaction was conducted in bulk monomer although a concentrated solution of $CoCp_2$ in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.03 mL) was used to reduce the catalyst prior to the addition of the monomer. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of terminal olefin ($[\text{terminal olefin}]_0$ = 3.99 M). See also Figure 3.

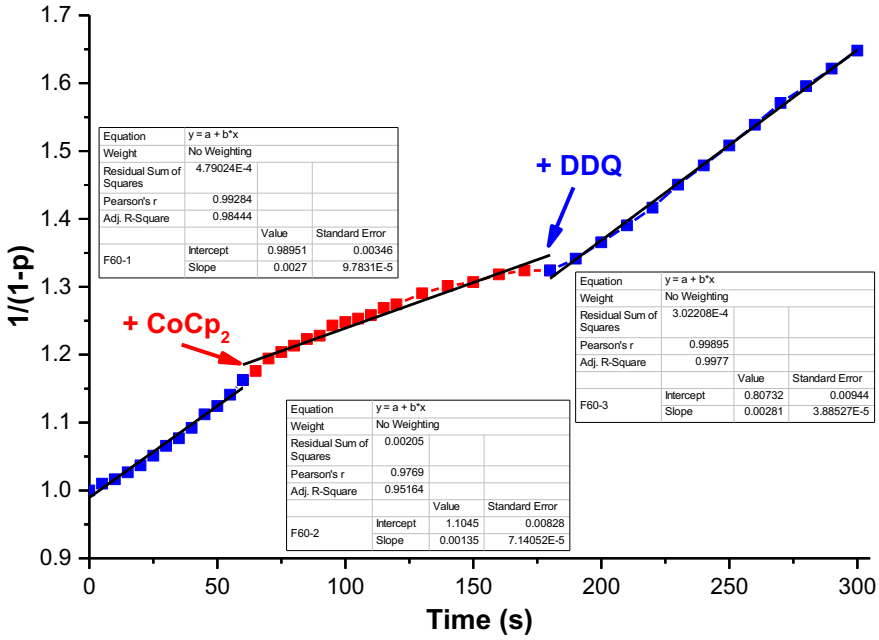

Figure S9. Plot of 1 / (1 - p) versus time for the conversion of **6** to its ADMET product using **1** as the initiator followed by the in situ reduction and re-oxidation of the catalyst using $CoCp_2$ (1.0 equiv. rel. to **1**) and DDQ (1.5 equiv. rel. to **1**), respectively (indicated). Conditions: $\mathbf{6}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 µmol, $\mathbf{6}_0/\mathbf{1}_0$ = 450, 60 °C. Note: the reaction was conducted in bulk monomer although $CoCp_2$ and DDQ were added as their respective concentrated solutions in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.03 mL; $[DDQ]_0$ = 0.05 M, 0.09 mL). As noted above, the corresponding rate constants were calculated by dividing the slopes of the fitted lines by the concentrations of terminal olefin at the indicated times ($[\text{terminal olefin}]_0$ = 4.17 M, $[\text{terminal olefin}]_{t,\,60\,s}$ = 3.71 M, $[\text{terminal olefin}]_{t,\,180\,s}$ = 3.22 M). The concentration calculations considered the initial volume of **6** and as well as the added solvent. Volume changes due to the consumption of monomer and the formation of polymer were neglected. See also Figure 3.

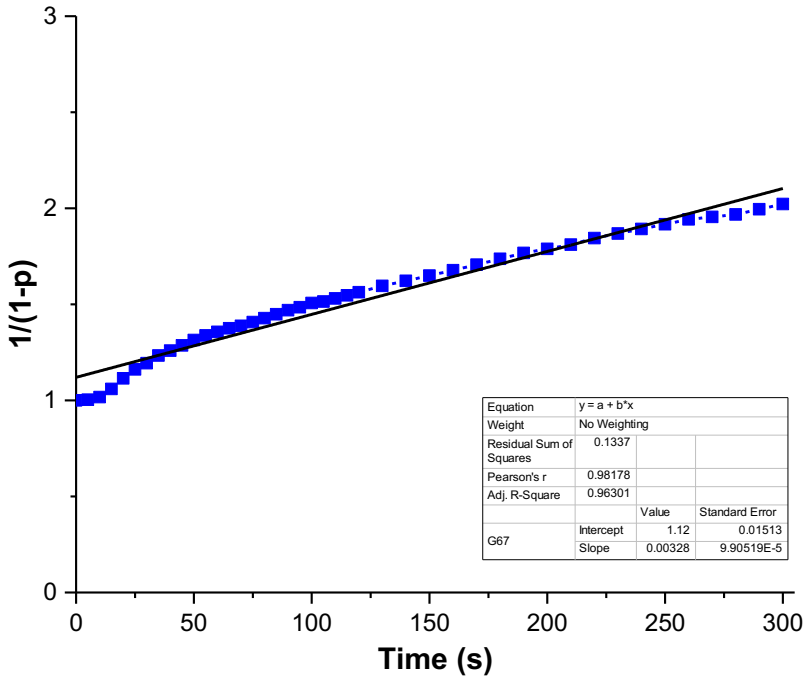

Figure S10. Plot of 1 / (1 - p) versus time for the conversion of **8** to its ADMET product using **1** as the initiator. Conditions: $\mathbf{8}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 µmol, $\mathbf{8}_0/\mathbf{1}_0$ = 450, 60 °C. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of terminal olefin ($[\text{terminal olefin}]_0$ = 4.13 M). See also Figure 4.

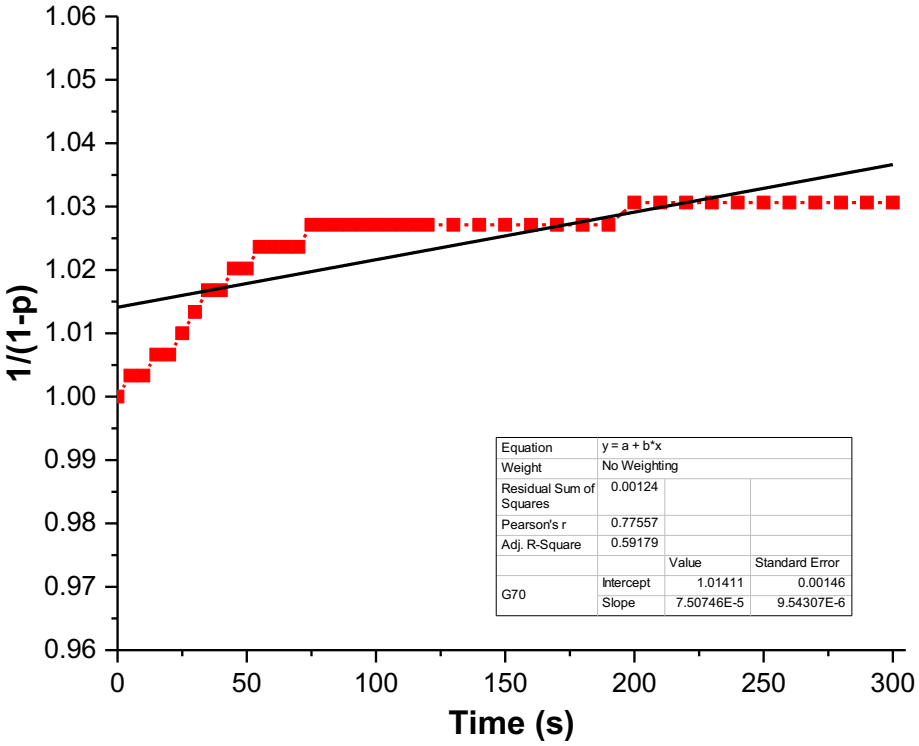

Figure S11. Plot of 1 / (1 - p) versus time for the conversion of **8** to its ADMET product using $\mathbf{1}_{red}$ as the initiator (prepared by using 1.0 equiv. of $CoCp_2$ rel. to **1**). Conditions: $\mathbf{8}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 μmol, $\mathbf{8}_0/\mathbf{1}_0$ = 450, 60 °C. Note: the reaction was conducted in bulk monomer although a concentrated solution of $CoCp_2$ in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.03 mL) was used to reduce the catalyst prior to the addition of the monomer. As noted above, the corresponding rate constant was calculated by dividing the slope of the fitted line by the initial concentration of terminal olefin ($[\text{terminal olefin}]_0$ = 3.95 M). See also Figure 4.

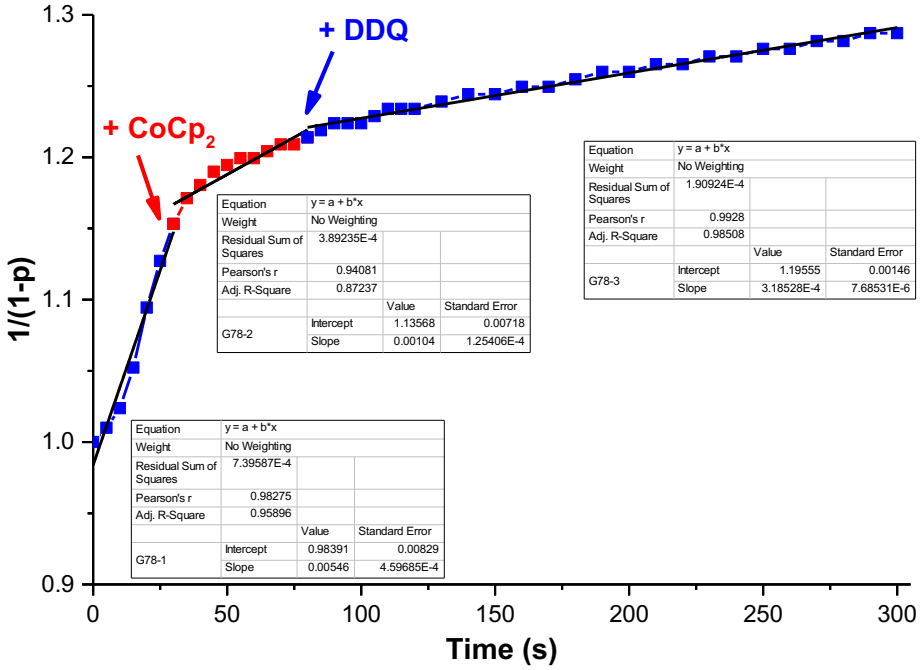

Figure S12. Plot of 1 / (1 - p) versus time for the conversion of **8** to its ADMET product using **1** as the initiator followed by the in situ reduction and re-oxidation of the catalyst using $CoCp_2$ (1.0 equiv. rel. to **1**) and DDQ (1.5 equiv. rel. to **1**), respectively (indicated). Conditions: $\mathbf{8}_0$ = 1.35 mmol, $\mathbf{1}_0$ = 3 µmol, $\mathbf{8}_0/\mathbf{1}_0$ = 450, 60 °C . Note: the reaction was conducted in bulk monomer although $CoCp_2$ and DDQ were added as their respective concentrated solutions in 1,2-dichlorobenzene ($[CoCp_2]_0$ = 0.1 M, 0.03 mL; $[DDQ]_0$ = 0.05 M, 0.09 mL). As noted above, the corresponding rate constants were calculated by dividing the slopes of the fitted lines by the concentrations of terminal olefin at the indicated times ($[\text{terminal olefin}]_0$ = 4.13 M, $[\text{terminal olefin}]_{t,\,30\text{ s}}$ = 3.69 M, $[\text{terminal olefin}]_{t,\,80\text{ s}}$ = 3.30 M). The concentration calculations considered the initial volume of **8** and as well as the added solvent. Volume changes due to the consumption of monomer and the formation of polymer were neglected. See also Figure 4.

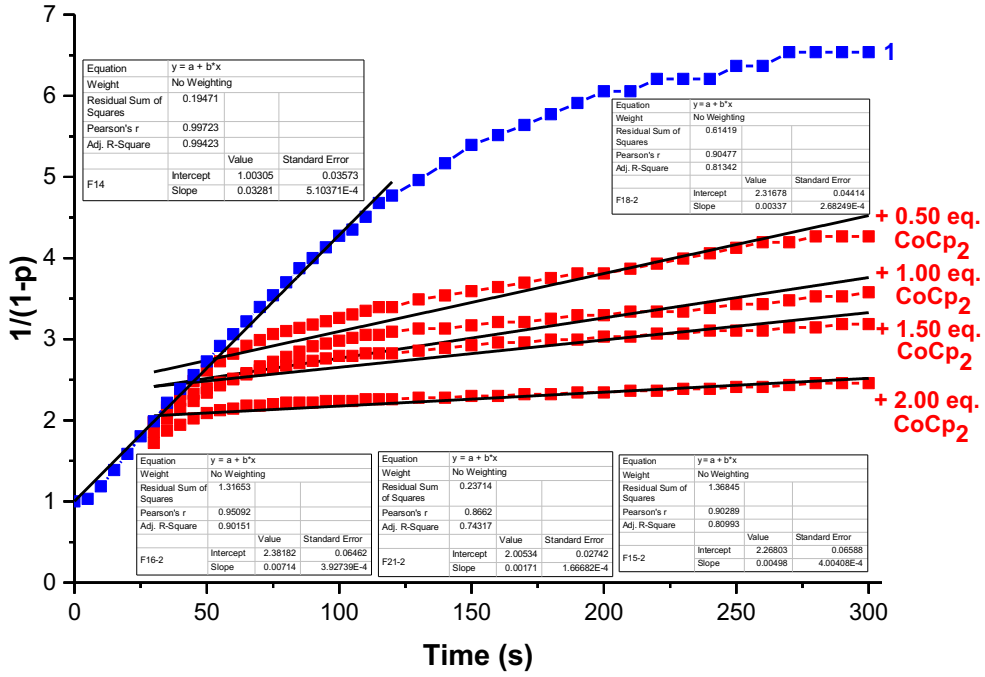

Figure S13. Plots of 1 / (1 - p) versus time for the conversion of **2** to its CM product using **1** as the initiator (blue line) and various equivalents of $CoCp_2$ (red lines) (indicated). Conditions: $\mathbf{2}_0$ = 2.25 mmol, $\mathbf{1}_0$ = 5 µmol, $\mathbf{2}_0/\mathbf{1}_0$ = 450, 65 °C. A stock solution of $CoCp_2$ in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide ($[CoCp_2]_0$ = 62.5 mM) was used. See also Figure 5 and the main text for more details.

5.) NMR Data

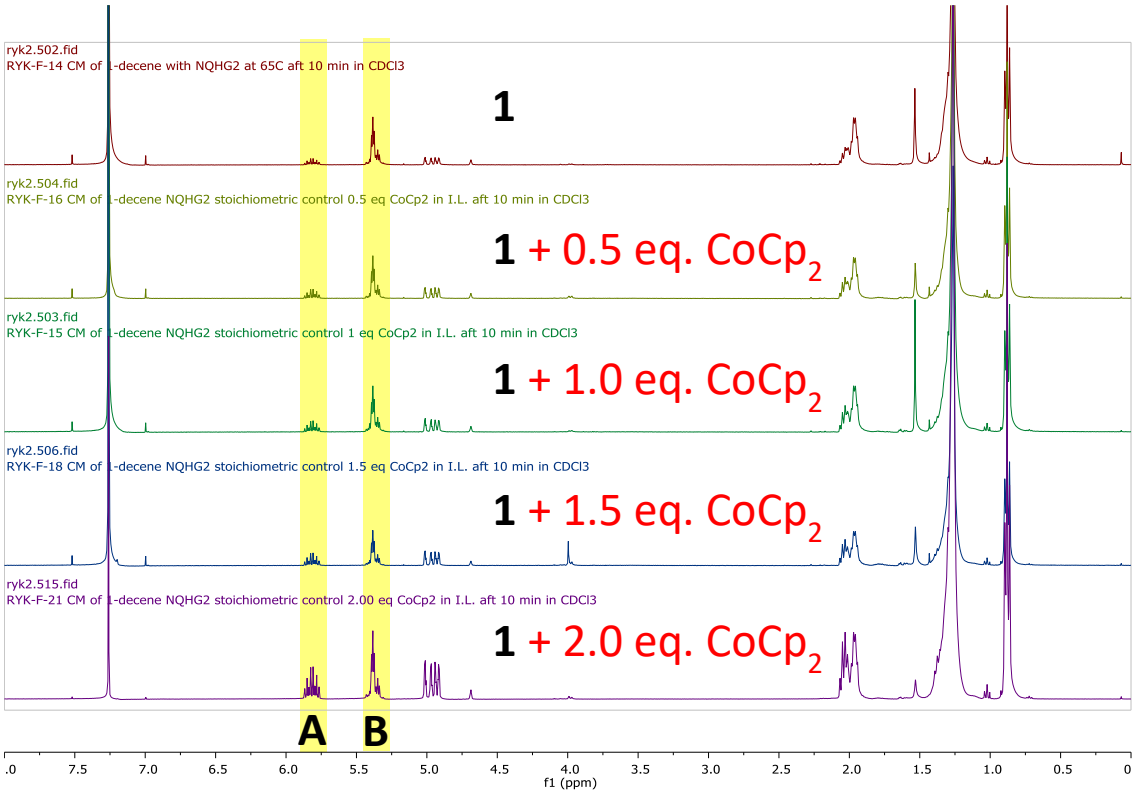

Figure S14. ^{1}H NMR spectra recorded for the CM of **2** using **1** in conjunction with various quantities of added $CoCp_2$ (indicated). Conditions: $\mathbf{2}_0$ = 2.25 mmol, $\mathbf{2}_0/\mathbf{1}_0$ = 450, 65 °C. The signals labeled as "A" were assigned to the internal proton on olefin in **2**. The signals labels as "B" were assigned to the two protons connected to the internal olefin in **3**. The integrated values were used to determine conversions (see Table S1).

Table S1. ^{1}H NMR integration values as obtained from the spectra shown in Figure S13 and generated using a data analysis option implemented in the Mestrelab Mnova software package (v.10.0.2).

Equivalents of $CoCp_2$ added relative to **1**	Integrated value of **A** (I_A)	Integrated value of **B** (I_B)	$I_B/(I_A+I_B)$ × 100%	Conv. as determined by CH_2CH_2 evolution (%)
0.00	1.00	6.58	87	82
0.50	1.00	4.07	80	79
1.00	1.00	3.77	79	74
1.50	1.00	2.58	72	70
2.00	1.00	1.80	64	63

6.) GPC Data

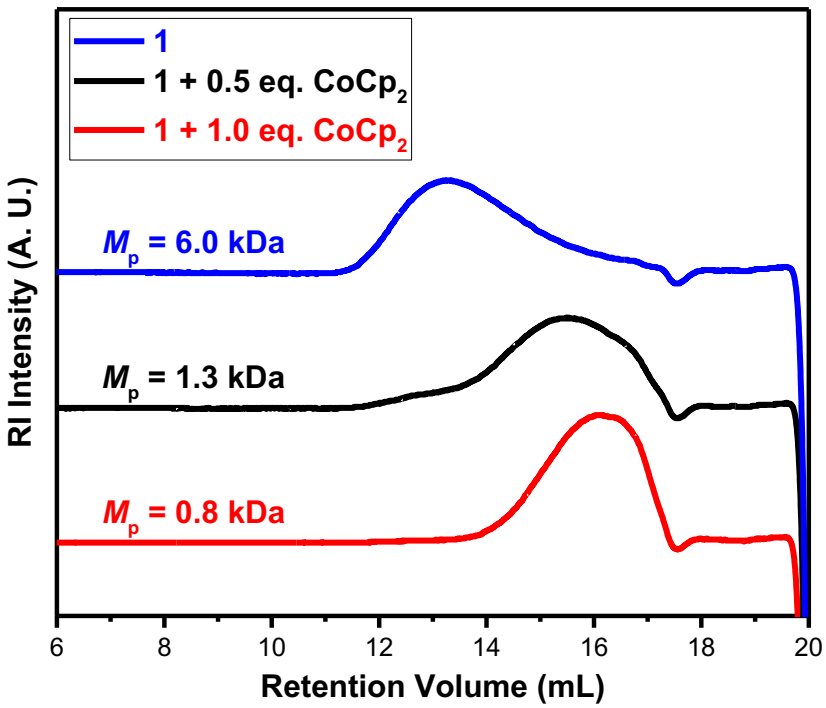

Figure S15. Gel permeation chromatograms acquired for polymers that were obtained using 1,9-decadiene **6** as monomer and **1** (blue line), **1** + 0.5 eq. $CoCp_2$ (black line), or **1** + 1.0 eq. $CoCp_2$ (red line) as the catalyst. Conditions: $[\mathbf{6}]_0$ = 1.85 M; $\mathbf{6}_0/\mathbf{1}_0$ = 450; $\mathbf{1}_0$ = 24.11 µmol; $CoCp_2$ = 0 µmol (blue line), 12.06 µmol (black line) or 24.11 µmol (red line); 75 °C for 5 days under vacuum (ca. 0.1 mmHg).

7.) Computational Details

All geometry optimizations were performed using the dispersion-corrected B3LYP functional,[1–4] with a mixed basis set of SDD[5] for Ru and 6-31G(d) for other atoms. Single point energies were calculated with M06[6] and a mixed basis set of SDD for Ru and 6-311+G(d,p) for other atoms. Solvation effects were considered by performing single point calculations with the SMD model in 1,2-dichlorobenzene (ε = 9.93).[7,8] All calculations were performed with Gaussian 16.[9]

Reaction energy profiles presented in this study were obtained by optimizing molecular geometries and calculating energies of the reaction intermediates (local minima) and transition states (1st order saddle point) along plausible reaction pathways. Vibrational frequencies were computed at the same level of theory in geometry optimization to confirm whether the structures are intermediates (no imaginary frequency) or transition states (only one imaginary frequency). The reported Gibbs free energies and enthalpies include zero-point vibrational energies and thermal corrections at 298 K calculated using a harmonic-oscillator model. Since the harmonic-oscillator approximation may lead to spurious results for the computed entropies in molecules with low-frequency vibrational modes, the quasiharmonic approximation from Cramer and Truhlar was applied to compute the thermal corrections.[10,11] In the quasiharmonic approximation, vibrational frequencies lower than 100 cm^{-1} were raised to 100 cm^{-1} as a way to avoid spurious results associated with the harmonic-oscillator model for very low-frequency vibrations. The reported energies in the text were corrected using the quasiharmonic approximation. The Gibbs free energies in solution were calculated under standard conditions (1 atm of ethylene and 1 mol/L for other species).

The reaction energy profile of the propagation cycle of the cross metathesis of 1-pentene as a model substrate is shown in Figure S16. The red line represents reaction with reduced ligand $\mathbf{L1_{red}}$ while the blue line with neutral ligand **L1**. The 1-pentene substrate binds onto Ru-methylidene catalyst **10** to form the Dewar–Chatt–Duncanson adduct **14**. Subsequent [2+2] cycloaddition (**TS5**) affords ruthenacyclobutane intermediate **15**, which then undergoes retro-[2+2] cycloaddition (**TS6**) to release one molecule of ethylene and alkylidene intermediate **16**. Coordination of another molecule of 1-pentene substrate forms intermediate **17**, which further undergoes [2+2] cycloaddition (**TS7**) to form the ruthenacyclobutane intermediate **18**. DFT calculations indicate the rate-determining step is the second retro-[2+2] cycloaddition to release the product (**TS8**). Under standard conditions (1 atm of ethylene and

1 mol/L of other species), the catalyst resting state is the monosubstituted ruthenacyclobutane intermediate **15**. Although computations indicated the monosubstituted ruthenacyclobutane intermediate **15** is more stable than **18** under standard conditions (1 atm ethylene and 1 mol/L 1-pentene), under the experimental conditions, a lower pressure of ethylene and a relatively high concentration of the terminal olefin substrate would favor the formation of the disubstituted ruthenacyclobutane intermediate **18**.

8.) Computed Energy Profile for the Cross Metathesis of 1-Pentene

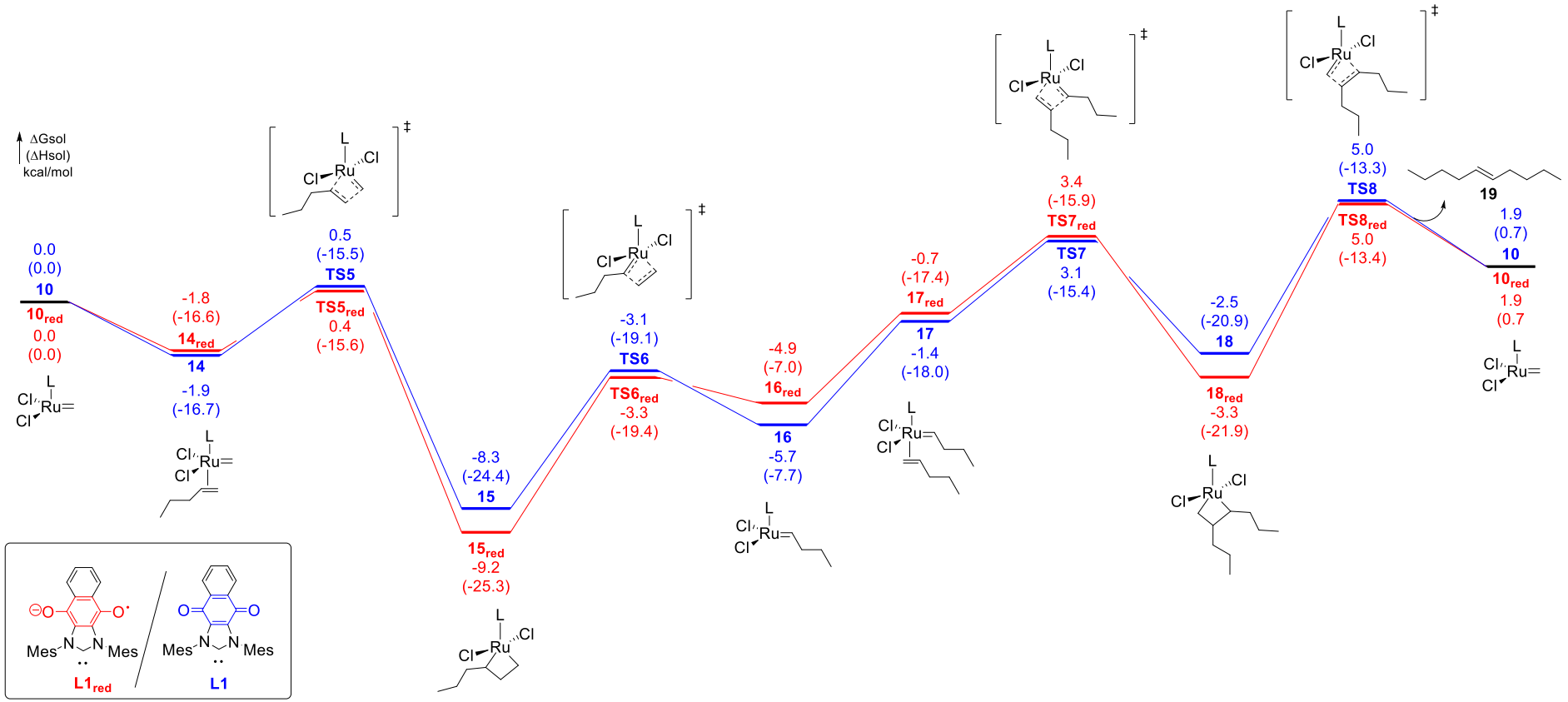

Figure S16. Computed reaction energy profile of cross metathesis with 1-pentene as catalyzed by **1** (blue line) or $\mathbf{1}_{red}$ (red line).

When **15** is used as the resting state in the activation energy calculations, the reaction employing the neutral ligand (**L1**) requires 0.9 kcal/mol lower barrier for the retro-[2+2] cycloaddition than the reaction with the reduced ligand (**L1**$_{red}$). This is in agreement with the faster reaction rate with the neutral catalyst observed in the cross-metathesis experiment, although computations underestimated the rate difference. The experimental rate constant ratio (k/k_{red} = 35) that was measured for 1-decene can be compared to the rate constant ratio (k/k_{red} = 4.6) calculated for 1-pentene. The faster reaction rate with the neutral ligand in retro-[2+2] cycloaddition is also attributed to an electronic effect. The stronger donor ligand **L1**$_{red}$ stabilizes the Ru(IV) metallacyclobutane resting state (**15**), and thus requires higher barrier for the subsequent retro-[2+2] cycloaddition.

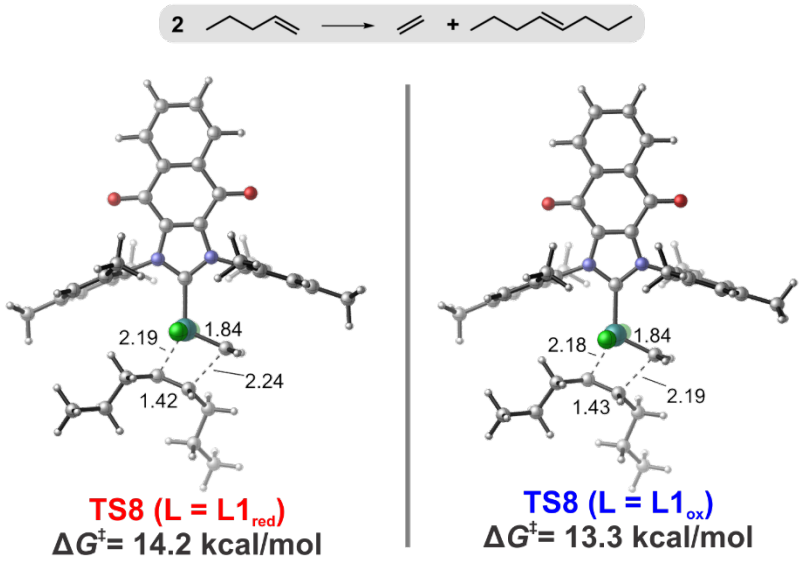

Figure S17. Computed structures of **TS8** as formed during the cross metathesis of 1-pentene (see Figure S16). The activation free energies were calculated with respect to **15**.

When the disubstituted ruthenacyclobutane **18** was used as the resting state in the activation energy calculations, the computed Gibbs free energies of activation for the retro-[2+2] cycloadditions with **L1** and **L1**$_{red}$ are 7.5 and 8.3 kcal/mol, respectively. Therefore, these results also indicate that **L1**$_{red}$ suppresses the CM reactivity by stabilization of the ruthenacyclobutane resting state.

9.) Computed Energies and Coordinates of Optimized Structures

11a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2826.591137 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2826.540751 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2826.539807 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2826.683109 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2826.562243 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2826.665558 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.164940	-1.823148	0.375993
2	17	0	0.673368	-1.845509	-2.003843
3	17	0	-0.363533	-1.961649	2.753332
4	6	0	-0.052160	-3.777900	0.286583
5	1	0	-0.233065	-4.178847	-0.710439
6	6	0	-1.077348	-0.191600	0.154789
7	7	0	-2.399806	-0.219259	-0.162006
8	7	0	-0.730121	1.115130	0.298715
9	6	0	-2.908609	1.092688	-0.221979
10	6	0	-1.849597	1.940000	0.071582
11	6	0	-4.246067	1.528260	-0.523726
12	6	0	-1.937056	3.374877	0.122603
13	6	0	-4.384267	2.996716	-0.484994
14	6	0	-3.294018	3.868723	-0.179698

15	8	0	-5.195796	0.747494	-0.793418
16	8	0	-0.967245	4.129331	0.396492
17	6	0	-5.648869	3.557672	-0.761940
18	1	0	-6.456934	2.868949	-0.990502
19	6	0	-3.518534	5.261541	-0.164606
20	1	0	-2.670302	5.897495	0.071246
21	6	0	-5.844964	4.927888	-0.741373
22	1	0	-6.828101	5.341630	-0.957613
23	6	0	-4.768669	5.788742	-0.439510
24	1	0	-4.922111	6.866095	-0.423039
25	6	0	2.043020	-2.165429	0.904859
26	6	0	3.263924	-1.749384	0.103454
27	1	0	2.178558	-2.006587	1.978204
28	1	0	3.341479	-0.656761	0.161038
29	1	0	3.130585	-2.000617	-0.952594
30	6	0	-3.161439	-1.427628	-0.397660
31	6	0	-3.276139	-1.916634	-1.710144
32	6	0	-3.816135	-2.042591	0.682127
33	6	0	-3.967297	-3.116982	-1.900823
34	6	0	-4.495403	-3.240876	0.436241
35	6	0	-4.568354	-3.802319	-0.840982
36	1	0	-4.052372	-3.512742	-2.911203
37	1	0	-4.996591	-3.733935	1.267084
38	6	0	0.598355	1.582778	0.628675
39	6	0	0.927184	1.807201	1.976312
40	6	0	1.493870	1.880082	-0.412499
41	6	0	2.222894	2.245374	2.268121

42	6	0	2.776087	2.320690	-0.065542
43	6	0	3.164919	2.494044	1.266136
44	1	0	2.489441	2.422759	3.308242
45	1	0	3.476493	2.561463	-0.863265
46	6	0	-3.859342	-1.404269	2.047141
47	1	0	-4.446048	-2.019935	2.736920
48	1	0	-2.858804	-1.279914	2.471201
49	1	0	-4.334291	-0.417751	1.984247
50	6	0	-2.746391	-1.141588	-2.889300
51	1	0	-1.669213	-0.969684	-2.812542
52	1	0	-2.937175	-1.685553	-3.820236
53	1	0	-3.251308	-0.170075	-2.952673
54	6	0	-5.335300	-5.082909	-1.083756
55	1	0	-6.368423	-4.876713	-1.396641
56	1	0	-4.872366	-5.684307	-1.874671
57	1	0	-5.386289	-5.697169	-0.177877
58	6	0	1.074774	1.804369	-1.858852
59	1	0	1.894796	2.123734	-2.510523
60	1	0	0.787279	0.788055	-2.146503
61	1	0	0.219790	2.466452	-2.040137
62	6	0	-0.097418	1.661518	3.071899
63	1	0	-0.495671	0.643583	3.121379
64	1	0	0.346541	1.901150	4.043699
65	1	0	-0.931506	2.352028	2.899155
66	6	0	4.563508	2.950767	1.613797
67	1	0	4.578142	3.512816	2.554417
68	1	0	5.246678	2.098456	1.733350

69	1	0	4.981595	3.592626	0.829907
70	6	0	4.557543	-2.391278	0.647788
71	1	0	4.439515	-3.484386	0.652491
72	1	0	4.703164	-2.095223	1.697593
73	6	0	1.479564	-3.645719	0.638996
74	1	0	2.052547	-4.053510	-0.195345
75	1	0	1.627505	-4.181019	1.578871
76	1	0	-0.646754	-4.225753	1.082073
77	6	0	5.819593	-2.044494	-0.161284
78	1	0	6.652807	-2.665646	0.200403
79	1	0	5.661343	-2.327916	-1.212357
80	6	0	6.241517	-0.569938	-0.094240
81	1	0	5.437531	0.067612	-0.484234
82	1	0	6.376740	-0.281351	0.959607
83	6	0	7.534753	-0.279756	-0.867619
84	1	0	7.408200	-0.567715	-1.920441
85	1	0	8.346241	-0.910432	-0.473853
86	6	0	7.964077	1.199048	-0.801864
87	1	0	7.172587	1.832681	-1.222985
88	1	0	8.063889	1.486616	0.256671
89	6	0	9.261939	1.467107	-1.513973
90	1	0	10.128556	0.916893	-1.140334
91	6	0	9.420870	2.291799	-2.550561
92	1	0	8.587405	2.858706	-2.961275
93	1	0	10.387113	2.434687	-3.028157

Ethylene

SCF Energy(B3LYP/SDD-6-31g(d)) = -78.536237 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -78.533195 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -78.532251 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -78.557767 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -78.540495 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -78.557767 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.665433	0.000000
2	1	0	0.923689	1.239527	0.000000
3	1	0	-0.923651	1.239571	0.000000
4	6	0	-0.000000	-0.665433	0.000000
5	1	0	-0.923689	-1.239527	0.000000
6	1	0	0.923651	-1.239571	0.000000

TS4a

SCF Energy(B3LYP/SDD-6-31g(d)) = -3139.637563 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -3139.576591 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -3139.575647 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -3139.745336 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -3139.644876 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -3139.721343 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.485130	-0.221186	-0.006338
2	17	0	-0.720228	-1.347246	-2.165697
3	17	0	-0.350890	0.919877	2.156021
4	6	0	-2.206515	0.972066	-0.650123
5	1	0	-2.282924	0.787214	-1.723613
6	6	0	1.567239	-0.542633	-0.034227
7	7	0	2.475464	0.323682	-0.566081
8	7	0	2.279244	-1.610305	0.428469
9	6	0	3.778460	-0.191844	-0.446716
10	6	0	3.654644	-1.419920	0.186338
11	6	0	5.020117	0.391546	-0.876367
12	6	0	4.758222	-2.288189	0.503036
13	6	0	6.182124	-0.461642	-0.567634
14	6	0	6.057825	-1.727634	0.083978
15	8	0	5.107887	1.508168	-1.453169
16	8	0	4.636613	-3.404401	1.071384
17	6	0	7.466291	-0.005788	-0.933653
18	1	0	7.527071	0.959726	-1.427369
19	6	0	7.224064	-2.479583	0.338929
20	1	0	7.096860	-3.437505	0.834693
21	6	0	8.596257	-0.761412	-0.672103
22	1	0	9.578453	-0.392710	-0.961855

23	6	0	8.473838	-2.011419	-0.029121
24	1	0	9.361691	-2.606321	0.176777
25	6	0	-2.868230	0.021561	0.172334
26	6	0	-1.425151	-1.567366	0.815356
27	1	0	-3.057371	0.329701	1.200806
28	1	0	-1.603574	-1.565285	1.895750
29	6	0	2.122124	1.595816	-1.154581
30	6	0	1.870824	1.666020	-2.536459
31	6	0	2.118300	2.745099	-0.343860
32	6	0	1.487029	2.901706	-3.069318
33	6	0	1.732972	3.956327	-0.927877
34	6	0	1.392726	4.051723	-2.280830
35	1	0	1.286214	2.967188	-4.136918
36	1	0	1.724699	4.852032	-0.309677
37	6	0	1.716912	-2.768729	1.084034
38	6	0	1.575054	-2.758796	2.480988
39	6	0	1.382359	-3.894416	0.314064
40	6	0	0.997004	-3.878782	3.088312
41	6	0	0.807804	-4.988212	0.969654
42	6	0	0.590865	-4.994118	2.350576
43	1	0	0.881494	-3.882163	4.170684
44	1	0	0.543243	-5.865996	0.382809
45	6	0	2.597577	2.701208	1.084545
46	1	0	2.533175	3.695218	1.539312
47	1	0	2.003836	2.011645	1.691197
48	1	0	3.645218	2.378865	1.115943
49	6	0	2.103709	0.482101	-3.439635

50	1	0	1.499478	-0.381134	-3.147622
51	1	0	1.854090	0.736761	-4.474920
52	1	0	3.161482	0.194423	-3.404102
53	6	0	0.950359	5.368436	-2.877992
54	1	0	1.192241	5.425127	-3.945294
55	1	0	-0.135782	5.508373	-2.783793
56	1	0	1.429934	6.216755	-2.376422
57	6	0	1.686500	-3.956052	-1.160952
58	1	0	1.359922	-4.913973	-1.579366
59	1	0	1.183990	-3.154229	-1.711022
60	1	0	2.766511	-3.863482	-1.326589
61	6	0	2.077920	-1.607675	3.314970
62	1	0	1.557608	-0.675091	3.073055
63	1	0	1.929298	-1.814471	4.380085
64	1	0	3.150305	-1.454465	3.145486
65	6	0	-0.060657	-6.178356	3.028627
66	1	0	0.161367	-7.113399	2.501659
67	1	0	0.281639	-6.284758	4.064324
68	1	0	-1.154576	-6.075021	3.057840
69	1	0	-1.762628	-2.448515	0.262165
70	6	0	-2.044768	2.436519	-0.279491
71	1	0	-1.092576	2.815781	-0.674548
72	1	0	-1.995528	2.538704	0.806194
73	6	0	-3.190160	3.289016	-0.866276
74	1	0	-4.149072	2.954359	-0.443241
75	1	0	-3.252892	3.109711	-1.949186
76	6	0	-3.863684	-0.961730	-0.429388

77	1	0	-3.432597	-1.396124	-1.338461
78	1	0	-4.053921	-1.783193	0.270297
79	6	0	-5.196484	-0.263204	-0.767638
80	1	0	-5.618169	0.191245	0.141900
81	1	0	-4.992378	0.564864	-1.458366
82	6	0	-3.026753	4.799726	-0.626178
83	1	0	-2.064713	5.128194	-1.046324
84	1	0	-3.806071	5.333166	-1.190833
85	6	0	-3.105485	5.224398	0.847309
86	1	0	-2.299934	4.744073	1.417515
87	1	0	-4.048620	4.855967	1.279653
88	6	0	-3.020846	6.744074	1.041444
89	1	0	-2.083471	7.120619	0.609286
90	1	0	-3.833346	7.231437	0.481339
91	6	0	-3.096425	7.170598	2.520665
92	1	0	-2.269384	6.713230	3.079205
93	1	0	-4.025955	6.767047	2.952494
94	6	0	-6.245775	-1.191537	-1.404306
95	1	0	-7.089983	-0.577457	-1.750809
96	1	0	-5.816664	-1.655965	-2.304063
97	6	0	-6.787196	-2.288728	-0.476059
98	1	0	-5.970447	-2.953150	-0.163686
99	1	0	-7.174705	-1.826006	0.444584
100	6	0	-7.894594	-3.131086	-1.123263
101	1	0	-7.517036	-3.592148	-2.046247
102	1	0	-8.723271	-2.473848	-1.426636
103	6	0	-8.436312	-4.236841	-0.196241

104	1	0	-7.620433	-4.915822	0.084869
105	1	0	-8.788841	-3.768506	0.736304
106	6	0	-9.560594	-5.023407	-0.813445
107	1	0	-10.445985	-4.446097	-1.088848
108	6	0	-9.544992	-6.334877	-1.057368
109	1	0	-8.684267	-6.951739	-0.805495
110	1	0	-10.388860	-6.843844	-1.516457
111	6	0	-3.070231	8.663514	2.704939
112	1	0	-3.881896	9.213833	2.223485
113	6	0	-2.142442	9.344410	3.379848
114	1	0	-1.311957	8.841863	3.872222
115	1	0	-2.175170	10.427632	3.467684

TS6a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.372644 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.328473 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.327529 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.453002 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.322954 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.441605 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.722847	1.189321	0.050488

2	17	0	-1.907788	1.134759	-2.389365
3	17	0	-1.620915	1.490064	2.478510
4	6	0	-2.678798	3.148298	-0.023565
5	1	0	-2.444252	3.531224	-1.013352
6	6	0	0.074190	0.137806	0.020248
7	7	0	1.281068	0.775600	-0.004243
8	7	0	0.351952	-1.196827	0.034126
9	6	0	2.334978	-0.154152	-0.002566
10	6	0	1.746023	-1.409674	0.021662
11	6	0	3.752094	0.088390	-0.015482
12	6	0	2.472434	-2.652234	0.029383
13	6	0	4.539751	-1.157917	-0.009247
14	6	0	3.934735	-2.452578	0.012006
15	8	0	4.266973	1.238171	-0.024466
16	8	0	1.929115	-3.787635	0.044568
17	6	0	5.947471	-1.062956	-0.023104
18	1	0	6.376442	-0.065254	-0.038282
19	6	0	4.765798	-3.592666	0.017017
20	1	0	4.276194	-4.562014	0.033148
21	6	0	6.742190	-2.196387	-0.017817
22	1	0	7.826492	-2.102680	-0.029125
23	6	0	6.145096	-3.474669	0.002399
24	1	0	6.769121	-4.366408	0.006717
25	6	0	-3.793543	2.315475	0.139162
26	6	0	-5.333249	-1.275107	-0.115005
27	6	0	-3.198539	0.082517	0.308320
28	6	0	-4.001901	-0.731400	-0.667294

29	1	0	-5.139059	-1.808329	0.825957
30	1	0	-4.250148	2.226992	1.120281
31	1	0	-5.712908	-2.028109	-0.819020
32	1	0	-3.481642	-0.069949	1.360872
33	1	0	-3.359704	-1.583524	-0.933658
34	1	0	-4.139969	-0.183851	-1.605662
35	6	0	1.417596	2.214786	-0.043613
36	6	0	1.445778	2.863810	-1.291187
37	6	0	1.596253	2.921384	1.159767
38	6	0	1.509740	4.261918	-1.299541
39	6	0	1.656921	4.316494	1.094820
40	6	0	1.588169	5.006104	-0.119607
41	1	0	1.524517	4.775735	-2.258812
42	1	0	1.784695	4.874326	2.020500
43	6	0	-0.625684	-2.256844	0.042669
44	6	0	-1.127745	-2.713325	1.270978
45	6	0	-1.003756	-2.841546	-1.177076
46	6	0	-2.076734	-3.742888	1.248774
47	6	0	-1.947088	-3.873810	-1.144190
48	6	0	-2.497781	-4.336061	0.055957
49	1	0	-2.475098	-4.104161	2.195161
50	1	0	-2.247299	-4.335419	-2.083209
51	6	0	1.826940	2.204283	2.464332
52	1	0	1.869948	2.918986	3.292561
53	1	0	1.032956	1.485830	2.680262
54	1	0	2.784366	1.670774	2.419002
55	6	0	1.513821	2.087510	-2.582008

56	1	0	0.640129	1.445351	-2.721167
57	1	0	1.568342	2.771971	-3.434935
58	1	0	2.412783	1.459187	-2.590688
59	6	0	1.616549	6.517267	-0.154701
60	1	0	2.226399	6.925582	0.659475
61	1	0	2.023667	6.888309	-1.102078
62	1	0	0.607805	6.939563	-0.046449
63	6	0	-0.396800	-2.393731	-2.482472
64	1	0	-0.812069	-2.969932	-3.315934
65	1	0	-0.590181	-1.331697	-2.670202
66	1	0	0.688390	-2.546989	-2.470744
67	6	0	-0.629265	-2.154841	2.580420
68	1	0	-0.839229	-1.084030	2.677929
69	1	0	-1.100036	-2.674303	3.421780
70	1	0	0.455820	-2.290453	2.663043
71	6	0	-3.484037	-5.482393	0.063656
72	1	0	-2.966925	-6.451913	0.065049
73	1	0	-4.124954	-5.454637	0.951960
74	1	0	-4.130846	-5.463115	-0.821182
75	1	0	-2.286436	3.688194	0.833952
76	1	0	-4.404867	2.067654	-0.722227
77	6	0	-6.412740	-0.210438	0.110124
78	1	0	-7.347800	-0.661395	0.464296
79	1	0	-6.100328	0.528084	0.857654
80	1	0	-6.634165	0.330063	-0.819153

TS8a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.221594 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.173192 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.172248 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.307967 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.193923 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.294307 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.557675	0.470946	0.092873
2	17	0	1.624096	0.685644	-2.344180
3	17	0	1.592787	0.276055	2.532329
4	6	0	3.607743	-0.276703	-0.103396
5	1	0	3.716316	-0.503325	-1.166021
6	6	0	-0.485087	0.097802	0.028804
7	7	0	-1.038848	-1.143614	-0.074947
8	7	0	-1.524510	0.980924	0.060134
9	6	0	-2.442023	-1.057146	-0.113001
10	6	0	-2.751270	0.292321	-0.025827
11	6	0	-3.406774	-2.117594	-0.220499
12	6	0	-4.089104	0.823670	-0.031642
13	6	0	-4.794764	-1.620587	-0.225493
14	6	0	-5.116550	-0.230870	-0.136405
15	8	0	-3.102294	-3.337411	-0.301505

16	8	0	-4.361148	2.050262	0.041052
17	6	0	-5.843969	-2.558895	-0.323712
18	1	0	-5.566552	-3.606896	-0.390147
19	6	0	-6.473230	0.156149	-0.150259
20	1	0	-6.685345	1.219120	-0.081768
21	6	0	-7.167909	-2.154818	-0.334600
22	1	0	-7.963446	-2.893708	-0.410783
23	6	0	-7.485865	-0.782868	-0.247017
24	1	0	-8.526519	-0.464144	-0.255693
25	6	0	3.877631	1.071165	0.254266
26	6	0	1.971712	2.250376	0.274941
27	1	0	4.059593	1.256794	1.312974
28	1	0	2.048892	2.723083	1.259696
29	6	0	-0.267180	-2.364955	-0.123463
30	6	0	0.115168	-2.885284	-1.372776
31	6	0	0.013015	-3.043063	1.076285
32	6	0	0.900578	-4.043251	-1.386140
33	6	0	0.797213	-4.199299	1.006315
34	6	0	1.268591	-4.702563	-0.210043
35	1	0	1.205808	-4.452870	-2.347118
36	1	0	1.023072	-4.730694	1.928823
37	6	0	-1.398835	2.415782	0.175397
38	6	0	-1.378887	2.997197	1.453306
39	6	0	-1.359720	3.194282	-0.992713
40	6	0	-1.223104	4.384990	1.538821
41	6	0	-1.203407	4.577025	-0.852402
42	6	0	-1.115661	5.189444	0.401138

43	1	0	-1.205524	4.846856	2.524353
44	1	0	-1.170377	5.190513	-1.750979
45	6	0	-0.580140	-2.597295	2.388250
46	1	0	-0.257302	-3.260104	3.197826
47	1	0	-0.278344	-1.577781	2.644306
48	1	0	-1.674743	-2.633258	2.333365
49	6	0	-0.383028	-2.283026	-2.661441
50	1	0	-0.091809	-1.233888	-2.762263
51	1	0	0.019306	-2.831268	-3.519682
52	1	0	-1.477376	-2.345483	-2.698716
53	6	0	2.140929	-5.936781	-0.252647
54	1	0	1.911328	-6.617948	0.574658
55	1	0	2.009920	-6.487345	-1.191123
56	1	0	3.206627	-5.679285	-0.174237
57	6	0	-1.542361	2.576394	-2.355371
58	1	0	-1.491579	3.344979	-3.133863
59	1	0	-0.773161	1.826539	-2.565386
60	1	0	-2.523659	2.091385	-2.420198
61	6	0	-1.575070	2.169068	2.697980
62	1	0	-0.775613	1.431434	2.823565
63	1	0	-1.589042	2.810982	3.585175
64	1	0	-2.530315	1.632763	2.652125
65	6	0	-0.915254	6.683372	0.522308
66	1	0	-1.351600	7.071842	1.449582
67	1	0	0.151576	6.947943	0.530184
68	1	0	-1.374209	7.218296	-0.317098
69	1	0	2.073690	2.905488	-0.595029

70	6	0	3.866039	-1.459549	0.814167
71	1	0	3.102769	-2.231774	0.649502
72	1	0	3.777556	-1.152418	1.859579
73	6	0	5.253762	-2.080947	0.553485
74	1	0	6.031351	-1.325103	0.733073
75	1	0	5.337092	-2.363590	-0.505791
76	6	0	5.517222	-3.308620	1.432371
77	1	0	4.767826	-4.088963	1.251737
78	1	0	6.506494	-3.739383	1.234327
79	1	0	5.470450	-3.048686	2.497067
80	6	0	4.580019	2.003677	-0.723034
81	1	0	4.117877	1.903024	-1.711361
82	1	0	4.463089	3.049251	-0.410472
83	6	0	6.085741	1.687914	-0.815616
84	1	0	6.535165	1.735275	0.186943
85	1	0	6.216629	0.655318	-1.164033
86	6	0	6.826107	2.647342	-1.754070
87	1	0	6.738242	3.685635	-1.410160
88	1	0	7.893856	2.404215	-1.812537
89	1	0	6.414644	2.599533	-2.769620

TS4

SCF Energy(B3LYP/SDD-6-31g(d)) = -3139.560676 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -3139.499722 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -3139.498778 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -3139.667706 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -3139.513490 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -3139.644031 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.481815	-0.233289	-0.018261
2	17	0	-0.678949	-1.322931	-2.190794
3	17	0	-0.357315	0.873296	2.151871
4	6	0	-2.218309	0.935959	-0.644105
5	1	0	-2.292456	0.764874	-1.719813
6	6	0	1.561649	-0.518276	-0.045097
7	7	0	2.476430	0.355359	-0.578836
8	7	0	2.296203	-1.578426	0.428922
9	6	0	3.758274	-0.152545	-0.442665
10	6	0	3.645511	-1.362107	0.189059
11	6	0	5.036759	0.434681	-0.869066
12	6	0	4.797150	-2.217096	0.519309
13	6	0	6.236422	-0.404714	-0.549574
14	6	0	6.123209	-1.652483	0.103230
15	8	0	5.121768	1.516043	-1.437811
16	8	0	4.693967	-3.297632	1.085032
17	6	0	7.497454	0.073525	-0.915157
18	1	0	7.558988	1.034355	-1.415685
19	6	0	7.274155	-2.396091	0.376778
20	1	0	7.162935	-3.351607	0.878836

21	6	0	8.640879	-0.676144	-0.637481
22	1	0	9.617867	-0.297922	-0.924523
23	6	0	8.529168	-1.910407	0.008178
24	1	0	9.419152	-2.494449	0.224484
25	6	0	-2.865356	-0.044557	0.163813
26	6	0	-1.436819	-1.590405	0.775454
27	1	0	-3.064374	0.253814	1.193394
28	1	0	-1.621771	-1.606582	1.853922
29	6	0	2.124287	1.632635	-1.176414
30	6	0	1.897334	1.694472	-2.562478
31	6	0	2.102970	2.776437	-0.357933
32	6	0	1.528173	2.932350	-3.099724
33	6	0	1.732380	3.986619	-0.952136
34	6	0	1.420285	4.082367	-2.312432
35	1	0	1.341533	2.997938	-4.169015
36	1	0	1.706047	4.880974	-0.333878
37	6	0	1.752132	-2.752941	1.088742
38	6	0	1.628758	-2.743506	2.487415
39	6	0	1.429990	-3.876111	0.310264
40	6	0	1.087938	-3.881574	3.094193
41	6	0	0.893564	-4.985713	0.971359
42	6	0	0.699577	-5.003738	2.355962
43	1	0	0.982538	-3.891754	4.176685
44	1	0	0.635544	-5.864356	0.384475
45	6	0	2.521410	2.734529	1.090741
46	1	0	2.478240	3.737090	1.526041
47	1	0	1.871149	2.082938	1.682729

48	1	0	3.553723	2.375706	1.189277
49	6	0	2.112203	0.505369	-3.464937
50	1	0	1.471588	-0.337704	-3.189811
51	1	0	1.889006	0.771715	-4.502066
52	1	0	3.158121	0.175008	-3.426002
53	6	0	0.989422	5.398890	-2.915393
54	1	0	1.497106	6.243667	-2.437439
55	1	0	1.201073	5.436656	-3.988951
56	1	0	-0.090272	5.555978	-2.789354
57	6	0	1.683619	-3.920204	-1.176015
58	1	0	1.390478	-4.892497	-1.582727
59	1	0	1.117623	-3.146953	-1.706269
60	1	0	2.748789	-3.777568	-1.398631
61	6	0	2.091396	-1.577358	3.325109
62	1	0	1.530862	-0.665425	3.092755
63	1	0	1.954679	-1.795921	4.388215
64	1	0	3.157654	-1.373352	3.164740
65	6	0	0.088807	-6.206154	3.037488
66	1	0	-1.003858	-6.114144	3.099063
67	1	0	0.306501	-7.129894	2.490986
68	1	0	0.462786	-6.319621	4.060567
69	1	0	-1.760349	-2.465760	0.206446
70	6	0	-2.093007	2.398059	-0.253545
71	1	0	-1.144443	2.802066	-0.633693
72	1	0	-2.061494	2.492001	0.833356
73	6	0	-3.248779	3.231375	-0.849837
74	1	0	-4.204290	2.876612	-0.437560

75	1	0	-3.296521	3.055094	-1.933730
76	6	0	-3.859671	-1.018782	-0.457420
77	1	0	-3.435090	-1.429414	-1.380269
78	1	0	-4.044042	-1.856582	0.223373
79	6	0	-5.196286	-0.313441	-0.767187
80	1	0	-5.604444	0.126272	0.155076
81	1	0	-5.001435	0.524444	-1.448704
82	6	0	-3.114413	4.743340	-0.600023
83	1	0	-2.153754	5.091767	-1.008325
84	1	0	-3.895525	5.262135	-1.174050
85	6	0	-3.221591	5.162839	0.873109
86	1	0	-2.419848	4.691514	1.457152
87	1	0	-4.167087	4.782249	1.288521
88	6	0	-3.157497	6.683071	1.071326
89	1	0	-2.216818	7.070938	0.656203
90	1	0	-3.964861	7.161482	0.497254
91	6	0	-3.264320	7.106424	2.549261
92	1	0	-2.447387	6.650429	3.124113
93	1	0	-4.201278	6.700232	2.961579
94	6	0	-6.252589	-1.235475	-1.401538
95	1	0	-7.097347	-0.614535	-1.731687
96	1	0	-5.835009	-1.690018	-2.311663
97	6	0	-6.787389	-2.340282	-0.478509
98	1	0	-5.969961	-3.010341	-0.178398
99	1	0	-7.166800	-1.885231	0.449057
100	6	0	-7.900891	-3.174977	-1.125358
101	1	0	-7.530940	-3.627619	-2.055544

102	1	0	-8.730165	-2.513399	-1.415985
103	6	0	-8.436985	-4.288369	-0.204626
104	1	0	-7.618976	-4.968930	0.067125
105	1	0	-8.786189	-3.828316	0.733157
106	6	0	-9.562146	-5.071803	-0.824839
107	1	0	-10.451288	-4.495374	-1.088492
108	6	0	-9.541436	-6.380521	-1.081633
109	1	0	-8.677121	-6.996290	-0.839318
110	1	0	-10.385607	-6.888995	-1.540074
111	6	0	-3.243689	8.599466	2.735284
112	1	0	-4.047333	9.149505	2.241115
113	6	0	-2.328810	9.278395	3.429110
114	1	0	-1.508636	8.774763	3.937617
115	1	0	-2.364514	10.360895	3.520777

TS6

SCF Energy(B3LYP/SDD-6-31g(d)) =	-2631.295569 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2631.251419 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2631.250474 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2631.375580 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2631.191379 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-2631.364080 A.U.

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

1	44	0	-1.735515	1.187870	0.075989
2	17	0	-1.905328	1.205848	-2.353884
3	17	0	-1.608643	1.402986	2.502077
4	6	0	-2.681283	3.129014	0.068812
5	1	0	-2.463263	3.557390	-0.906115
6	6	0	0.058930	0.155993	0.019571
7	7	0	1.283482	0.780886	-0.013215
8	7	0	0.335361	-1.187741	0.037709
9	6	0	2.300736	-0.158124	-0.011038
10	6	0	1.708761	-1.392130	0.023473
11	6	0	3.756027	0.051730	-0.046275
12	6	0	2.461301	-2.655916	0.049037
13	6	0	4.560865	-1.212305	-0.030480
14	6	0	3.951362	-2.486050	0.015002
15	8	0	4.272603	1.161286	-0.085757
16	8	0	1.928586	-3.757344	0.095899
17	6	0	5.954295	-1.112172	-0.060568
18	1	0	6.399301	-0.123092	-0.095179
19	6	0	4.748766	-3.633351	0.030016
20	1	0	4.258818	-4.600879	0.065769
21	6	0	6.742016	-2.263633	-0.045905
22	1	0	7.824621	-2.178005	-0.069607
23	6	0	6.139418	-3.523600	-0.000482
24	1	0	6.752341	-4.420344	0.011254
25	6	0	-3.800198	2.282424	0.203229
26	6	0	-5.414301	-1.182323	-0.161960

27	6	0	-3.253663	0.121835	0.306338
28	6	0	-4.062875	-0.661185	-0.689495
29	1	0	-5.246814	-1.728974	0.776557
30	1	0	-4.266464	2.190001	1.179494
31	1	0	-5.792580	-1.920790	-0.881062
32	1	0	-3.531258	-0.059369	1.354412
33	1	0	-3.434909	-1.526101	-0.950276
34	1	0	-4.174397	-0.104731	-1.625533
35	6	0	1.451219	2.225027	-0.047127
36	6	0	1.499422	2.869868	-1.296109
37	6	0	1.639846	2.915567	1.163764
38	6	0	1.610781	4.264161	-1.296714
39	6	0	1.747327	4.307864	1.099864
40	6	0	1.709366	5.002204	-0.113558
41	1	0	1.640684	4.781025	-2.253028
42	1	0	1.882507	4.859851	2.027031
43	6	0	-0.649730	-2.252383	0.032827
44	6	0	-1.123388	-2.742733	1.259563
45	6	0	-1.042531	-2.794869	-1.201259
46	6	0	-2.060797	-3.780980	1.219701
47	6	0	-1.974006	-3.838453	-1.179821
48	6	0	-2.496416	-4.343127	0.015937
49	1	0	-2.443642	-4.170856	2.160147
50	1	0	-2.291829	-4.270809	-2.125966
51	6	0	1.809771	2.197833	2.479123
52	1	0	1.888422	2.919111	3.297478
53	1	0	0.965265	1.539245	2.697408

54	1	0	2.731564	1.601633	2.473407
55	6	0	1.515022	2.103677	-2.595421
56	1	0	0.599248	1.522851	-2.738740
57	1	0	1.608063	2.793214	-3.439357
58	1	0	2.371890	1.418744	-2.631370
59	6	0	1.788383	6.510462	-0.144774
60	1	0	2.386262	6.897823	0.687101
61	1	0	2.231023	6.869572	-1.079793
62	1	0	0.789239	6.958764	-0.063494
63	6	0	-0.487801	-2.289003	-2.510367
64	1	0	-0.889976	-2.871398	-3.344391
65	1	0	-0.746899	-1.236616	-2.675210
66	1	0	0.605131	-2.377583	-2.543104
67	6	0	-0.626253	-2.207265	2.579604
68	1	0	-0.839459	-1.138645	2.696200
69	1	0	-1.099965	-2.740197	3.409210
70	1	0	0.458329	-2.344963	2.675472
71	6	0	-3.472453	-5.496730	0.007700
72	1	0	-2.943529	-6.458922	0.027731
73	1	0	-4.132598	-5.470290	0.880914
74	1	0	-4.096757	-5.488415	-0.892039
75	1	0	-2.306957	3.652296	0.944517
76	1	0	-4.419068	2.090635	-0.666841
77	6	0	-6.480165	-0.102603	0.053571
78	1	0	-7.429833	-0.546912	0.372484
79	1	0	-6.180962	0.616073	0.825336
80	1	0	-6.669314	0.457334	-0.870890

TS5

SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.292308 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.248058 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.247114 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.373197 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.185501 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.360752 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.635607	1.211288	0.156843
2	17	0	-1.844948	1.219772	-2.269161
3	17	0	-1.545019	1.257651	2.593038
4	6	0	-1.349082	3.025285	0.120462
5	1	0	-1.302717	3.576808	-0.823931
6	6	0	0.148636	0.198736	0.061155
7	7	0	1.434018	0.680203	-0.010380
8	7	0	0.267118	-1.169559	0.064988
9	6	0	1.601576	-1.534474	-0.000477
10	6	0	2.331909	-0.377170	-0.048996
11	6	0	2.193151	-2.880015	-0.016359
12	6	0	3.801084	-0.346587	-0.128914
13	6	0	3.689428	-2.893482	-0.096790

14	6	0	4.445524	-1.701158	-0.149701
15	8	0	1.525867	-3.905952	0.032250
16	8	0	4.451960	0.689080	-0.175485
17	6	0	4.342052	-4.128828	-0.118915
18	1	0	3.739931	-5.030614	-0.077062
19	6	0	5.839145	-1.769650	-0.223858
20	1	0	6.399216	-0.841106	-0.263498
21	6	0	5.734077	-4.186891	-0.193115
22	1	0	6.234559	-5.150828	-0.209950
23	6	0	6.482162	-3.007782	-0.245609
24	1	0	7.565962	-3.052499	-0.303389
25	6	0	-3.564345	2.594916	0.228673
26	6	0	-3.849204	1.237464	0.459810
27	6	0	-4.587007	0.351465	-0.522368
28	1	0	-3.546659	3.275084	1.075253
29	1	0	-4.446177	0.714661	-1.543803
30	1	0	-3.936173	0.943058	1.505115
31	1	0	-4.174090	-0.665931	-0.488090
32	6	0	1.808616	2.082754	-0.041774
33	6	0	2.086891	2.734090	1.170853
34	6	0	1.939094	2.718197	-1.287228
35	6	0	2.435651	4.087047	1.110339
36	6	0	2.291636	4.071657	-1.286299
37	6	0	2.529246	4.776830	-0.102468
38	1	0	2.652856	4.608845	2.039600
39	1	0	2.396012	4.581278	-2.241485
40	6	0	-0.869549	-2.073815	0.115435

41	6	0	-1.326337	-2.520411	1.368046
42	6	0	-1.424181	-2.529117	-1.094669
43	6	0	-2.447892	-3.356660	1.383486
44	6	0	-2.541017	-3.366474	-1.016029
45	6	0	-3.081256	-3.772715	0.208846
46	1	0	-2.820084	-3.706304	2.343541
47	1	0	-2.986955	-3.723744	-1.941359
48	6	0	2.051599	2.010995	2.494258
49	1	0	2.757959	1.171232	2.504826
50	1	0	2.334354	2.688621	3.305105
51	1	0	1.052692	1.618632	2.713901
52	6	0	1.746063	1.978389	-2.587727
53	1	0	0.725318	1.592921	-2.686947
54	1	0	1.940048	2.642709	-3.434887
55	1	0	2.439048	1.131245	-2.667414
56	6	0	2.878461	6.246640	-0.132711
57	1	0	3.399732	6.515523	-1.057516
58	1	0	1.975753	6.869478	-0.074942
59	1	0	3.518304	6.523721	0.711799
60	6	0	-0.813490	-2.194933	-2.432717
61	1	0	-1.378477	-2.674777	-3.237010
62	1	0	-0.812627	-1.117054	-2.620950
63	1	0	0.219852	-2.559683	-2.490979
64	6	0	-0.606916	-2.185472	2.650548
65	1	0	-0.578532	-1.107050	2.832911
66	1	0	-1.109597	-2.655866	3.500485
67	1	0	0.423755	-2.561611	2.625777

68	6	0	-4.310329	-4.649928	0.257738
69	1	0	-4.329464	-5.359403	-0.576616
70	1	0	-4.359520	-5.219685	1.191348
71	1	0	-5.227186	-4.048720	0.193031
72	6	0	-6.090285	0.283846	-0.176466
73	1	0	-6.518606	1.293988	-0.231143
74	1	0	-6.213680	-0.047930	0.863879
75	1	0	-3.754995	3.020314	-0.752949
76	6	0	-6.859486	-0.656013	-1.110535
77	1	0	-6.471011	-1.680155	-1.047567
78	1	0	-7.924684	-0.685700	-0.854306
79	1	0	-6.774066	-0.333500	-2.155152
80	1	0	-1.178201	3.601192	1.035459

TS8

SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.145433 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.096990 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.096046 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.231523 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.062538 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.217744 A.U.

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

1	44	0	1.569483	0.469368	0.084694
2	17	0	1.630029	0.632766	-2.347906
3	17	0	1.586902	0.309433	2.517470
4	6	0	3.617453	-0.271024	-0.092330
5	1	0	3.733468	-0.511808	-1.150807
6	6	0	-0.458822	0.095766	0.022533
7	7	0	-1.032256	-1.147441	-0.081164
8	7	0	-1.506837	0.984006	0.058163
9	6	0	-2.412901	-1.035997	-0.112718
10	6	0	-2.709808	0.297789	-0.024205
11	6	0	-3.425065	-2.096712	-0.219852
12	6	0	-4.083414	0.826401	-0.022037
13	6	0	-4.839117	-1.600234	-0.219862
14	6	0	-5.148377	-0.224870	-0.127223
15	8	0	-3.144419	-3.285972	-0.303143
16	8	0	-4.346563	2.019124	0.058445
17	6	0	-5.871473	-2.537022	-0.315965
18	1	0	-5.609093	-3.587601	-0.386309
19	6	0	-6.484238	0.184861	-0.132645
20	1	0	-6.697776	1.246299	-0.060609
21	6	0	-7.202288	-2.118152	-0.320353
22	1	0	-7.999541	-2.852139	-0.395233
23	6	0	-7.508440	-0.757769	-0.228759
24	1	0	-8.544445	-0.431190	-0.232241
25	6	0	3.879339	1.089501	0.243506
26	6	0	2.017664	2.246806	0.238974
27	1	0	4.062539	1.284864	1.300320

28	1	0	2.095250	2.735882	1.214876
29	6	0	-0.275455	-2.387500	-0.126616
30	6	0	0.084903	-2.917710	-1.377790
31	6	0	-0.000349	-3.053566	1.081350
32	6	0	0.841461	-4.094493	-1.384504
33	6	0	0.754845	-4.228183	1.011395
34	6	0	1.203171	-4.752630	-0.205493
35	1	0	1.135551	-4.515689	-2.342961
36	1	0	0.981804	-4.754192	1.935814
37	6	0	-1.385869	2.427581	0.169409
38	6	0	-1.378824	3.006649	1.448410
39	6	0	-1.336177	3.193421	-1.006467
40	6	0	-1.238170	4.396111	1.525691
41	6	0	-1.195906	4.577896	-0.867875
42	6	0	-1.135287	5.197073	0.384424
43	1	0	-1.221405	4.861982	2.508428
44	1	0	-1.145951	5.186879	-1.767757
45	6	0	-0.542022	-2.572431	2.404373
46	1	0	-0.249550	-3.258125	3.204810
47	1	0	-0.164071	-1.577618	2.659855
48	1	0	-1.638520	-2.533023	2.386909
49	6	0	-0.379430	-2.302343	-2.673988
50	1	0	-0.035647	-1.269388	-2.782045
51	1	0	0.004210	-2.874243	-3.523785
52	1	0	-1.475197	-2.312769	-2.735789
53	6	0	2.046695	-6.005474	-0.242939
54	1	0	1.765955	-6.701330	0.555040

55	1	0	1.948029	-6.526848	-1.200664
56	1	0	3.110768	-5.769245	-0.107807
57	6	0	-1.463141	2.570744	-2.374446
58	1	0	-1.428471	3.343415	-3.148060
59	1	0	-0.655719	1.857715	-2.571846
60	1	0	-2.419456	2.042529	-2.479131
61	6	0	-1.547395	2.184680	2.702072
62	1	0	-0.725864	1.472044	2.832812
63	1	0	-1.573462	2.834977	3.581347
64	1	0	-2.488400	1.620497	2.681134
65	6	0	-1.016297	6.699161	0.500185
66	1	0	-0.454712	7.122881	-0.339166
67	1	0	-2.006504	7.174201	0.502163
68	1	0	-0.513678	6.991295	1.428210
69	1	0	2.123378	2.885259	-0.641902
70	6	0	3.886668	-1.437088	0.842232
71	1	0	3.128329	-2.217136	0.689010
72	1	0	3.801179	-1.117499	1.883932
73	6	0	5.277835	-2.053340	0.582588
74	1	0	6.050659	-1.292535	0.757226
75	1	0	5.361169	-2.341936	-0.474717
76	6	0	5.546635	-3.273284	1.470115
77	1	0	4.805210	-4.062004	1.291554
78	1	0	6.539070	-3.695786	1.275362
79	1	0	5.497143	-3.008014	2.533033
80	6	0	4.603390	1.997791	-0.743110
81	1	0	4.161642	1.878418	-1.738489

82	1	0	4.487205	3.049776	-0.454648
83	6	0	6.108872	1.669819	-0.796088
84	1	0	6.535491	1.733031	0.215000
85	1	0	6.240718	0.630702	-1.123889
86	6	0	6.873389	2.609422	-1.734839
87	1	0	6.786113	3.653390	-1.409770
88	1	0	7.939404	2.357301	-1.764143
89	1	0	6.485302	2.546160	-2.758507

TS7

SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.146080 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.097772 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.096828 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.231622 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.066129 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.218298 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.634852	0.448241	0.177168
2	17	0	1.746318	0.676365	-2.247014
3	17	0	1.581541	0.384000	2.615019
4	6	0	2.908688	-0.923759	0.071551
5	1	0	3.252480	-1.148744	-0.944595

6	6	0	-0.407583	0.091508	0.055900
7	7	0	-1.101563	-1.086887	-0.035853
8	7	0	-1.358480	1.082934	0.035437
9	6	0	-2.623090	0.528061	-0.070472
10	6	0	-2.463893	-0.830900	-0.116415
11	6	0	-3.929435	1.202143	-0.123853
12	6	0	-3.583026	-1.778734	-0.234855
13	6	0	-5.098137	0.271168	-0.239532
14	6	0	-4.934808	-1.131102	-0.292226
15	8	0	-4.058832	2.418895	-0.078254
16	8	0	-3.436031	-2.993120	-0.284125
17	6	0	-6.381377	0.821330	-0.297117
18	1	0	-6.481597	1.901000	-0.255094
19	6	0	-6.058723	-1.954070	-0.401860
20	1	0	-5.908986	-3.028068	-0.441192
21	6	0	-7.497504	-0.008651	-0.406048
22	1	0	-8.491938	0.426189	-0.450193
23	6	0	-7.336145	-1.395734	-0.458501
24	1	0	-8.204878	-2.042284	-0.543585
25	6	0	3.940485	0.918690	0.357534
26	6	0	3.020471	2.022210	0.339191
27	1	0	4.263994	0.619339	1.352734
28	1	0	2.793994	2.516173	1.281517
29	6	0	-0.515242	-2.415027	-0.022800
30	6	0	-0.390958	-3.079943	1.208025
31	6	0	-0.176738	-3.016613	-1.244817
32	6	0	0.143351	-4.372099	1.191389

33	6	0	0.354956	-4.310080	-1.199983
34	6	0	0.529542	-5.000712	0.003107
35	1	0	0.244454	-4.904660	2.134388
36	1	0	0.620808	-4.794409	-2.136843
37	6	0	-1.055036	2.502965	0.122462
38	6	0	-1.001545	3.104674	1.392225
39	6	0	-0.906577	3.239546	-1.066158
40	6	0	-0.661490	4.460160	1.448195
41	6	0	-0.568546	4.590910	-0.947076
42	6	0	-0.416470	5.213069	0.296025
43	1	0	-0.606975	4.940731	2.422221
44	1	0	-0.439794	5.174433	-1.855696
45	6	0	-0.844189	-2.454760	2.504860
46	1	0	-1.914265	-2.213367	2.477048
47	1	0	-0.685685	-3.147508	3.336484
48	1	0	-0.294893	-1.532076	2.723504
49	6	0	-0.412134	-2.329804	-2.567171
50	1	0	0.142639	-1.387925	-2.642034
51	1	0	-0.097236	-2.975284	-3.392309
52	1	0	-1.477105	-2.106744	-2.711076
53	6	0	1.126127	-6.388733	0.021177
54	1	0	0.946152	-6.914475	-0.922314
55	1	0	2.213309	-6.349111	0.171224
56	1	0	0.708377	-6.993577	0.833115
57	6	0	-1.178465	2.638900	-2.422425
58	1	0	-0.973816	3.370691	-3.209133
59	1	0	-0.554484	1.761623	-2.612658

60	1	0	-2.233122	2.346816	-2.508739
61	6	0	-1.367501	2.358462	2.651055
62	1	0	-0.695207	1.515343	2.835439
63	1	0	-1.311069	3.025963	3.515726
64	1	0	-2.395511	1.978476	2.593012
65	6	0	-0.012691	6.665726	0.390610
66	1	0	-0.370223	7.238173	-0.471920
67	1	0	-0.408075	7.133478	1.298430
68	1	0	1.080128	6.769749	0.419805
69	1	0	2.982458	2.640736	-0.556009
70	6	0	4.982468	0.811057	-0.746252
71	1	0	5.464505	-0.172527	-0.726015
72	1	0	4.490540	0.917514	-1.719277
73	6	0	6.071062	1.891432	-0.587524
74	1	0	5.605981	2.884373	-0.639799
75	1	0	6.523291	1.814251	0.411395
76	6	0	7.163603	1.775596	-1.655759
77	1	0	7.924343	2.554300	-1.529777
78	1	0	7.669484	0.803655	-1.603517
79	1	0	6.742826	1.877483	-2.663334
80	6	0	3.295969	-1.949315	1.117268
81	1	0	3.977345	-1.499145	1.852236
82	1	0	2.402181	-2.208561	1.692037
83	6	0	3.920475	-3.232385	0.531570
84	1	0	3.934494	-3.985890	1.330388
85	1	0	3.258042	-3.629830	-0.248420
86	6	0	5.338797	-3.069950	-0.024618

87	1	0	5.739321	-4.031753	-0.365300
88	1	0	5.366084	-2.386360	-0.880882
89	1	0	6.021596	-2.676970	0.739396

18a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.234553 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.186223 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.185279 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.320760 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.209802 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.307089 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.562294	0.391777	0.078503
2	17	0	1.567318	0.667314	-2.345289
3	17	0	1.617358	0.249545	2.507300
4	6	0	3.211654	-0.682168	-0.143337
5	1	0	3.366057	-0.950067	-1.193407
6	6	0	-0.472890	0.084871	0.024988
7	7	0	-1.103668	-1.115499	-0.077470
8	7	0	-1.439290	1.041030	0.063567
9	6	0	-2.499253	-0.925641	-0.108948
10	6	0	-2.711937	0.442607	-0.018258

11	6	0	-3.540225	-1.912518	-0.214296
12	6	0	-4.005910	1.071063	-0.018316
13	6	0	-4.888472	-1.313703	-0.210141
14	6	0	-5.108291	0.095314	-0.117570
15	8	0	-3.329050	-3.150579	-0.301277
16	8	0	-4.183457	2.315165	0.053789
17	6	0	-6.003454	-2.173086	-0.304120
18	1	0	-5.803316	-3.238289	-0.373926
19	6	0	-6.433188	0.580278	-0.123407
20	1	0	-6.567257	1.655717	-0.052637
21	6	0	-7.294585	-1.673795	-0.306878
22	1	0	-8.142007	-2.352827	-0.379710
23	6	0	-7.511692	-0.282698	-0.215538
24	1	0	-8.526486	0.110602	-0.217912
25	6	0	2.762953	1.947322	0.216554
26	1	0	2.751834	2.459342	1.178621
27	6	0	-0.430368	-2.395146	-0.122821
28	6	0	-0.098789	-2.950869	-1.369758
29	6	0	-0.196794	-3.082297	1.080921
30	6	0	0.580558	-4.174160	-1.379233
31	6	0	0.479193	-4.304870	1.014617
32	6	0	0.893728	-4.857261	-0.201105
33	1	0	0.846659	-4.613204	-2.338830
34	1	0	0.667161	-4.845877	1.940104
35	6	0	-1.182803	2.460311	0.188736
36	6	0	-1.097400	3.025138	1.472939
37	6	0	-1.097697	3.245840	-0.972578

38	6	0	-0.795784	4.387369	1.568187
39	6	0	-0.794491	4.603000	-0.820969
40	6	0	-0.616240	5.187008	0.435834
41	1	0	-0.721665	4.835370	2.557352
42	1	0	-0.718517	5.220947	-1.713609
43	6	0	-0.715540	-2.563683	2.397960
44	1	0	-0.476110	-3.264680	3.204315
45	1	0	-0.277736	-1.593041	2.650697
46	1	0	-1.805350	-2.450867	2.357739
47	6	0	-0.528910	-2.303286	-2.661051
48	1	0	-0.124740	-1.291884	-2.765319
49	1	0	-0.189221	-2.896059	-3.516799
50	1	0	-1.623236	-2.243554	-2.701409
51	6	0	1.652599	-6.164431	-0.238548
52	1	0	1.327834	-6.839353	0.561838
53	1	0	1.512777	-6.681165	-1.194566
54	1	0	2.732549	-6.005860	-0.109162
55	6	0	-1.412410	2.679259	-2.333041
56	1	0	-1.259231	3.437713	-3.107840
57	1	0	-0.781391	1.818983	-2.571502
58	1	0	-2.462406	2.363875	-2.366716
59	6	0	-1.401103	2.220330	2.711401
60	1	0	-0.702445	1.388219	2.838198
61	1	0	-1.336938	2.854329	3.601876
62	1	0	-2.417905	1.813229	2.656586
63	6	0	-0.252731	6.648449	0.569489
64	1	0	-0.719345	7.098567	1.453517

65	1	0	0.832926	6.783941	0.672897
66	1	0	-0.569389	7.221588	-0.309120
67	6	0	3.828878	0.780656	0.138606
68	1	0	4.271777	0.707757	1.136940
69	1	0	2.772025	2.606667	-0.652168
70	6	0	4.877102	1.097480	-0.951841
71	1	0	5.537309	0.228612	-1.073509
72	1	0	4.353270	1.234884	-1.904936
73	6	0	5.738245	2.327362	-0.630153
74	1	0	5.097788	3.212814	-0.529558
75	1	0	6.224584	2.187394	0.346476
76	6	0	6.805662	2.589836	-1.698536
77	1	0	7.412939	3.468688	-1.450475
78	1	0	7.484286	1.733444	-1.801266
79	1	0	6.346282	2.766018	-2.678897
80	6	0	3.626412	-1.800436	0.798580
81	1	0	2.909958	-2.623738	0.676018
82	1	0	3.547389	-1.472612	1.838728
83	6	0	5.043475	-2.336762	0.512372
84	1	0	5.121542	-2.624320	-0.546087
85	1	0	5.781521	-1.537463	0.669910
86	6	0	5.402567	-3.536932	1.395750
87	1	0	4.702750	-4.366339	1.234271
88	1	0	6.414200	-3.904815	1.184086
89	1	0	5.357183	-3.271385	2.459165

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2552.830193 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2552.787874 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2552.786930 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2552.911269 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2552.760414 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2552.897684 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.627072	1.501428	0.151112
2	17	0	1.503604	2.123996	2.429753
3	17	0	1.693386	2.113679	-2.134488
4	6	0	0.114960	0.216742	0.071368
5	7	0	-1.193697	0.637774	0.006573
6	7	0	0.056813	-1.154230	0.057879
7	6	0	-2.070109	-0.457982	-0.048894
8	6	0	-1.279579	-1.595460	-0.017634
9	6	0	-3.506936	-0.461652	-0.124607
10	6	0	-1.781322	-2.943902	-0.060203
11	6	0	-4.069299	-1.824144	-0.165201
12	6	0	-3.253809	-2.996986	-0.134818
13	8	0	-4.213175	0.580952	-0.154102
14	8	0	-1.052631	-3.970616	-0.038446
15	6	0	-5.470828	-1.969792	-0.238150

16	1	0	-6.062825	-1.059495	-0.259969
17	6	0	-3.877128	-4.261904	-0.179014
18	1	0	-3.230059	-5.133857	-0.154830
19	6	0	-6.059952	-3.221866	-0.279842
20	1	0	-7.143020	-3.313751	-0.335773
21	6	0	-5.254693	-4.380075	-0.249980
22	1	0	-5.716978	-5.364885	-0.282843
23	6	0	5.574201	0.511938	-0.357463
24	6	0	3.097046	0.453837	0.258458
25	6	0	4.438701	1.093820	0.511029
26	1	0	5.581898	-0.580548	-0.238592
27	1	0	6.535548	0.874349	0.032814
28	1	0	3.109109	-0.635124	0.181416
29	1	0	4.664476	0.917780	1.577278
30	1	0	4.395372	2.186639	0.392064
31	6	0	-1.606237	2.023110	0.004956
32	6	0	-1.897560	2.650742	1.228550
33	6	0	-1.796227	2.680748	-1.222800
34	6	0	-2.238342	4.006410	1.204022
35	6	0	-2.138836	4.035819	-1.192798
36	6	0	-2.335492	4.722845	0.008167
37	1	0	-2.451747	4.506540	2.146697
38	1	0	-2.274547	4.559113	-2.137312
39	6	0	1.176307	-2.055832	0.122472
40	6	0	1.762432	-2.499592	-1.072037
41	6	0	1.637158	-2.478222	1.378403
42	6	0	2.863373	-3.357332	-0.982292

43	6	0	2.739831	-3.337469	1.416328
44	6	0	3.366794	-3.787125	0.249806
45	1	0	3.330929	-3.705849	-1.901397
46	1	0	3.110576	-3.669792	2.384319
47	6	0	-1.762989	1.931717	-2.530444
48	1	0	-1.778964	2.628231	-3.374749
49	1	0	-0.873635	1.306545	-2.628095
50	1	0	-2.649199	1.287584	-2.597477
51	6	0	-1.969156	1.869862	2.516201
52	1	0	-1.084437	1.250954	2.676391
53	1	0	-2.065663	2.545490	3.371979
54	1	0	-2.849967	1.215298	2.492738
55	6	0	-2.656916	6.199805	0.012824
56	1	0	-3.201013	6.494655	-0.891836
57	1	0	-3.267416	6.474615	0.880639
58	1	0	-1.741765	6.806587	0.053923
59	6	0	0.965250	-2.022302	2.649824
60	1	0	1.441112	-2.481053	3.522721
61	1	0	1.016821	-0.933352	2.765280
62	1	0	-0.093466	-2.306342	2.650493
63	6	0	1.219212	-2.071449	-2.412478
64	1	0	1.237345	-0.981495	-2.527350
65	1	0	1.806784	-2.511134	-3.225069
66	1	0	0.179888	-2.400828	-2.526910
67	6	0	4.531049	-4.749641	0.317872
68	1	0	4.184793	-5.792467	0.320308
69	1	0	5.200194	-4.632505	-0.542067

70	1	0	5.121735	-4.602598	1.229248
71	6	0	5.449855	0.870925	-1.842131
72	1	0	6.261582	0.419531	-2.426039
73	1	0	4.495139	0.529842	-2.255875
74	1	0	5.491460	1.956976	-1.988327

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.370482 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.325153 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.324209 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.453287 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.319024 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.440231 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.641253	1.193068	0.098370
2	17	0	-1.830309	1.196449	-2.338938
3	17	0	-1.659300	1.249331	2.547902
4	6	0	-1.010447	2.896015	0.086368
5	1	0	-0.817325	3.430331	-0.850991
6	6	0	0.157771	0.214881	0.034239
7	7	0	1.440232	0.688718	0.002275
8	7	0	0.260225	-1.148255	0.030743

9	6	0	1.608112	-1.546229	0.000306
10	6	0	2.358276	-0.380393	-0.019345
11	6	0	2.155037	-2.876065	-0.007665
12	6	0	3.796814	-0.336286	-0.051779
13	6	0	3.628912	-2.881512	-0.043211
14	6	0	4.404296	-1.681195	-0.064197
15	8	0	1.454889	-3.923265	0.012793
16	8	0	4.470178	0.727083	-0.066667
17	6	0	4.295861	-4.124830	-0.056393
18	1	0	3.678465	-5.018244	-0.039602
19	6	0	5.811314	-1.779817	-0.097223
20	1	0	6.372502	-0.850070	-0.112179
21	6	0	5.677932	-4.196242	-0.089257
22	1	0	6.174275	-5.164837	-0.099094
23	6	0	6.443698	-3.011298	-0.109899
24	1	0	7.530396	-3.066406	-0.135670
25	6	0	-3.811431	2.427808	-0.008168
26	6	0	-4.048414	1.156359	0.431035
27	6	0	-4.520389	0.005508	-0.427189
28	1	0	-3.691365	3.238742	0.703765
29	1	0	-4.422055	0.259740	-1.487333
30	1	0	-4.080309	0.989646	1.506397
31	1	0	-3.885818	-0.873507	-0.252270
32	6	0	1.830057	2.076469	-0.022000
33	6	0	2.089995	2.735501	1.192116
34	6	0	2.013907	2.711442	-1.262914
35	6	0	2.466536	4.081406	1.139083

36	6	0	2.392895	4.057210	-1.260291
37	6	0	2.617606	4.760605	-0.073089
38	1	0	2.663400	4.604125	2.073281
39	1	0	2.531465	4.561294	-2.215020
40	6	0	-0.875305	-2.042071	0.044514
41	6	0	-1.377231	-2.494138	1.278546
42	6	0	-1.390899	-2.510564	-1.177611
43	6	0	-2.502241	-3.326215	1.261978
44	6	0	-2.512479	-3.345481	-1.137572
45	6	0	-3.096394	-3.745407	0.068236
46	1	0	-2.902269	-3.677754	2.211080
47	1	0	-2.922948	-3.709668	-2.077390
48	6	0	2.008591	2.009731	2.510470
49	1	0	2.713995	1.170395	2.524398
50	1	0	2.266100	2.683067	3.334749
51	1	0	1.004317	1.612269	2.693344
52	6	0	1.844236	1.961790	-2.559539
53	1	0	0.825377	1.575482	-2.674259
54	1	0	2.060468	2.615804	-3.410781
55	1	0	2.534977	1.111266	-2.600716
56	6	0	3.066342	6.204305	-0.101709
57	1	0	4.161380	6.279657	-0.154513
58	1	0	2.663153	6.733268	-0.972828
59	1	0	2.747459	6.741828	0.798483
60	6	0	-0.710874	-2.204398	-2.487157
61	1	0	-1.258945	-2.661323	-3.317707
62	1	0	-0.651672	-1.128143	-2.671342

63	1	0	0.305870	-2.615054	-2.481821
64	6	0	-0.672715	-2.185954	2.574707
65	1	0	-0.600565	-1.110104	2.755617
66	1	0	-1.208888	-2.636157	3.416629
67	1	0	0.340558	-2.604995	2.551683
68	6	0	-4.329453	-4.620366	0.080548
69	1	0	-4.368358	-5.269356	-0.801682
70	1	0	-4.359081	-5.257623	0.971662
71	1	0	-5.248993	-4.018472	0.081712
72	1	0	-3.868941	2.686717	-1.060971
73	6	0	-5.977639	-0.392650	-0.097465
74	1	0	-6.201950	-1.324167	-0.634168
75	1	0	-6.056078	-0.627549	0.973372
76	6	0	-7.015470	0.670995	-0.470137
77	1	0	-8.031937	0.332484	-0.234818
78	1	0	-6.841126	1.608135	0.070815
79	1	0	-6.977083	0.897086	-1.543171
80	1	0	-0.844538	3.461570	1.010520

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SCF Energy(B3LYP/SDD-6-31g(d)) =	-2434.888141 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2434.850153 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2434.849209 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2434.962135 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2434.736952 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2434.951097 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.309052	-2.656525	2.243358
2	17	0	-1.314098	-2.658665	-2.239971
3	6	0	0.862936	-3.427114	-0.000647
4	1	0	1.902063	-3.104173	-0.002251
5	6	0	-0.071534	-0.611874	0.000058
6	7	0	1.183345	-0.030378	-0.000034
7	7	0	-0.954768	0.461675	0.000067
8	6	0	-0.260382	1.656297	0.000071
9	6	0	1.073499	1.352993	-0.000008
10	6	0	-0.785923	3.031326	0.000196
11	6	0	2.140553	2.365590	-0.000144
12	6	0	0.269287	4.095017	0.000137
13	6	0	1.646540	3.781419	-0.000010
14	8	0	-1.982176	3.293029	0.000299
15	8	0	3.333788	2.089499	-0.000302
16	6	0	-0.136289	5.432158	0.000246
17	1	0	-1.199639	5.648342	0.000358
18	6	0	2.590054	4.811910	-0.000043
19	1	0	3.642360	4.547236	-0.000159
20	6	0	0.813343	6.454490	0.000213
21	1	0	0.490566	7.491653	0.000301
22	6	0	2.175791	6.144433	0.000069

23	1	0	2.915456	6.939940	0.000046
24	6	0	2.449328	-0.729624	-0.000407
25	6	0	3.041157	-1.048658	-1.231504
26	6	0	3.041935	-1.048726	1.230213
27	6	0	4.261047	-1.731422	-1.202895
28	6	0	4.261865	-1.731528	1.200713
29	6	0	4.887510	-2.080123	-0.001274
30	1	0	4.733138	-1.995041	-2.146552
31	1	0	4.734588	-1.995196	2.144028
32	6	0	-2.401883	0.337104	-0.000172
33	6	0	-3.080548	0.322627	-1.231218
34	6	0	-3.081111	0.322651	1.230493
35	6	0	-4.467088	0.150688	-1.201069
36	6	0	-4.467703	0.150620	1.199633
37	6	0	-5.174834	0.034861	-0.000863
38	1	0	-5.006863	0.119989	-2.144595
39	1	0	-5.007932	0.119880	2.142893
40	6	0	2.387481	-0.689325	-2.543992
41	1	0	2.243643	0.394235	-2.636380
42	1	0	3.010190	-1.012708	-3.382860
43	1	0	1.405380	-1.165060	-2.650096
44	6	0	2.389301	-0.689344	2.543200
45	1	0	1.407259	-1.165011	2.650093
46	1	0	3.012665	-1.012737	3.381579
47	1	0	2.245627	0.394233	2.635663
48	6	0	6.222707	-2.787117	-0.001920
49	1	0	7.049311	-2.064224	-0.009486

50	1	0	6.345773	-3.412976	0.888063
51	1	0	6.339225	-3.423730	-0.885183
52	6	0	-2.381450	0.596045	2.539165
53	1	0	-3.015791	0.306412	3.381309
54	1	0	-1.440561	0.051512	2.635296
55	1	0	-2.172751	1.670705	2.632735
56	6	0	-2.380009	0.595604	-2.539512
57	1	0	-1.440080	0.049384	-2.635628
58	1	0	-3.014625	0.307578	-3.381998
59	1	0	-2.169306	1.669921	-2.632475
60	6	0	-6.666444	-0.201882	-0.001369
61	1	0	-7.141018	0.226074	0.887989
62	1	0	-7.141752	0.234579	-0.886230
63	1	0	-6.891762	-1.276488	-0.006515
64	44	0	-0.666168	-2.474998	0.000869
65	1	0	0.702053	-4.520064	-0.000135

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SCF Energy(B3LYP/SDD-6-31g(d)) =	-2826.511852 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2826.461416 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2826.460472 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2826.603277 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2826.429363 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-2826.585889 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.184961	-1.825626	0.370565
2	17	0	0.687490	-1.842143	-2.001384
3	17	0	-0.351943	-1.946446	2.740214
4	6	0	-0.035633	-3.781986	0.288033
5	1	0	-0.217277	-4.184697	-0.707600
6	6	0	-1.062698	-0.211244	0.150963
7	7	0	-2.398030	-0.239301	-0.154254
8	7	0	-0.729788	1.109593	0.285992
9	6	0	-2.891992	1.055517	-0.206661
10	6	0	-1.849591	1.899359	0.068352
11	6	0	-4.260199	1.514741	-0.495517
12	6	0	-1.971752	3.365112	0.106696
13	6	0	-4.428032	3.004096	-0.465589
14	6	0	-3.351556	3.874522	-0.182613
15	8	0	-5.186279	0.752782	-0.740307
16	8	0	-1.032761	4.110878	0.353128
17	6	0	-5.694587	3.533042	-0.727723
18	1	0	-6.506013	2.845328	-0.942413
19	6	0	-3.564263	5.255523	-0.167652
20	1	0	-2.722721	5.904285	0.052289
21	6	0	-5.897138	4.913358	-0.710515
22	1	0	-6.884609	5.316950	-0.915214
23	6	0	-4.832505	5.774179	-0.430617
24	1	0	-4.990024	6.848840	-0.417098

25	6	0	2.064852	-2.160963	0.906285
26	6	0	3.286828	-1.746358	0.109564
27	1	0	2.192097	-2.003291	1.980100
28	1	0	3.366911	-0.653799	0.169243
29	1	0	3.160760	-1.997587	-0.947071
30	6	0	-3.168936	-1.451144	-0.390029
31	6	0	-3.282721	-1.932313	-1.705518
32	6	0	-3.824477	-2.056421	0.694850
33	6	0	-3.993617	-3.120885	-1.895474
34	6	0	-4.521530	-3.242675	0.443314
35	6	0	-4.605141	-3.798869	-0.836256
36	1	0	-4.081047	-3.516709	-2.904717
37	1	0	-5.024293	-3.733921	1.273164
38	6	0	0.601879	1.600917	0.603163
39	6	0	0.932998	1.833326	1.948224
40	6	0	1.476891	1.904735	-0.454346
41	6	0	2.221956	2.303658	2.221090
42	6	0	2.749920	2.376774	-0.120106
43	6	0	3.147238	2.568402	1.207772
44	1	0	2.498237	2.486327	3.256816
45	1	0	3.440210	2.620190	-0.924690
46	6	0	-3.839439	-1.440584	2.071638
47	1	0	-4.436146	-2.053214	2.753594
48	1	0	-2.832362	-1.354729	2.491051
49	1	0	-4.290606	-0.440318	2.046709
50	6	0	-2.718079	-1.183910	-2.887139
51	1	0	-1.630691	-1.081218	-2.821345

52	1	0	-2.948985	-1.713535	-3.815867
53	1	0	-3.158137	-0.181161	-2.961063
54	6	0	-5.388204	-5.067910	-1.080763
55	1	0	-6.419885	-4.842820	-1.382672
56	1	0	-4.939834	-5.667262	-1.880318
57	1	0	-5.439532	-5.686931	-0.179202
58	6	0	1.061786	1.785155	-1.899796
59	1	0	1.867733	2.128495	-2.554808
60	1	0	0.824524	0.750807	-2.170435
61	1	0	0.180166	2.403943	-2.109490
62	6	0	-0.062630	1.645456	3.065399
63	1	0	-0.403686	0.607431	3.134029
64	1	0	0.388606	1.916063	4.024305
65	1	0	-0.940623	2.287767	2.920946
66	6	0	4.537995	3.059710	1.534194
67	1	0	4.583449	3.495862	2.537211
68	1	0	5.265420	2.238198	1.498580
69	1	0	4.872728	3.818130	0.817782
70	6	0	4.575973	-2.389959	0.665503
71	1	0	4.456287	-3.482419	0.669473
72	1	0	4.712620	-2.092697	1.715735
73	6	0	1.494605	-3.640059	0.635034
74	1	0	2.066626	-4.042791	-0.201411
75	1	0	1.643644	-4.170224	1.577130
76	1	0	-0.627716	-4.225970	1.086789
77	6	0	5.843129	-2.043100	-0.135240
78	1	0	6.671063	-2.661662	0.239655

79	1	0	5.696611	-2.334050	-1.185645
80	6	0	6.263917	-0.568006	-0.071858
81	1	0	5.468116	0.067248	-0.484249
82	1	0	6.379850	-0.271246	0.982133
83	6	0	7.571104	-0.284480	-0.824165
84	1	0	7.464473	-0.584085	-1.875732
85	1	0	8.374469	-0.909980	-0.408023
86	6	0	7.997642	1.195175	-0.766038
87	1	0	7.212012	1.823744	-1.206560
88	1	0	8.081862	1.493208	0.291132
89	6	0	9.305270	1.458141	-1.462720
90	1	0	10.168622	0.918615	-1.067986
91	6	0	9.473142	2.268553	-2.508748
92	1	0	8.642437	2.825085	-2.939058
93	1	0	10.444693	2.410527	-2.974841

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2434.967228 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2434.929212 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2434.928268 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2435.042300 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2434.868274 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2435.030679 A.U.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	17	0	1.305318	-2.669523	-2.254658
2	17	0	1.300330	-2.658087	2.266383
3	6	0	-0.859583	-3.428521	0.005578
4	1	0	-1.895224	-3.093134	0.004530
5	6	0	0.066670	-0.582653	0.001000
6	7	0	-1.181712	-0.015624	0.000673
7	7	0	0.949714	0.471817	0.000201
8	6	0	0.262938	1.696972	-0.000344
9	6	0	-1.088412	1.390434	0.000106
10	6	0	0.799600	3.032139	-0.000991
11	6	0	-2.149802	2.363106	0.000782
12	6	0	-0.252062	4.065729	-0.001259
13	6	0	-1.645359	3.749561	-0.000412
14	8	0	2.031075	3.296294	-0.001206
15	8	0	-3.374846	2.073176	0.002580
16	6	0	0.139610	5.421253	-0.002124
17	1	0	1.205675	5.628729	-0.002691
18	6	0	-2.583493	4.803308	-0.000404
19	1	0	-3.634726	4.530428	0.000366
20	6	0	-0.799443	6.438396	-0.002202
21	1	0	-0.477623	7.478101	-0.002896
22	6	0	-2.175393	6.126198	-0.001328
23	1	0	-2.914411	6.925215	-0.001356
24	6	0	-2.438262	-0.717432	-0.001382
25	6	0	-3.039468	-1.038440	1.224506

26	6	0	-3.032539	-1.043151	-1.229327
27	6	0	-4.249459	-1.738882	1.196436
28	6	0	-4.242866	-1.743384	-1.205315
29	6	0	-4.866170	-2.100695	-0.005524
30	1	0	-4.724298	-1.999913	2.140434
31	1	0	-4.712445	-2.008014	-2.150931
32	6	0	2.389267	0.337861	-0.001171
33	6	0	3.076728	0.324880	1.224725
34	6	0	3.073575	0.320716	-1.228781
35	6	0	4.461649	0.136411	1.195967
36	6	0	4.458570	0.132459	-1.203021
37	6	0	5.165975	0.008638	-0.004228
38	1	0	5.002785	0.109402	2.139758
39	1	0	4.997249	0.102204	-2.148113
40	6	0	-2.405073	-0.638365	2.533214
41	1	0	-2.300054	0.451226	2.592387
42	1	0	-3.021248	-0.967052	3.376397
43	1	0	-1.406783	-1.075985	2.648758
44	6	0	-2.390325	-0.649413	-2.536215
45	1	0	-1.394870	-1.094672	-2.647309
46	1	0	-3.005684	-0.974971	-3.381208
47	1	0	-2.276731	0.439207	-2.597049
48	6	0	-6.194402	-2.823174	-0.007667
49	1	0	-7.033101	-2.113266	-0.003441
50	1	0	-6.307515	-3.453288	-0.897109
51	1	0	-6.305935	-3.461642	0.876053
52	6	0	2.370313	0.624423	-2.527195

53	1	0	3.022676	0.408531	-3.379221
54	1	0	1.454710	0.043284	-2.650521
55	1	0	2.109717	1.690386	-2.553756
56	6	0	2.377039	0.633626	2.523848
57	1	0	1.460410	0.054910	2.650794
58	1	0	3.030809	0.418731	3.375052
59	1	0	2.118954	1.700263	2.547748
60	6	0	6.656126	-0.244497	-0.005707
61	1	0	7.134515	0.182462	-0.894620
62	1	0	7.137195	0.187751	0.879206
63	1	0	6.877300	-1.320787	-0.002817
64	44	0	0.666690	-2.476990	0.004724
65	1	0	-0.713292	-4.525298	0.007883

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.293812 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.248471 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.247527 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.376234 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.187784 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.363124 A.U.

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

1	44	0	-1.665946	1.158956	0.105446
2	17	0	-1.849867	1.180299	-2.321785
3	17	0	-1.677925	1.180936	2.543376
4	6	0	-1.080297	2.879588	0.103874
5	1	0	-0.923953	3.430863	-0.830152
6	6	0	0.129034	0.217123	0.037393
7	7	0	1.414416	0.713809	-0.000104
8	7	0	0.271219	-1.153138	0.033099
9	6	0	1.611440	-1.497988	-0.002373
10	6	0	2.326970	-0.331231	-0.024304
11	6	0	2.222818	-2.835202	-0.013001
12	6	0	3.796924	-0.279802	-0.065688
13	6	0	3.720675	-2.827513	-0.055572
14	6	0	4.461038	-1.624690	-0.080374
15	8	0	1.570227	-3.871390	0.011407
16	8	0	4.435056	0.764965	-0.086673
17	6	0	4.390763	-4.053562	-0.070238
18	1	0	3.800408	-4.963825	-0.050356
19	6	0	5.856895	-1.673292	-0.119518
20	1	0	6.404734	-0.736834	-0.137909
21	6	0	5.784929	-4.091900	-0.109444
22	1	0	6.299064	-5.048708	-0.120666
23	6	0	6.517545	-2.902248	-0.134119
24	1	0	7.602984	-2.931568	-0.164604
25	6	0	-3.833762	2.395101	0.028994
26	6	0	-4.071422	1.107446	0.423030
27	6	0	-4.556630	-0.010684	-0.469177

28	1	0	-3.726504	3.181616	0.769907
29	1	0	-4.458311	0.273369	-1.521362
30	1	0	-4.107177	0.908336	1.492978
31	1	0	-3.932192	-0.902349	-0.319244
32	6	0	1.786109	2.114654	-0.018728
33	6	0	2.037364	2.763980	1.202393
34	6	0	1.958005	2.750935	-1.260557
35	6	0	2.407946	4.111396	1.152143
36	6	0	2.330942	4.098155	-1.248839
37	6	0	2.555143	4.796640	-0.057899
38	1	0	2.597026	4.633076	2.087546
39	1	0	2.459425	4.609799	-2.199976
40	6	0	-0.843985	-2.084347	0.049105
41	6	0	-1.316259	-2.556742	1.287183
42	6	0	-1.351246	-2.551517	-1.176938
43	6	0	-2.409431	-3.429200	1.269098
44	6	0	-2.441067	-3.426780	-1.131837
45	6	0	-2.998458	-3.858942	0.075905
46	1	0	-2.792647	-3.798943	2.217268
47	1	0	-2.850639	-3.793027	-2.070314
48	6	0	1.938502	2.043879	2.523984
49	1	0	2.636867	1.198388	2.565486
50	1	0	2.191417	2.720185	3.345646
51	1	0	0.928850	1.656513	2.701553
52	6	0	1.770391	2.017986	-2.565434
53	1	0	0.747403	1.640426	-2.675907
54	1	0	1.978929	2.682963	-3.408520

55	1	0	2.455326	1.163976	-2.641239
56	6	0	2.991858	6.242923	-0.080299
57	1	0	4.085829	6.322295	-0.135313
58	1	0	2.583742	6.771820	-0.948011
59	1	0	2.672162	6.772537	0.823179
60	6	0	-0.717260	-2.191322	-2.497181
61	1	0	-1.247741	-2.682120	-3.318218
62	1	0	-0.742711	-1.112615	-2.678715
63	1	0	0.327234	-2.526180	-2.531349
64	6	0	-0.635956	-2.214817	2.588957
65	1	0	-0.635076	-1.137543	2.779218
66	1	0	-1.148678	-2.701953	3.423352
67	1	0	0.402665	-2.569476	2.586331
68	6	0	-4.198068	-4.777241	0.090879
69	1	0	-4.224319	-5.416529	-0.797856
70	1	0	-4.197600	-5.422469	0.975703
71	1	0	-5.134178	-4.203287	0.107243
72	1	0	-3.899089	2.691028	-1.013717
73	6	0	-6.019832	-0.397187	-0.145925
74	1	0	-6.256752	-1.307476	-0.712036
75	1	0	-6.098603	-0.665304	0.916819
76	6	0	-7.041970	0.692503	-0.483359
77	1	0	-8.061315	0.356034	-0.262246
78	1	0	-6.861770	1.607617	0.092203
79	1	0	-6.999577	0.955405	-1.547491
80	1	0	-0.920753	3.439003	1.032447

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.304260 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.260019 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.259075 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.386115 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.202196 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.372638 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.627644	1.230003	0.160537
2	17	0	-1.807867	1.307313	-2.255403
3	17	0	-1.462349	1.300492	2.587049
4	6	0	-2.130111	3.135316	0.208798
5	1	0	-1.984980	3.674823	-0.726234
6	6	0	0.134982	0.183854	0.061156
7	7	0	1.401268	0.701420	-0.010343
8	7	0	0.278621	-1.177638	0.064659
9	6	0	2.325961	-0.331591	-0.048704
10	6	0	1.624688	-1.506504	-0.000879
11	6	0	3.793795	-0.259505	-0.128371
12	6	0	2.253756	-2.836316	-0.018715
13	6	0	4.474608	-1.595005	-0.151458
14	6	0	3.750257	-2.807139	-0.099857

15	8	0	4.412664	0.795565	-0.172619
16	8	0	1.616836	-3.880689	0.028988
17	6	0	5.869642	-1.625735	-0.225982
18	1	0	6.404609	-0.682449	-0.264470
19	6	0	4.436120	-4.024364	-0.123647
20	1	0	3.858727	-4.942191	-0.082690
21	6	0	6.545565	-2.846064	-0.249505
22	1	0	7.630127	-2.861725	-0.307582
23	6	0	5.829175	-4.044794	-0.198304
24	1	0	6.355258	-4.994953	-0.216441
25	6	0	-3.548215	0.820773	0.429247
26	6	0	-4.421693	0.067447	-0.554773
27	1	0	-3.738644	0.529276	1.465029
28	1	0	-4.094629	-0.981223	-0.561063
29	1	0	-4.277957	0.447645	-1.569644
30	6	0	1.714768	2.122329	-0.045690
31	6	0	1.811258	2.760006	-1.294285
32	6	0	1.973164	2.787714	1.164136
33	6	0	2.071856	4.133574	-1.295701
34	6	0	2.228764	4.161195	1.099681
35	6	0	2.267005	4.854399	-0.113521
36	1	0	2.137195	4.647593	-2.251958
37	1	0	2.417125	4.697059	2.027096
38	6	0	-0.824665	-2.124207	0.111329
39	6	0	-1.258233	-2.597057	1.361146
40	6	0	-1.363772	-2.588091	-1.100961
41	6	0	-2.331403	-3.494180	1.371866

42	6	0	-2.431144	-3.488458	-1.027271
43	6	0	-2.941044	-3.938579	0.194957
44	1	0	-2.684552	-3.867983	2.330061
45	1	0	-2.863060	-3.857403	-1.954717
46	6	0	2.035921	2.061761	2.484693
47	1	0	2.272932	2.762225	3.290661
48	1	0	1.085467	1.577889	2.728987
49	1	0	2.822356	1.296197	2.471540
50	6	0	1.696295	2.004385	-2.594777
51	1	0	0.706847	1.552770	-2.716510
52	1	0	1.863472	2.678650	-3.439665
53	1	0	2.449517	1.208398	-2.653806
54	6	0	2.572492	6.333803	-0.152060
55	1	0	3.646572	6.511127	-0.297317
56	1	0	2.047634	6.829736	-0.975519
57	1	0	2.283626	6.826866	0.781806
58	6	0	-0.798385	-2.182369	-2.439363
59	1	0	-1.317394	-2.709597	-3.245004
60	1	0	-0.907533	-1.107008	-2.615281
61	1	0	0.266811	-2.435410	-2.511742
62	6	0	-0.573043	-2.210955	2.648092
63	1	0	-0.629842	-1.133017	2.831182
64	1	0	-1.041215	-2.721758	3.494438
65	1	0	0.485002	-2.501699	2.631242
66	6	0	-4.117383	-4.885615	0.239687
67	1	0	-4.119459	-5.479157	1.159715
68	1	0	-5.067892	-4.336620	0.203061

69	1	0	-4.109005	-5.575269	-0.611222
70	6	0	-5.913526	0.117326	-0.164435
71	1	0	-6.258174	1.160969	-0.163636
72	1	0	-6.035342	-0.248004	0.865004
73	6	0	-3.532844	2.424137	0.307804
74	1	0	-4.100645	2.673219	-0.589143
75	1	0	-3.985463	2.774127	1.237130
76	6	0	-6.791909	-0.708282	-1.110641
77	1	0	-6.494223	-1.764216	-1.104512
78	1	0	-7.847593	-0.656531	-0.820512
79	1	0	-6.709467	-0.347478	-2.142959
80	1	0	-1.847655	3.677576	1.109780

1_9_decadiene

SCF Energy(B3LYP/SDD-6-31g(d)) =	-391.609857 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-391.597122 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-391.596178 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-391.650464 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-391.647091 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-391.648039 A.U.

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

1	6	0	5.482030	-0.051039	-0.479526

2	1	0	5.455864	0.714240	-1.253217
3	1	0	6.385451	-0.652716	-0.423651
4	6	0	4.460011	-0.235282	0.357036
5	1	0	4.532598	-1.017470	1.115594
6	6	0	3.172422	0.542759	0.344037
7	1	0	3.045146	1.053599	1.311381
8	1	0	3.224373	1.330175	-0.419758
9	6	0	1.936745	-0.342782	0.093124
10	1	0	1.905305	-1.143207	0.846902
11	1	0	2.047243	-0.843405	-0.878670
12	6	0	0.616964	0.438224	0.125457
13	1	0	0.651379	1.240867	-0.626126
14	1	0	0.515055	0.939227	1.099602
15	6	0	-0.616957	-0.438100	-0.125595
16	1	0	-0.651337	-1.240773	0.625958
17	1	0	-0.515047	-0.939084	-1.099748
18	6	0	-1.936773	0.342855	-0.093224
19	1	0	-1.905392	1.143308	-0.846979
20	1	0	-2.047233	0.843488	0.878570
21	6	0	-3.172411	-0.542727	-0.344078
22	1	0	-3.224287	-1.330183	0.419677
23	1	0	-3.045197	-1.053535	-1.311446
24	6	0	-4.460064	0.235221	-0.356947
25	1	0	-4.532933	1.017148	-1.115737
26	6	0	-5.481940	0.050925	0.479772
27	1	0	-5.455645	-0.714400	1.253408
28	1	0	-6.385505	0.652384	0.423901

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SCF Energy(B3LYP/SDD-6-31g(d)) =	-2552.753132 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2552.710785 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2552.709841 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2552.833492 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2552.630183 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-2552.820166 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.636761	1.481842	0.168683
2	17	0	1.494239	2.083346	2.437130
3	17	0	1.719584	2.122593	-2.093083
4	6	0	0.141969	0.229630	0.074193
5	7	0	-1.182231	0.653662	0.006527
6	7	0	0.061706	-1.152719	0.058452
7	6	0	-2.035447	-0.431212	-0.048156
8	6	0	-1.262927	-1.560053	-0.016207
9	6	0	-3.504737	-0.448968	-0.126115
10	6	0	-1.810080	-2.923975	-0.055789
11	6	0	-4.104515	-1.821596	-0.168000
12	6	0	-3.306548	-2.986495	-0.134876
13	8	0	-4.188328	0.566880	-0.154621

14	8	0	-1.114966	-3.932440	-0.026905
15	6	0	-5.495036	-1.936715	-0.241745
16	1	0	-6.086944	-1.027576	-0.265977
17	6	0	-3.915913	-4.243036	-0.176136
18	1	0	-3.282801	-5.123872	-0.149472
19	6	0	-6.094728	-3.196019	-0.282443
20	1	0	-7.176388	-3.277746	-0.339641
21	6	0	-5.305481	-4.348529	-0.249638
22	1	0	-5.771771	-5.329125	-0.281252
23	6	0	5.585672	0.526265	-0.324446
24	6	0	3.106030	0.426634	0.276422
25	6	0	4.430576	1.091383	0.530863
26	1	0	5.624489	-0.563362	-0.187672
27	1	0	6.530165	0.922143	0.070801
28	1	0	3.130325	-0.662011	0.203104
29	1	0	4.648074	0.924748	1.600612
30	1	0	4.368132	2.182947	0.407840
31	6	0	-1.595491	2.045584	-0.001071
32	6	0	-1.890994	2.671408	1.222617
33	6	0	-1.767664	2.695430	-1.235828
34	6	0	-2.236320	4.025310	1.188098
35	6	0	-2.116163	4.048552	-1.209515
36	6	0	-2.327456	4.737608	-0.011422
37	1	0	-2.452343	4.529944	2.126842
38	1	0	-2.237825	4.571571	-2.155161
39	6	0	1.176469	-2.071625	0.110650
40	6	0	1.756514	-2.495059	-1.094202

41	6	0	1.625110	-2.515734	1.363546
42	6	0	2.837411	-3.378893	-1.014864
43	6	0	2.708640	-3.399178	1.385228
44	6	0	3.326473	-3.843575	0.210953
45	1	0	3.305112	-3.714844	-1.937558
46	1	0	3.075400	-3.751006	2.346864
47	6	0	-1.696344	1.956356	-2.549273
48	1	0	-1.642574	2.661305	-3.383377
49	1	0	-0.824659	1.302915	-2.615480
50	1	0	-2.600512	1.347129	-2.684895
51	6	0	-1.951602	1.906624	2.521918
52	1	0	-1.091683	1.249318	2.662400
53	1	0	-1.980812	2.594970	3.370953
54	1	0	-2.865259	1.297289	2.554593
55	6	0	-2.653268	6.212398	-0.013704
56	1	0	-3.191101	6.503133	-0.922377
57	1	0	-3.266846	6.489215	0.850161
58	1	0	-1.736841	6.815619	0.030052
59	6	0	0.979595	-2.052519	2.647214
60	1	0	1.464621	-2.518553	3.509666
61	1	0	1.050752	-0.964878	2.766166
62	1	0	-0.083482	-2.321098	2.679716
63	6	0	1.251132	-2.010060	-2.431617
64	1	0	1.327342	-0.920010	-2.522082
65	1	0	1.829663	-2.457561	-3.244831
66	1	0	0.199598	-2.282649	-2.584363
67	6	0	4.471036	-4.828562	0.264392

68	1	0	4.099903	-5.862029	0.253995
69	1	0	5.139574	-4.714404	-0.595258
70	1	0	5.064346	-4.705774	1.176595
71	6	0	5.465624	0.862184	-1.814430
72	1	0	6.303889	0.438099	-2.379245
73	1	0	4.533823	0.474129	-2.240048
74	1	0	5.464962	1.946540	-1.974869

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SCF Energy(B3LYP/SDD-6-31g(d)) =	-2749.152482 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2749.102699 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2749.101755 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2749.240607 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2749.070361 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-2749.226189 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.657981	-0.554498	2.603997
2	17	0	-1.806859	-0.538949	-2.259774
3	6	0	0.343585	-0.071983	0.060129
4	7	0	1.235644	-1.128848	0.021230
5	7	0	1.128814	1.056026	-0.024095
6	6	0	2.532248	-0.663998	-0.089301

7	6	0	2.469504	0.703052	-0.119469
8	6	0	3.785575	-1.429830	-0.160083
9	6	0	3.653754	1.567368	-0.233140
10	6	0	5.018358	-0.586295	-0.272556
11	6	0	4.955626	0.824337	-0.306456
12	8	0	3.825698	-2.653802	-0.129100
13	8	0	3.599311	2.790492	-0.267202
14	6	0	6.258046	-1.226898	-0.345440
15	1	0	6.280232	-2.311450	-0.317609
16	6	0	6.135196	1.565463	-0.412991
17	1	0	6.062934	2.647846	-0.437800
18	6	0	7.430575	-0.478107	-0.451150
19	1	0	8.390884	-0.982706	-0.507251
20	6	0	7.368949	0.917445	-0.484935
21	1	0	8.281442	1.501037	-0.567413
22	6	0	-3.529912	3.441811	0.722343
23	6	0	-2.270393	1.289437	0.127422
24	6	0	-2.935628	2.104872	1.204383
25	1	0	-2.751190	4.009674	0.198549
26	1	0	-3.800789	4.034551	1.606362
27	1	0	-2.176895	1.808274	-0.837657
28	1	0	-2.176578	2.288631	1.977528
29	1	0	-3.694790	1.503622	1.719453
30	6	0	0.831416	-2.522366	0.104438
31	6	0	0.766957	-3.132219	1.371368
32	6	0	0.609377	-3.241574	-1.084750
33	6	0	0.319313	-4.455564	1.428417

34	6	0	0.164677	-4.562234	-0.964950
35	6	0	-0.013962	-5.177425	0.277925
36	1	0	0.251459	-4.938138	2.400564
37	1	0	-0.023482	-5.129335	-1.873608
38	6	0	0.669651	2.428910	0.012778
39	6	0	0.426491	3.094211	-1.198967
40	6	0	0.580180	3.071491	1.258605
41	6	0	0.051489	4.440472	-1.132111
42	6	0	0.204449	4.417870	1.265601
43	6	0	-0.058709	5.120778	0.084450
44	1	0	-0.143405	4.972451	-2.060486
45	1	0	0.128692	4.932445	2.220977
46	6	0	0.934220	-2.669327	-2.441392
47	1	0	0.623841	-3.360945	-3.229829
48	1	0	0.430193	-1.716382	-2.618371
49	1	0	2.017807	-2.520722	-2.538059
50	6	0	1.254189	-2.439537	2.619302
51	1	0	0.751079	-1.483732	2.782475
52	1	0	1.068465	-3.064313	3.497459
53	1	0	2.336507	-2.264710	2.558426
54	6	0	-0.533374	-6.592654	0.374972
55	1	0	-0.271620	-7.177511	-0.513102
56	1	0	-0.131421	-7.107668	1.253956
57	1	0	-1.627920	-6.605564	0.462831
58	6	0	0.893498	2.353028	2.548796
59	1	0	0.774434	3.028920	3.400695
60	1	0	0.237322	1.488559	2.705785

61	1	0	1.928578	1.988627	2.559928
62	6	0	0.586677	2.405287	-2.531622
63	1	0	-0.044718	1.512526	-2.610242
64	1	0	0.319336	3.084101	-3.346706
65	1	0	1.626961	2.093496	-2.690411
66	6	0	-0.416543	6.588447	0.123641
67	1	0	0.485787	7.210952	0.187800
68	1	0	-0.960295	6.893306	-0.776327
69	1	0	-1.037272	6.827476	0.993954
70	6	0	-4.758082	3.294333	-0.181789
71	1	0	-5.143261	4.273632	-0.488508
72	1	0	-4.521710	2.733257	-1.094194
73	1	0	-5.569189	2.766116	0.335328
74	44	0	-1.636844	-0.437240	0.173414
75	6	0	-4.169064	-1.114840	0.362293
76	6	0	-3.296962	-2.154298	0.231550
77	1	0	-4.337201	-0.717900	1.362637
78	1	0	-3.172900	-2.651619	-0.727896
79	1	0	-2.859699	-2.624673	1.108541
80	6	0	-5.081480	-0.636942	-0.734384
81	1	0	-5.206791	0.450393	-0.677362
82	1	0	-4.635646	-0.862166	-1.709048
83	6	0	-6.473168	-1.299737	-0.622442
84	1	0	-6.357854	-2.388856	-0.698887
85	1	0	-6.896173	-1.103342	0.372729
86	6	0	-7.441705	-0.802062	-1.700395
87	1	0	-7.054805	-1.010133	-2.705120

88	1	0	-8.418986	-1.289579	-1.609269
89	1	0	-7.599327	0.280597	-1.622903

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SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.155834 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.107439 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.106494 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.241452 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.076978 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.228014 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.578755	0.393392	0.073105
2	17	0	1.579021	0.610300	-2.352165
3	17	0	1.612615	0.304008	2.495736
4	6	0	3.233748	-0.680220	-0.125972
5	1	0	3.391697	-0.960856	-1.171300
6	6	0	-0.445596	0.087101	0.018259
7	7	0	-1.089126	-1.117342	-0.083793
8	7	0	-1.427188	1.042179	0.060334
9	6	0	-2.461200	-0.914232	-0.109054
10	6	0	-2.671955	0.435477	-0.018149
11	6	0	-3.542744	-1.906152	-0.211967

12	6	0	-4.007099	1.054413	-0.008564
13	6	0	-4.920765	-1.316238	-0.202743
14	6	0	-5.139144	0.076451	-0.107098
15	8	0	-3.342824	-3.110835	-0.298862
16	8	0	-4.186544	2.262494	0.072641
17	6	0	-6.012991	-2.183076	-0.293419
18	1	0	-5.820724	-3.248513	-0.366522
19	6	0	-6.445290	0.573006	-0.103864
20	1	0	-6.588554	1.646064	-0.029816
21	6	0	-7.313489	-1.677814	-0.289016
22	1	0	-8.157470	-2.357975	-0.359605
23	6	0	-7.529519	-0.300456	-0.194225
24	1	0	-8.541925	0.093148	-0.190883
25	6	0	2.768272	1.961652	0.177844
26	1	0	2.747945	2.495488	1.127223
27	6	0	-0.423148	-2.409607	-0.129296
28	6	0	-0.115533	-2.970366	-1.380146
29	6	0	-0.185282	-3.084622	1.080479
30	6	0	0.538628	-4.206784	-1.386785
31	6	0	0.465602	-4.320247	1.010511
32	6	0	0.852429	-4.888695	-0.207469
33	1	0	0.790173	-4.654508	-2.345355
34	1	0	0.660626	-4.856578	1.936321
35	6	0	-1.186651	2.472635	0.180661
36	6	0	-1.126696	3.039110	1.465111
37	6	0	-1.098899	3.245227	-0.989650
38	6	0	-0.858227	4.408749	1.551777

39	6	0	-0.830133	4.609176	-0.840099
40	6	0	-0.683614	5.205178	0.416188
41	1	0	-0.801028	4.864166	2.537686
42	1	0	-0.750927	5.222523	-1.734679
43	6	0	-0.648489	-2.540639	2.409104
44	1	0	-0.428921	-3.255084	3.207722
45	1	0	-0.151024	-1.596663	2.655444
46	1	0	-1.731973	-2.367389	2.409753
47	6	0	-0.519507	-2.313716	-2.676309
48	1	0	-0.070480	-1.321632	-2.787484
49	1	0	-0.201788	-2.924980	-3.525930
50	1	0	-1.610188	-2.207052	-2.736027
51	6	0	1.585858	-6.209008	-0.245617
52	1	0	1.259048	-6.872332	0.562428
53	1	0	1.429001	-6.727541	-1.197085
54	1	0	2.668017	-6.062893	-0.127795
55	6	0	-1.348772	2.663075	-2.358295
56	1	0	-1.236536	3.435410	-3.124692
57	1	0	-0.649012	1.854862	-2.590648
58	1	0	-2.371140	2.270581	-2.433114
59	6	0	-1.399304	2.235772	2.712493
60	1	0	-0.661206	1.439888	2.852322
61	1	0	-1.365340	2.882921	3.593666
62	1	0	-2.396974	1.779976	2.675923
63	6	0	-0.356109	6.674523	0.543063
64	1	0	-0.767418	7.098848	1.465091
65	1	0	0.729913	6.835567	0.566609

66	1	0	-0.751237	7.247826	-0.302283
67	6	0	3.833723	0.794876	0.135850
68	1	0	4.261246	0.742294	1.141466
69	1	0	2.778562	2.597078	-0.707743
70	6	0	4.892575	1.093102	-0.952999
71	1	0	5.551803	0.221662	-1.051631
72	1	0	4.379700	1.214822	-1.913872
73	6	0	5.750008	2.327694	-0.638672
74	1	0	5.110147	3.216321	-0.562866
75	1	0	6.221744	2.203053	0.346632
76	6	0	6.832392	2.567301	-1.697187
77	1	0	7.436260	3.449011	-1.454483
78	1	0	7.511164	1.708845	-1.773077
79	1	0	6.388375	2.727370	-2.687131
80	6	0	3.648208	-1.779069	0.835826
81	1	0	2.942294	-2.611973	0.713313
82	1	0	3.555204	-1.440182	1.870947
83	6	0	5.074493	-2.304220	0.569856
84	1	0	5.167736	-2.601133	-0.484388
85	1	0	5.801155	-1.495804	0.729202
86	6	0	5.432580	-3.491062	1.471118
87	1	0	4.746058	-4.331180	1.307889
88	1	0	6.450447	-3.847467	1.275313
89	1	0	5.371510	-3.215385	2.530828

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SCF Energy(B3LYP/SDD-6-31g(d)) = -314.258375 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -314.247723 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -314.246778 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -314.295092 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -314.300411 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -314.293804 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.548599	-0.665554	0.381126
2	1	0	-0.432313	-0.663440	1.467935
3	6	0	0.548586	-0.665440	-0.381176
4	1	0	0.432293	-0.662858	-1.467983
5	6	0	-1.964919	-0.654076	-0.126515
6	1	0	-2.493687	-1.549892	0.236196
7	1	0	-1.966505	-0.716916	-1.223294
8	6	0	-2.757753	0.590171	0.318083
9	1	0	-2.249915	1.488479	-0.057128
10	1	0	-2.732972	0.661099	1.414639
11	6	0	-4.212260	0.574870	-0.161848
12	1	0	-4.749205	-0.299259	0.227093
13	1	0	-4.751165	1.470612	0.167391
14	1	0	-4.268321	0.536254	-1.256779
15	6	0	1.964909	-0.654083	0.126434
16	1	0	1.966527	-0.717137	1.223200

17	1	0	2.493644	-1.549837	-0.236470
18	6	0	2.757752	0.590250	-0.317966
19	1	0	2.732894	0.661391	-1.414506
20	1	0	2.249954	1.488489	0.057463
21	6	0	4.212281	0.574810	0.161860
22	1	0	4.749183	-0.299261	-0.227276
23	1	0	4.751199	1.470596	-0.167244
24	1	0	4.268417	0.535992	1.256780

TS5a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.368972 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.324691 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.323747 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.450502 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.316899 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.437901 A.U.

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

1	44	0	-1.613436	1.224745	0.145311
2	17	0	-1.839577	1.196993	-2.288915
3	17	0	-1.521361	1.333643	2.589317
4	6	0	-1.297366	3.030112	0.071180
5	1	0	-1.245740	3.562201	-0.884701

6	6	0	0.178524	0.193491	0.057905
7	7	0	1.458371	0.661358	-0.009895
8	7	0	0.267101	-1.167134	0.063108
9	6	0	1.610781	-1.575795	-0.000203
10	6	0	2.368395	-0.414664	-0.048097
11	6	0	2.146051	-2.909655	-0.015673
12	6	0	3.805598	-0.382354	-0.120199
13	6	0	3.618313	-2.927045	-0.090051
14	6	0	4.401869	-1.732614	-0.139505
15	8	0	1.436544	-3.949988	0.027479
16	8	0	4.485982	0.675575	-0.160912
17	6	0	4.275333	-4.175487	-0.113266
18	1	0	3.651935	-5.064062	-0.074490
19	6	0	5.806681	-1.842389	-0.209498
20	1	0	6.374236	-0.917088	-0.245587
21	6	0	5.655455	-4.257674	-0.182435
22	1	0	6.144120	-5.230071	-0.199335
23	6	0	6.429231	-3.078761	-0.231056
24	1	0	7.514408	-3.142344	-0.285453
25	6	0	-3.548248	2.605856	0.199685
26	6	0	-3.826076	1.254366	0.457409
27	6	0	-4.560841	0.346248	-0.508326
28	1	0	-3.514869	3.303784	1.030990
29	1	0	-4.419987	0.693710	-1.535492
30	1	0	-3.907541	0.976525	1.507800
31	1	0	-4.140578	-0.667152	-0.459315
32	6	0	1.838488	2.054158	-0.044160

33	6	0	2.126935	2.712982	1.162206
34	6	0	1.965094	2.695934	-1.286832
35	6	0	2.466076	4.068554	1.102758
36	6	0	2.308076	4.052310	-1.291287
37	6	0	2.546570	4.759632	-0.109717
38	1	0	2.691249	4.589659	2.031517
39	1	0	2.409451	4.560302	-2.248661
40	6	0	-0.885262	-2.037642	0.120574
41	6	0	-1.367119	-2.453918	1.374534
42	6	0	-1.450171	-2.504897	-1.080071
43	6	0	-2.517451	-3.250641	1.401563
44	6	0	-2.596177	-3.302171	-0.996512
45	6	0	-3.158103	-3.666293	0.231280
46	1	0	-2.902463	-3.574765	2.366474
47	1	0	-3.044460	-3.665915	-1.919108
48	6	0	2.126803	1.977421	2.477953
49	1	0	2.854779	1.157892	2.453903
50	1	0	2.403405	2.653297	3.294006
51	1	0	1.141985	1.555226	2.703269
52	6	0	1.792250	1.942895	-2.581604
53	1	0	0.781192	1.533724	-2.680766
54	1	0	1.978567	2.603054	-3.435309
55	1	0	2.503480	1.110101	-2.635082
56	6	0	2.885416	6.232989	-0.141695
57	1	0	3.541214	6.511106	0.691304
58	1	0	3.389960	6.507395	-1.075090
59	1	0	1.983168	6.856111	-0.065325

60	6	0	-0.797361	-2.237213	-2.411705
61	1	0	-1.385198	-2.681784	-3.221461
62	1	0	-0.704091	-1.165898	-2.609762
63	1	0	0.203523	-2.684903	-2.429672
64	6	0	-0.621024	-2.142139	2.646587
65	1	0	-0.527909	-1.065286	2.812412
66	1	0	-1.139955	-2.574151	3.508572
67	1	0	0.385393	-2.575482	2.601125
68	6	0	-4.417110	-4.501499	0.289246
69	1	0	-4.469875	-5.205191	-0.549466
70	1	0	-4.472472	-5.078145	1.219378
71	1	0	-5.318352	-3.874018	0.242108
72	6	0	-6.063365	0.273431	-0.165237
73	1	0	-6.499526	1.280179	-0.232636
74	1	0	-6.186477	-0.046145	0.879337
75	1	0	-3.735990	3.014129	-0.789810
76	6	0	-6.827187	-0.683569	-1.086750
77	1	0	-6.428098	-1.702739	-1.012628
78	1	0	-7.893357	-0.720729	-0.831444
79	1	0	-6.742937	-0.373153	-2.135483
80	1	0	-1.118032	3.623028	0.974329

TS7a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2749.222976 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2749.174674 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2749.173729 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2749.309187 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2749.196902 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2749.294475 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.598889	0.481429	0.140300
2	17	0	1.695134	0.853856	-2.271782
3	17	0	1.578728	0.349437	2.590469
4	6	0	2.701841	-0.975287	-0.048066
5	1	0	3.030408	-1.187751	-1.076711
6	6	0	-0.440953	0.070508	0.037401
7	7	0	-1.128568	-1.102389	-0.061209
8	7	0	-1.381410	1.061233	0.043239
9	6	0	-2.674415	0.519007	-0.054632
10	6	0	-2.515866	-0.856994	-0.121705
11	6	0	-3.939106	1.202532	-0.087542
12	6	0	-3.598281	-1.799545	-0.231653
13	6	0	-5.080709	0.276129	-0.196936
14	6	0	-4.919293	-1.142237	-0.265232
15	8	0	-4.061534	2.455320	-0.034176
16	8	0	-3.444801	-3.047519	-0.290219
17	6	0	-6.383297	0.817126	-0.237133
18	1	0	-6.472414	1.898272	-0.183938
19	6	0	-6.068300	-1.954250	-0.369885

20	1	0	-5.912682	-3.027972	-0.420028
21	6	0	-7.495783	-0.000204	-0.339815
22	1	0	-8.492563	0.435928	-0.369015
23	6	0	-7.336641	-1.400629	-0.406913
24	1	0	-8.210749	-2.044068	-0.487879
25	6	0	3.979431	0.860826	0.269379
26	6	0	3.196709	2.021843	0.398329
27	1	0	4.305709	0.402430	1.201240
28	1	0	2.969861	2.414668	1.384782
29	6	0	-0.543648	-2.420878	-0.080024
30	6	0	-0.438932	-3.133434	1.125297
31	6	0	-0.163642	-2.982782	-1.308901
32	6	0	0.115791	-4.417299	1.081502
33	6	0	0.395073	-4.265933	-1.297201
34	6	0	0.549422	-4.996030	-0.115515
35	1	0	0.196834	-4.981660	2.008722
36	1	0	0.692038	-4.712916	-2.244215
37	6	0	-1.061982	2.468107	0.149826
38	6	0	-0.969597	3.052402	1.425910
39	6	0	-0.932958	3.234596	-1.022580
40	6	0	-0.590388	4.397108	1.503606
41	6	0	-0.554977	4.574130	-0.888717
42	6	0	-0.351303	5.165787	0.361415
43	1	0	-0.507074	4.857518	2.486233
44	1	0	-0.441496	5.174022	-1.789667
45	6	0	-0.937698	-2.554232	2.424975
46	1	0	-2.011501	-2.343470	2.362230

47	1	0	-0.778146	-3.261264	3.245828
48	1	0	-0.421066	-1.620057	2.672278
49	6	0	-0.400978	-2.258894	-2.610386
50	1	0	0.138141	-1.306346	-2.654068
51	1	0	-0.077099	-2.875321	-3.455663
52	1	0	-1.469197	-2.045102	-2.736501
53	6	0	1.173575	-6.373373	-0.129784
54	1	0	0.986826	-6.887097	-1.079616
55	1	0	2.263523	-6.323759	0.003126
56	1	0	0.777350	-7.000339	0.677021
57	6	0	-1.302296	2.675703	-2.372034
58	1	0	-1.055692	3.390336	-3.164000
59	1	0	-0.777981	1.741835	-2.585640
60	1	0	-2.382983	2.488835	-2.400738
61	6	0	-1.374061	2.299485	2.667843
62	1	0	-0.789590	1.386298	2.803367
63	1	0	-1.232992	2.924634	3.555645
64	1	0	-2.435417	2.029160	2.605331
65	6	0	0.096749	6.605312	0.474049
66	1	0	-0.280400	7.208807	-0.359620
67	1	0	-0.251913	7.061453	1.407577
68	1	0	1.192680	6.686137	0.462516
69	1	0	3.113847	2.701865	-0.446827
70	6	0	4.898815	0.698288	-0.929878
71	1	0	5.197250	-0.348321	-1.060059
72	1	0	4.356471	0.990591	-1.835055
73	6	0	6.171015	1.555231	-0.775472

74	1	0	5.884121	2.610486	-0.678248
75	1	0	6.686037	1.289738	0.159375
76	6	0	7.134117	1.387384	-1.955837
77	1	0	8.028926	2.009530	-1.833193
78	1	0	7.462927	0.345183	-2.054566
79	1	0	6.652942	1.672551	-2.899235
80	6	0	3.063367	-2.062407	0.932912
81	1	0	3.113086	-1.669045	1.952590
82	1	0	2.180673	-2.717943	0.926346
83	6	0	4.301813	-2.920351	0.589501
84	1	0	4.132928	-3.934278	0.976350
85	1	0	4.386386	-3.026259	-0.501800
86	6	0	5.624331	-2.401670	1.168387
87	1	0	6.454247	-3.077574	0.926756
88	1	0	5.884317	-1.410867	0.781011
89	1	0	5.565534	-2.322487	2.261080

1_pentene

SCF Energy(B3LYP/SDD-6-31g(d)) = -196.397316 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -196.390771 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -196.389827 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -196.427117 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -196.421026 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -196.427089 A.U.

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.485212	-0.214993	-0.304573
2	1	0	-2.455155	-1.226309	-0.706183
3	1	0	-3.429850	0.314686	-0.396238
4	6	0	-1.419213	0.340260	0.273036
5	1	0	-1.498497	1.358678	0.659233
6	6	0	-0.074445	-0.314691	0.432564
7	1	0	0.174501	-0.382145	1.503412
8	1	0	-0.117915	-1.346144	0.057467
9	6	0	1.056941	0.448473	-0.282927
10	1	0	1.079005	1.485649	0.080070
11	1	0	0.826119	0.504925	-1.354802
12	6	0	2.431707	-0.195396	-0.079188
13	1	0	2.448946	-1.223382	-0.461662
14	1	0	3.216054	0.366239	-0.599120
15	1	0	2.698133	-0.234119	0.984348

17a

SCF Energy(B3LYP/SDD-6-31g(d)) =	-2749.228168 A.U.
SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction =	-2749.178389 A.U.
Enthalpies(B3LYP/SDD-6-31g(d)) =	-2749.177444 A.U.
Gibbs Free Energy(B3LYP/SDD-6-31g(d)) =	-2749.316801 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution =	-2749.200604 A.U.
SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction =	-2749.302301 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.661284	-0.488555	2.620574
2	17	0	-1.821933	-0.541679	-2.265498
3	6	0	0.374683	-0.062855	0.057635
4	7	0	1.229210	-1.133718	0.022308
5	7	0	1.166845	1.046439	-0.024728
6	6	0	2.562104	-0.707235	-0.085913
7	6	0	2.526080	0.678188	-0.118727
8	6	0	3.758228	-1.501603	-0.153756
9	6	0	3.688144	1.520558	-0.233129
10	6	0	4.977606	-0.681359	-0.262634
11	6	0	4.943773	0.746869	-0.300174
12	8	0	3.765162	-2.761735	-0.125241
13	8	0	3.650066	2.777970	-0.274708
14	6	0	6.225219	-1.336623	-0.334419
15	1	0	6.217032	-2.422296	-0.303990
16	6	0	6.159752	1.453959	-0.408178
17	1	0	6.101028	2.538120	-0.435200
18	6	0	7.405415	-0.620781	-0.439064
19	1	0	8.358221	-1.144159	-0.492866
20	6	0	7.372375	0.789337	-0.476387
21	1	0	8.299738	1.353096	-0.558946
22	6	0	-3.476112	3.500030	0.674320
23	6	0	-2.247626	1.320573	0.109746

24	6	0	-2.893492	2.166347	1.178434
25	1	0	-2.693309	4.047192	0.135266
26	1	0	-3.737888	4.115850	1.546218
27	1	0	-2.141465	1.828999	-0.860084
28	1	0	-2.122206	2.362034	1.935552
29	1	0	-3.654831	1.585563	1.713963
30	6	0	0.782477	-2.506275	0.104383
31	6	0	0.685168	-3.118854	1.367903
32	6	0	0.543443	-3.225919	-1.081440
33	6	0	0.179163	-4.421709	1.426631
34	6	0	0.039945	-4.526052	-0.966581
35	6	0	-0.177100	-5.129991	0.275292
36	1	0	0.089092	-4.900819	2.399601
37	1	0	-0.159148	-5.087889	-1.877153
38	6	0	0.725315	2.417362	0.009894
39	6	0	0.481066	3.087166	-1.199088
40	6	0	0.640706	3.070875	1.250293
41	6	0	0.102625	4.432954	-1.137790
42	6	0	0.261892	4.416675	1.257914
43	6	0	-0.007086	5.115925	0.076658
44	1	0	-0.087772	4.963873	-2.068687
45	1	0	0.195497	4.935007	2.212898
46	6	0	0.933437	-2.673416	-2.427530
47	1	0	0.606138	-3.345405	-3.227597
48	1	0	0.493450	-1.690941	-2.611162
49	1	0	2.026070	-2.586312	-2.475977
50	6	0	1.219614	-2.449868	2.608077

51	1	0	0.770945	-1.467554	2.770462
52	1	0	1.014895	-3.062721	3.491842
53	1	0	2.306382	-2.330247	2.516477
54	6	0	-0.759413	-6.521975	0.370006
55	1	0	-0.504003	-7.123599	-0.509751
56	1	0	-0.394537	-7.049047	1.258968
57	1	0	-1.855952	-6.494232	0.436933
58	6	0	0.980609	2.357679	2.535486
59	1	0	0.883944	3.037319	3.388737
60	1	0	0.327130	1.494479	2.707822
61	1	0	2.013793	1.991472	2.509928
62	6	0	0.664166	2.396357	-2.526499
63	1	0	0.042622	1.497463	-2.608970
64	1	0	0.405391	3.070614	-3.349678
65	1	0	1.710443	2.092970	-2.652682
66	6	0	-0.362383	6.585425	0.112478
67	1	0	0.539253	7.210526	0.171721
68	1	0	-0.909517	6.888128	-0.787258
69	1	0	-0.982076	6.829138	0.983345
70	6	0	-4.709467	3.347177	-0.222457
71	1	0	-5.086384	4.323427	-0.551546
72	1	0	-4.480001	2.761796	-1.121022
73	1	0	-5.524587	2.837667	0.308209
74	44	0	-1.633880	-0.409025	0.174897
75	6	0	-4.152331	-1.074649	0.394880
76	6	0	-3.293736	-2.124782	0.266454
77	1	0	-4.307608	-0.663519	1.391241

78	1	0	-3.175587	-2.628741	-0.690272
79	1	0	-2.842593	-2.585896	1.141067
80	6	0	-5.065958	-0.598847	-0.704059
81	1	0	-5.196522	0.487951	-0.643426
82	1	0	-4.609489	-0.815110	-1.676104
83	6	0	-6.454188	-1.268196	-0.609185
84	1	0	-6.333052	-2.356519	-0.691561
85	1	0	-6.887426	-1.081369	0.383994
86	6	0	-7.418518	-0.770018	-1.691107
87	1	0	-7.021003	-0.968662	-2.693819
88	1	0	-8.395603	-1.262090	-1.613063
89	1	0	-7.580879	0.311893	-1.608867

15a

SCF Energy(B3LYP/SDD-6-31g(d)) = -2631.383210 A.U.

SCF Energy(B3LYP/SDD-6-31g(d)) with thermal correction = -2631.339078 A.U.

Enthalpies(B3LYP/SDD-6-31g(d)) = -2631.338134 A.U.

Gibbs Free Energy(B3LYP/SDD-6-31g(d)) = -2631.464307 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution = -2631.335027 A.U.

SCF Energy(M06/SDD-6-311+G(d,p)) in solution with quasiharmonic correction = -2631.452098 A.U.

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

1	44	0	-1.606789	1.230096	0.146225

2	17	0	-1.824473	1.247371	-2.276874
3	17	0	-1.423356	1.378914	2.574491
4	6	0	-2.121296	3.131077	0.145410
5	1	0	-1.991750	3.645669	-0.806460
6	6	0	0.161637	0.173169	0.053265
7	7	0	1.417011	0.691854	-0.013289
8	7	0	0.290104	-1.180569	0.059735
9	6	0	2.366595	-0.347938	-0.048112
10	6	0	1.651644	-1.536442	-0.001024
11	6	0	3.800810	-0.258021	-0.114318
12	6	0	2.239880	-2.848874	-0.014599
13	6	0	4.449805	-1.583028	-0.133842
14	6	0	3.712782	-2.806549	-0.086697
15	8	0	4.436414	0.827879	-0.147955
16	8	0	1.575572	-3.917374	0.028809
17	6	0	5.858058	-1.637782	-0.200159
18	1	0	6.389464	-0.691198	-0.234070
19	6	0	4.417749	-4.028479	-0.108613
20	1	0	3.829290	-4.940568	-0.071321
21	6	0	6.527895	-2.849098	-0.220871
22	1	0	7.614805	-2.870667	-0.272589
23	6	0	5.800202	-4.056976	-0.174620
24	1	0	6.326151	-5.009680	-0.190663
25	6	0	-3.521451	0.824839	0.443545
26	6	0	-4.400669	0.041146	-0.514091
27	1	0	-3.703791	0.554612	1.487316
28	1	0	-4.059751	-1.002714	-0.508425

29	1	0	-4.273132	0.405372	-1.537298
30	6	0	1.715971	2.107656	-0.054169
31	6	0	1.792964	2.751309	-1.300557
32	6	0	1.988353	2.783932	1.146939
33	6	0	2.030091	4.130035	-1.309667
34	6	0	2.219704	4.161412	1.081569
35	6	0	2.221306	4.856216	-0.131308
36	1	0	2.086874	4.641277	-2.268815
37	1	0	2.425189	4.698032	2.005872
38	6	0	-0.818933	-2.108007	0.108905
39	6	0	-1.281262	-2.554792	1.357904
40	6	0	-1.354468	-2.592485	-1.096911
41	6	0	-2.376296	-3.425923	1.375215
42	6	0	-2.444200	-3.465891	-1.023137
43	6	0	-2.981803	-3.878429	0.200021
44	1	0	-2.745856	-3.777027	2.336765
45	1	0	-2.868414	-3.847249	-1.950055
46	6	0	2.116638	2.046582	2.455013
47	1	0	2.320833	2.748306	3.270408
48	1	0	1.204578	1.496328	2.702043
49	1	0	2.950163	1.335998	2.399647
50	6	0	1.705862	1.981318	-2.594053
51	1	0	0.734097	1.492871	-2.712504
52	1	0	1.853642	2.652466	-3.446569
53	1	0	2.486008	1.211486	-2.628470
54	6	0	2.436716	6.352220	-0.167746
55	1	0	3.076934	6.685132	0.657258

56	1	0	2.904564	6.666829	-1.107589
57	1	0	1.486007	6.896503	-0.080199
58	6	0	-0.738570	-2.245059	-2.428104
59	1	0	-1.274394	-2.748911	-3.239258
60	1	0	-0.769268	-1.167781	-2.618450
61	1	0	0.307534	-2.571961	-2.456601
62	6	0	-0.581454	-2.177668	2.638779
63	1	0	-0.595363	-1.096447	2.807871
64	1	0	-1.064458	-2.662309	3.493704
65	1	0	0.463890	-2.507343	2.607073
66	6	0	-4.182316	-4.796338	0.247366
67	1	0	-4.212747	-5.367704	1.181816
68	1	0	-5.122877	-4.231438	0.180662
69	1	0	-4.174776	-5.509128	-0.585350
70	6	0	-5.887702	0.078910	-0.108690
71	1	0	-6.246972	1.118222	-0.120631
72	1	0	-5.993209	-0.270551	0.928428
73	6	0	-3.524175	2.423007	0.286486
74	1	0	-4.108601	2.650547	-0.606445
75	1	0	-3.966882	2.798915	1.210950
76	6	0	-6.768782	-0.774001	-1.028273
77	1	0	-6.454606	-1.825055	-1.008706
78	1	0	-7.823025	-0.733160	-0.727504
79	1	0	-6.702407	-0.430630	-2.068058
80	1	0	-1.829330	3.702545	1.025767

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