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# Cover Page for Supporting Information

***Manuscript Title:***

$sp^2$-sp Cross-Carbanion Coupling at a Rare-Earth Center Leading to the Formation of Carbon-Carbon Double Bonds

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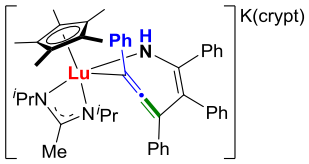
***Contents:***

## 1) Experimental Details and Characterization Data

Unless otherwise noted, all starting materials were commercially available and were used without further purification. Solvents were purified by Mbraun SPS-800 Solvent Purification System and dried over fresh Na chips and molecular sieves in a glovebox. THF-$d_8$ was purchased from Cambridge Isotope Laboratory, degassed, and vacuum transferred to 4 Å molecular sieves. All reactions were operated under an argon atmosphere in a glovebox. The argon in the glove box was constantly circulated through a copper/molecular sieves catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by an $O_2/H_2O$ Combi-Analyzer to ensure that both were always below 0.1 ppm.

Organometallic samples for NMR spectroscopic measurements were prepared in a glovebox using J. Young valve NMR tubes (Wilmad 528-JY). $^1$H and $^{13}$C NMR spectra were recorded on a Bruker Avance 400 MHz, 500 MHz or 600 MHz spectrometer. $^1$H and $^{13}$C NMR spectra were reported with reference to solvent resonances of THF-$d_8$ at 3.58 and 67.57 ppm, respectively. Elemental analyses were performed on a Vario MICRO cube elemental analyzer.

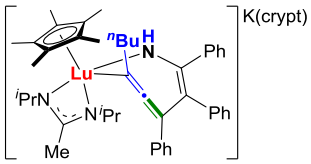
**1a** and **1b** were prepared following the literature procedure.[1]



**3a**

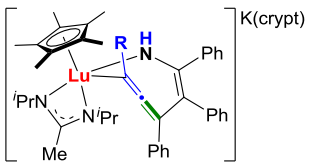
**Synthesis of 3a:** In the glovebox, to the THF solution of **1a** (52.3 mg, 0.050 mmol), PhCN (5.1 μL, 0.050 mmol) was added at −35 ℃. The reaction mixture was stirred at room temperature for 10 min before it was cooled to −35 ℃ again. After that, phenylacetylene (5.5 μL, 0.050 mmol). The reaction mixture was then stirred at room temperature for 2 h, resulting in a dark orange solution. After removal of the solvent under reduced pressure, the residue was stirred after adding hexane (10 mL) to yield orange participation. The mixture was filtered and the solid was washed with cooled $Et_2O$ thrice to obtain orange powder **3a** (56.8 mg, 0.042 mmol, 86% yield). The suitable crystals for X-ray diffraction of **3a·THF** could be obtained through gradually diffusing hexane into its THF solution at room temperature. $^1$H NMR (600 MHz, THF-$d_8$) of **3a·THF**: $\delta$ 0.84 (s, 3H, CC$H_3$), 0.96 (d, $J$ = 6.3 Hz, 6H, (C$H_3$)$_2$CH), 1.37 (d, $J$ = 6.5 Hz, 3H, (C$H_3$)$_2$CH), 1.48 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.76-1.80 (m, 4H, $\beta$-C$H_2$ for THF), 1.91 (s, 15H, C$_5$$Me_5$), 2.50 (t, $J$ = 4.5 Hz, 12H, NC$H_2$CH$_2$O), 3.24-3.29 (m, 1H, (CH$_3$)$_2$C$H$), 3.33-3.37 (m, 1H, (CH$_3$)$_2$C$H$), 3.48 (t, $J$ = 4.6 Hz, 12H, NCH$_2$C$H_2$O), 3.52 (s, 12H, OC$H_2$C$H_2$O), 3.61-3.63 (m, 4H, $\alpha$-C$H_2$ for THF), 4.55 (s, 1H, N$H$), 6.21-6.24 (m, 1H, Ar), 6.44-6.47 (m, 3H, Ar), 6.67-6.73 (m, 5H, Ar), 6.92-6.94 (m, 1H, Ar), 6.99-7.04 (m, 6H, Ar), 7.14-7.19 (m, 4H, Ar). $^{13}$C NMR of **3a·THF** (151 MHz, THF-$d_8$): $\delta$ 11.7 (C$C$H$_3$), 12.9 (C$_5$$Me_5$),

26.0 (*β-C* for THF), 26.6 ((*C*H$_3$)$_2$CH), 27.0 ((*C*H$_3$)$_2$CH), 27.1 ((*C*H$_3$)$_2$CH), 27.3 ((*C*H$_3$)$_2$CH), 47.5 ((CH$_3$)$_2$*C*H), 47.8 ((CH$_3$)$_2$*C*H), 54.9 (N*C*H$_2$CH$_2$O), 68.4 (*α-C* for THF), 68.6 (NCH$_2$*C*H$_2$O), 71.5 (O*C*H$_2$*C*H$_2$O), 94.2 (LuC=C=*C*), 100.3 (LuNH-C=*C*), 113.4 (*C*$_5$Me$_5$), 118.9 (Ar), 120.7 (Ar), 121.3 (Ar), 125.1 (Ar), 126.4 (Ar), 126.8 (Ar), 127.7 (Ar), 127.9 (Ar), 127.9 (Ar), 127.9 (Ar), 130.6 (Ar), 130.9 (Lu*C*), 131.3 (Ar), 145.0 (Ar), 146.4 (Ar), 147.4 (Ar), 151.8 (Ar), 155.6 (LuNH-*C*), 160.5 (LuC=*C*), 171.2 (N*C*N). Anal. Calcd for C$_{65}$H$_{89}$KLuN$_5$O$_6$ of **3a**: C, 62.43; H, 7.17; N, 5.60; Found: C, 61.88; H, 7.39; N, 5.54.



**3b**

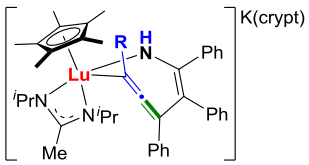
**Synthesis of 3b:** This complex was prepared by an analogous procedure as the synthesis of **3a**, except that phenylacetylene (5.5 μL, 0.050 mmol) was replaced by 1-hexyne (5.7 μL, 0.050 mmol). **3b**, yellow solid. Yield: 81% (49.8 mg, 0.041 mmol). The suitable crystals for X-ray diffraction of **3b** could be obtained through gradually diffusing hexane into its THF solution at room temperature. $^1$H NMR (400 MHz, THF-*d*$_8$) of **3b**: *δ* 0.81 (s, 3H, CC*H*$_3$), 0.87-0.92 (m, 9H, (C*H*$_3$)$_2$CH and C*H*$_3$(CH$_2$)$_3$), 1.27-1.30 (m, 6H, (C*H*$_3$)$_2$CH), 1.42-1.55 (m, 2H, CH$_3$C*H*$_2$(CH$_2$)$_2$), 1.58-1.65 (m, 2H, CH$_3$CH$_2$C*H*$_2$CH$_2$), 1.99 (s, 15H, C$_5$*Me*$_5$), 2.42 (t, *J* = 6.7 Hz, 2H, CH$_3$(CH$_2$)$_2$C*H*$_2$), 2.53 (t, *J* = 4.7 Hz, 12H, NC*H*$_2$CH$_2$O), 3.25-3.33 (m, 2H, (CH$_3$)$_2$C*H*), 3.51 (t, *J* = 4.7 Hz, 12H, NCH$_2$C*H*$_2$O), 3.55 (s, 12H, OC*H*$_2$C*H*$_2$O), 4.30 (s, 1H, N*H*), 6.16-6.20 (m, 1H, Ar), 6.33-6.37 (m, 1H, Ar), 6.41-6.45 (m, 2H, Ar), 6.64-6.66 (m, 4H, Ar), 6.87-6.91 (m, 1H, Ar), 6.94-6.98 (m, 2H, Ar), 7.14-7.16 (br, 4H, Ar). $^{13}$C NMR (151 MHz, THF-*d*$_8$) of **3b**: *δ* 11.6 (C*C*H$_3$), 13.0 (C$_5$*Me*$_5$), 15.0 (*C*H$_3$(CH$_2$)$_3$), 23.3 (CH$_3$*C*H$_2$(CH$_2$)$_2$), 27.0 ((*C*H$_3$)$_2$CH), 27.1 ((*C*H$_3$)$_2$CH), 30.7 (CH$_3$CH$_2$*C*H$_2$CH$_2$), 37.1 (CH$_3$(CH$_2$)$_2$*C*H$_2$), 47.4 ((CH$_3$)$_2$*C*H), 47.6 ((CH$_3$)$_2$*C*H), 54.9 (N*C*H$_2$CH$_2$O), 68.6 (NCH$_2$*C*H$_2$O), 71.5 (O*C*H$_2$*C*H$_2$O), 94.0 (LuC=C=*C*), 101.3 (LuNH-C=*C*), 112.8 (*C*$_5$Me$_5$), 118.6 (Ar), 119.5 (Ar), 124.8 (Ar), 126.3 (Ar), 126.6 (Ar), 127.1 (Ar), 127.7 (Ar), 127.8 (Ar), 130.7 (Lu*C*), 131.0 (Ar), 147.7 (Ar), 148.3 (Ar), 152.0 (Ar), 155.5 (LuNH-*C*), 159.4 (LuC=*C*), 171.0 (N*C*N). Anal. Calcd for C$_{63}$H$_{93}$KLuN$_5$O$_6$ of **3b**: C, 61.49; H, 7.62; N, 5.69; Found: C, 61.16; H, 7.58; N, 5.49.



**3c**, R = 4-Br-C$_6$H$_4$

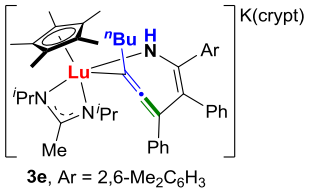
**Synthesis of 3c:** This complex was prepared by an analogous procedure as the synthesis of **3a**, except that phenylacetylene (5.5 μL, 0.050 mmol) was replaced by 4-bromophenylacetylene (9.1 mg, 0.050 mmol). **3c**, orange solid. Yield: 75% (49.8 mg, 0.038 mmol). The suitable crystals for X-ray diffraction of **3c·THF** could be

obtained through gradually diffusing hexane into its THF solution at room temperature. $^{1}$H NMR (400 MHz, THF-$d_8$) of **3c**: $\delta$ 0.83 (s, 3H, CC$H_3$), 0.95 (d, $J$ = 6.2 Hz, 6H, (C$H_3$)$_2$CH), 1.35 (d, $J$ = 6.5 Hz, 3H, (C$H_3$)$_2$CH), 1.44 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.91 (s, 15H, C$_5$*Me*$_5$), 2.51 (t, $J$ = 4.1 Hz, 12H, NC$H_2$CH$_2$O), 3.21-3.27 (m, 1H, (CH$_3$)$_2$C$H$), 3.31-3.37 (m, 1H, (CH$_3$)$_2$C$H$), 3.50 (t, $J$ = 4.2 Hz, 12H, NCH$_2$C$H_2$O), 3.54 (s, 12H, OC$H_2$C$H_2$O), 4.55 (s, 1H, N$H$), 6.21-6.25 (m, 1H, Ar), 6.44-6.50 (m, 3H, Ar), 6.66-6.75 (m, 4H, Ar), 6.92-6.95 (m, 3H, Ar), 6.98-7.02 (m, 2H, Ar), 7.13-7.18 (m, 6H, Ar). $^{13}$C NMR (151 MHz, THF-$d_8$) of **3c**: $\delta$ 11.7 (C$C$H$_3$), 12.9 (C$_5$*Me*$_5$), 26.9 ((*C*H$_3$)$_2$CH), 27.1 ((*C*H$_3$)$_2$CH), 27.2 ((*C*H$_3$)$_2$CH), 47.5 ((CH$_3$)$_2$*C*H), 47.8 ((CH$_3$)$_2$*C*H), 54.9 (N*C*H$_2$CH$_2$O), 68.6 (NCH$_2$*C*H$_2$O), 71.5 (O*C*H$_2$*C*H$_2$O), 95.2 (LuC=C=*C*), 99.8 (LuNH-C=*C*), 113.5 (*C*$_5$Me$_5$), 114.1 (Ar), 119.1 (Ar), 121.1 (Ar), 125.2 (Ar), 126.4 (Ar), 126.9 (Ar), 127.9 (Ar), 128.0 (Ar), 129.4 (Ar), 130.4 (Lu*C*), 130.5 (Ar), 130.7 (Ar), 131.3 (Ar), 144.8 (Ar), 145.9 (Ar), 147.2 (Ar), 151.6 (Ar), 155.7 (LuNH-*C*), 161.9 (LuC=*C*), 171.2 (N*C*N). Anal. Calcd for C$_{69}$H$_{96}$BrKLuN$_5$O$_7$ of **3c·THF**: C, 59.13; H, 6.90; N, 5.00; Found: C, 58.60; H, 6.85; N, 4.97.



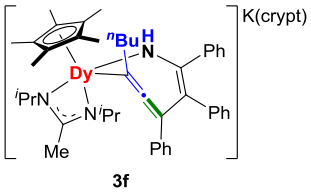
**3d**, R = 4-(CN)-C$_6$H$_4$

**Synthesis of 3d:** This complex was prepared by an analogous procedure as the synthesis of **3a**, except that phenylacetylene (5.5 μL, 0.050 mmol) was replaced by 4-ethynylbenzonitrile (6.4 mg, 0.050 mmol). **3d**, brown solid. Yield: 80% (51.0 mg, 0.040 mmol). The suitable crystals for X-ray diffraction of **3d** could be obtained through gradually diffusing hexane into its THF solution at room temperature. $^{1}$H NMR (400 MHz, THF-$d_8$) of **3d**: $\delta$ 0.83 (s, 3H, CC$H_3$), 0.94-0.97 (m, 6H, (C$H_3$)$_2$CH), 1.37 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.46 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.88 (s, 15H, C$_5$*Me*$_5$), 2.52 (t, $J$ = 4.7 Hz, 12H, NC$H_2$CH$_2$O), 3.19-3.25 (m, 1H, (CH$_3$)$_2$C$H$), 3.31-3.38 (m, 1H, (CH$_3$)$_2$C$H$), 3.51 (t, $J$ = 4.7 Hz, 12H, NCH$_2$C$H_2$O), 3.55 (s, 12H, OC$H_2$C$H_2$O), 4.62 (s, 1H, N$H$), 6.23-6.27 (m, 1H, Ar), 6.44-6.53 (m, 3H, Ar), 6.64-6.66 (m, 2H, Ar), 6.73-6.77 (m, 2H, Ar), 6.93-7.03 (m, 5H, Ar), 7.16-7.18 (m, 4H, Ar), 7.26-7.28 (m, 2H, Ar). $^{13}$C NMR (151 MHz, THF-$d_8$) of **3d**: $\delta$ 11.8 (C$C$H$_3$), 12.8 (C$_5$*Me*$_5$), 26.9 ((*C*H$_3$)$_2$CH), 27.1 ((*C*H$_3$)$_2$CH), 27.3 ((*C*H$_3$)$_2$CH), 47.5 ((CH$_3$)$_2$*C*H), 47.9 ((CH$_3$)$_2$*C*H), 54.9 (N*C*H$_2$CH$_2$O), 68.6 (NCH$_2$*C*H$_2$O), 71.5 (O*C*H$_2$*C*H$_2$O), 95.3 (LuC=C=*C*), 100.0 (LuNH-C=*C*), 103.1 (Ar*C*N), 113.7 (*C*$_5$Me$_5$), 119.4 (Ar), 121.3 (Ar), 121.5 (Ar), 125.3 (Ar), 126.5 (Ar), 126.7 (Ar), 127.0 (Ar), 128.0 (Ar), 128.2 (Ar), 130.4 (Ar), 130.6 (Lu*C*), 131.4 (Ar), 131.6 (Ar), 145.3 (Ar), 147.0 (Ar), 150.9 (Ar), 151.4 (Ar), 155.7 (LuNH-*C*), 158.8 (LuC=*C*), 171.3 (N*C*N).



**3e**, Ar = 2,6-$Me_2C_6H_3$

**Synthesis of 3e:** This complex was prepared by an analogous procedure as the synthesis of **3a**, except that PhCN (5.1 μL, 0.050 mmol) and phenylacetylene (5.5 μL, 0.050 mmol) were replaced by 2,6-$Me_2C_6H_3CN$ (6.6 mg, 0.050 mmol) and 1-hexyne (5.7 μL, 0.050 mmol), respectively. **3e**, green solid. Yield: 77% (48.4 mg, 0.039 mmol). $^1$H NMR (400 MHz, THF-$d_8$) of **3e**: $\delta$ 0.87-0.92 (m, 6H, C$H_3$(C$H_2$)$_3$ and (C$H_3$)$_2$CH), 0.96-0.99 (m, 6H, (C$H_3$)$_2$CH and CC$H_3$), 1.03 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.35 (d, $J$ = 6.4 Hz, 3H, (C$H_3$)$_2$CH), 1.47-1.62 (m, 4H, $CH_3CH_2CH_2CH_2$ and $CH_3CH_2CH_2CH_2$), 1.72 (s, 3H, C$H_3$ in 2,6-$Me_2C_6H_3$, overlaps with THF-$d_8$), 1.95 (s, 15H, $C_5Me_5$), 2.33-2.46 (m, 2H, $CH_3(CH_2)_2CH_2$), 2.51-2.54 (m, 12H, $NCH_2CH_2O$), 2.58 (s, 3H, C$H_3$ in 2,6-$Me_2C_6H_3$), 3.06-3.12 (m, 1H, $(CH_3)_2CH$), 3.49-3.52 (m, 13H, $NCH_2CH_2O$ and $(CH_3)_2CH$), 3.54 (s, 12H, $OCH_2CH_2O$), 3.86 (s, 1H, N$H$), 6.15-6.18 (m, 1H, Ar), 6.36-6.40 (m, 1H, Ar), 6.43-6.46 (m, 2H, Ar), 6.54-6.56 (m, 1H, Ar), 6.69-6.78 (m, 5H, Ar), 6.85-6.87 (m, 1H, Ar), 7.16 (br, 2H, Ar). $^{13}$C NMR (151 MHz, THF-$d_8$) of **3e**: $\delta$ 11.9 (C$CH_3$), 12.9 ($C_5Me_5$), 14.9 ($CH_3(CH_2)_3$), 19.8 ($CH_3$ in 2,6-$Me_2C_6H_3$), 21.7 ($CH_3$ in 2,6-$Me_2C_6H_3$), 23.5 ($CH_3CH_2(CH_2)_2$), 26.3 (($CH_3$)$_2$CH), 26.9 (($CH_3$)$_2$CH), 27.3 (($CH_3$)$_2$CH), 27.4 (($CH_3$)$_2$CH), 31.0 ($CH_3CH_2CH_2CH_2$), 37.3 ($CH_3(CH_2)_2CH_2$), 47.7 (($CH_3$)$_2$CH), 47.7 (($CH_3$)$_2$CH), 54.9 ($NCH_2CH_2O$), 68.6 ($NCH_2CH_2O$), 71.5 ($OCH_2CH_2O$), 91.7 (LuC=C=C), 101.2 (LuNH-C=C), 112.9 ($C_5Me_5$), 118.3 (Ar), 119.3 (Ar), 125.2 (Ar), 126.5 (Ar), 126.8 (Ar), 127.0 (LuC), 127.0 (Ar), 127.6 (Ar), 127.7 (Ar), 136.7 (Ar), 137.0 (Ar), 147.0 (Ar), 147.7 (Ar), 149.8 (Ar), 156.0 (LuNH-C), 161.2 (LuC=C), 171.0 (NCN). Anal. Calcd for $C_{65}H_{97}KLuN_5O_6$ of **3e**: C, 62.03; H, 7.77; N, 5.56; Found: C, 61.82; H, 7.74; N, 5.52.



**3f**

**Synthesis of 3f:** This complex was prepared by an analogous procedure as the synthesis of **3a**, except that **1a** (52.3 mg, 0.050 mmol) and phenylacetylene (5.5 μL, 0.050 mmol) were replaced by **1b** (51.6 mg, 0.050 mmol) and 1-hexyne (5.7 μL, 0.050 mmol), respectively. **3f**, orange solid. Yield: 85% (51.7 mg, 0.043 mmol). The suitable crystals for X-ray diffraction of **3f** could be obtained through gradually diffusing hexane into its THF solution at room temperature. Anal. Calcd for $C_{63}H_{93}DyKN_5O_6$ of **3f**: C, 62.12; H, 7.70; N, 5.75; Found: C, 61.89; H, 7.93; N, 5.64.

## 2) Copies of $^{1}$H NMR and $^{13}$C NMR Spectra

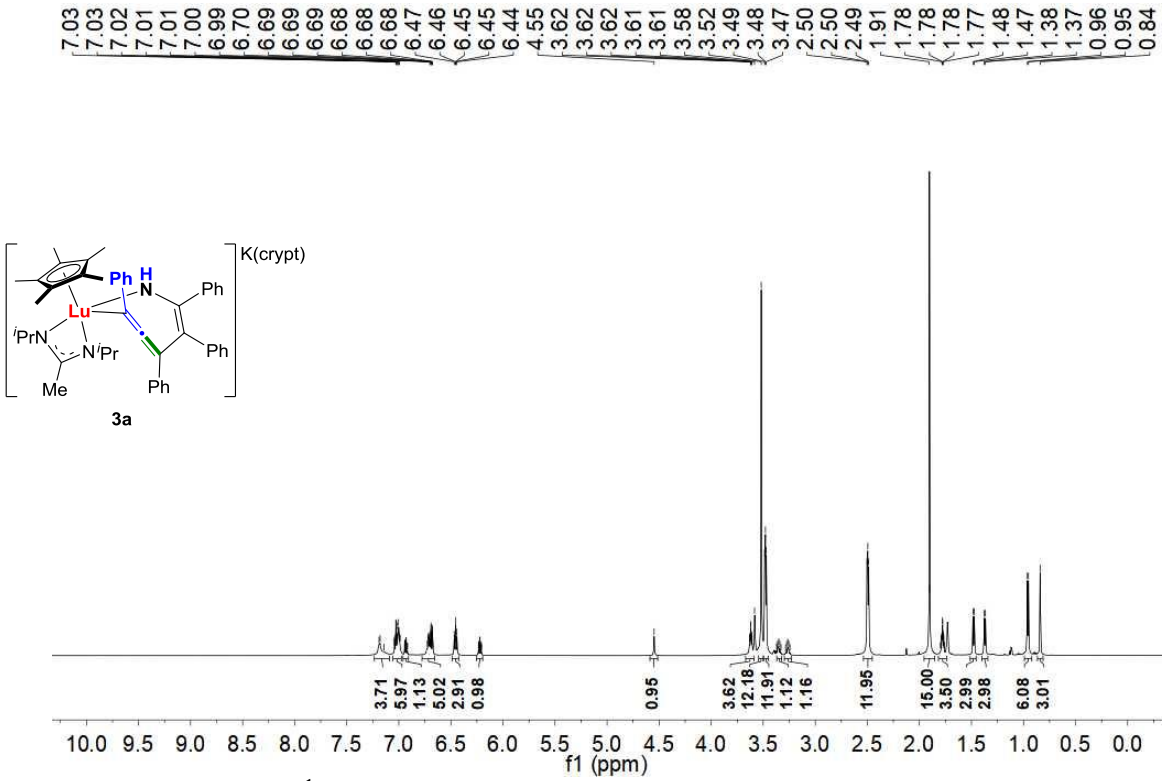



**Figure S1.** $^{1}$H NMR spectrum of **3a·THF** (25 °C, 600 MHz, THF-$d_8$).

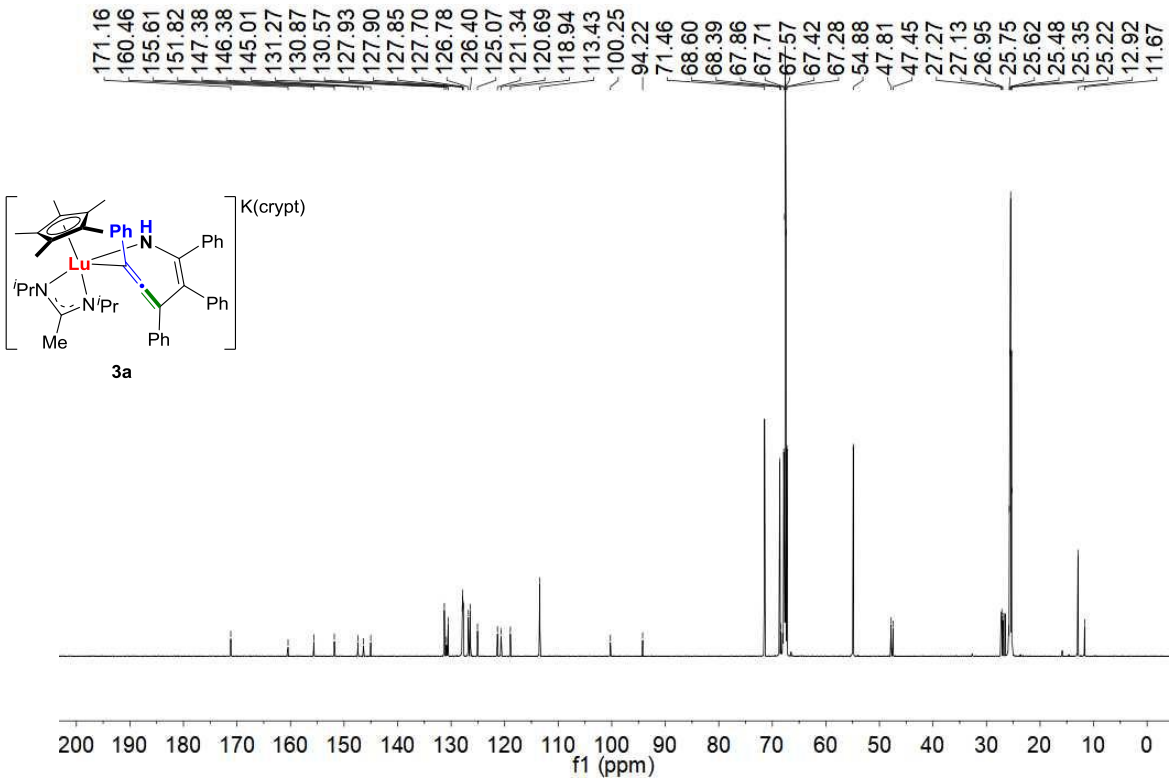



**Figure S2**. $^{13}$C NMR spectrum of **3a·THF** (25 °C, 151 MHz, THF-$d_8$).

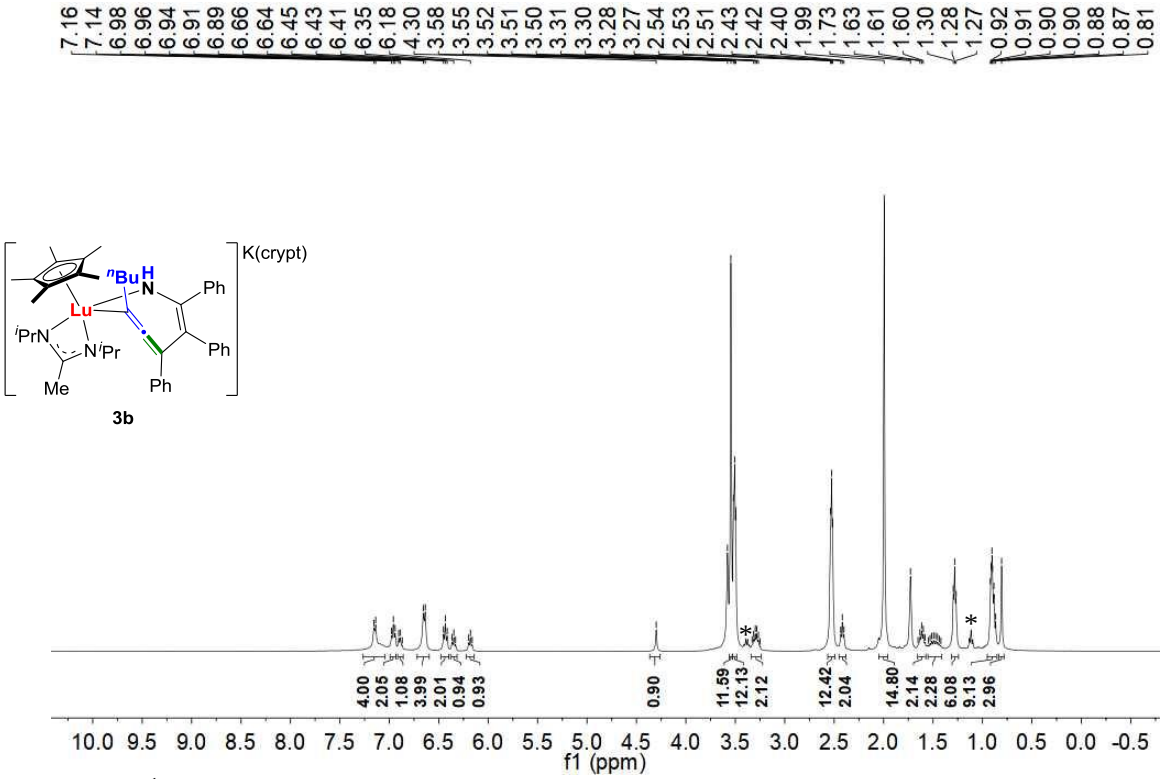



**Figure S3.** $^{1}$H NMR spectrum of **3b** (25 °C, 400 MHz, THF-$d_8$, "*" represents the residual $Et_2O$).

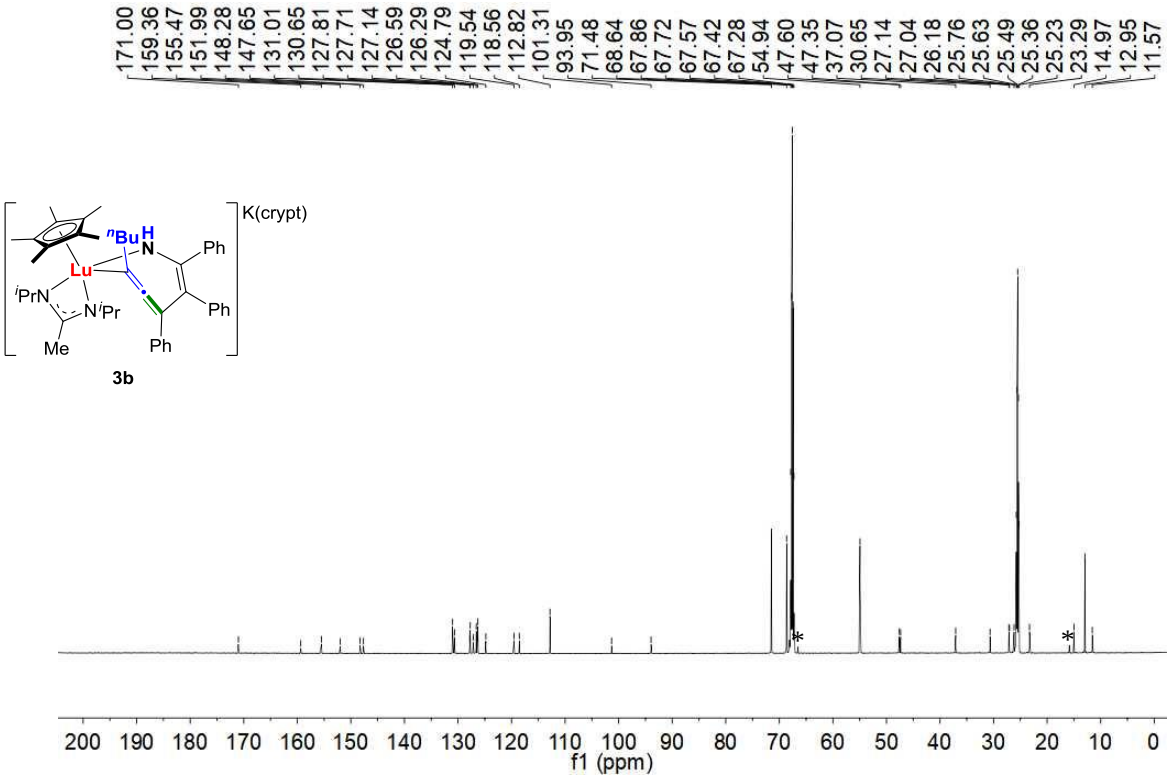



**Figure S4**. $^{13}$C NMR spectrum of **3b** (25 °C, 151 MHz, THF-$d_8$, "*" represents the residual $Et_2O$).

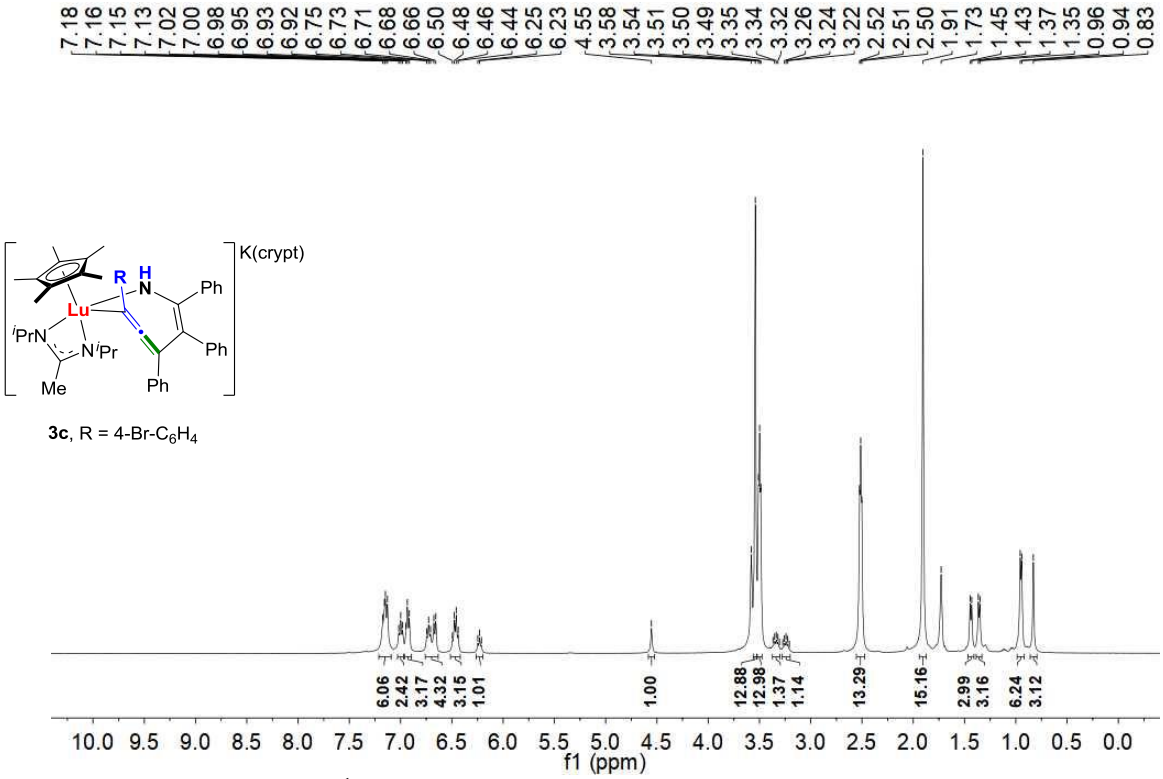



**Figure S5.** $^{1}$H NMR spectrum of **3c** (25 °C, 400 MHz, THF-$d_8$).

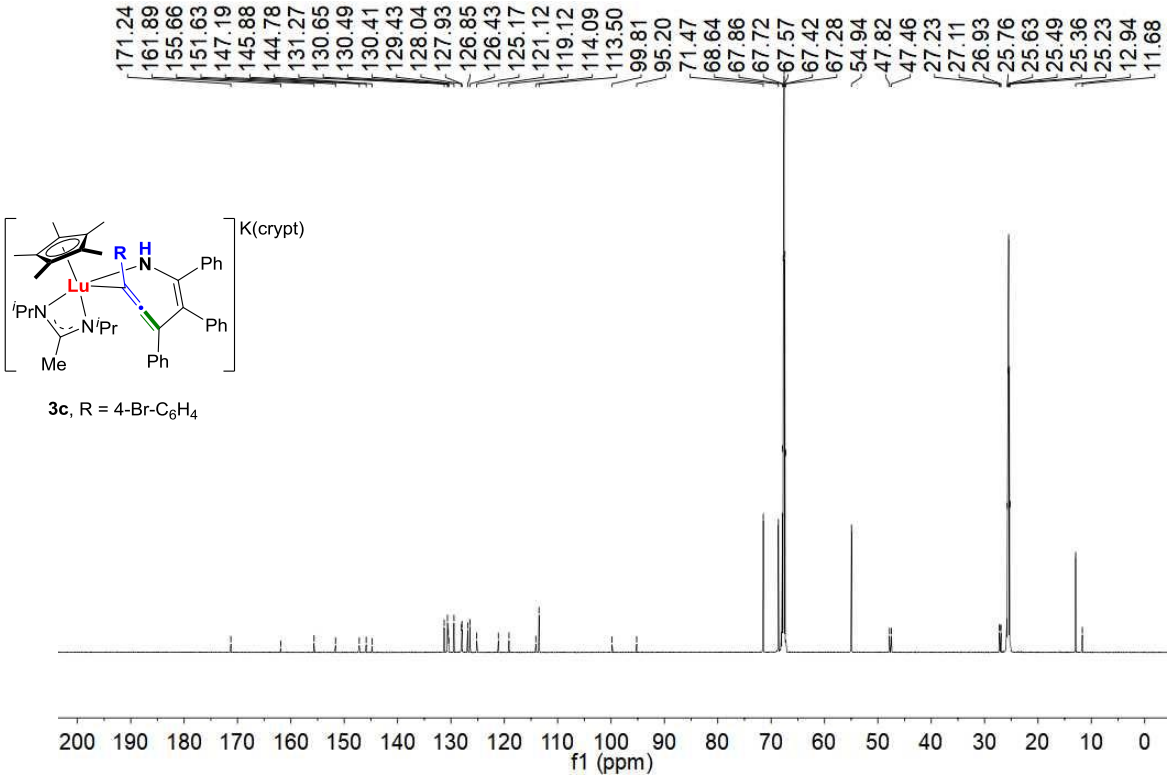



**Figure S6**. $^{13}$C NMR spectrum of **3c** (25 °C, 151 MHz, THF-$d_8$).

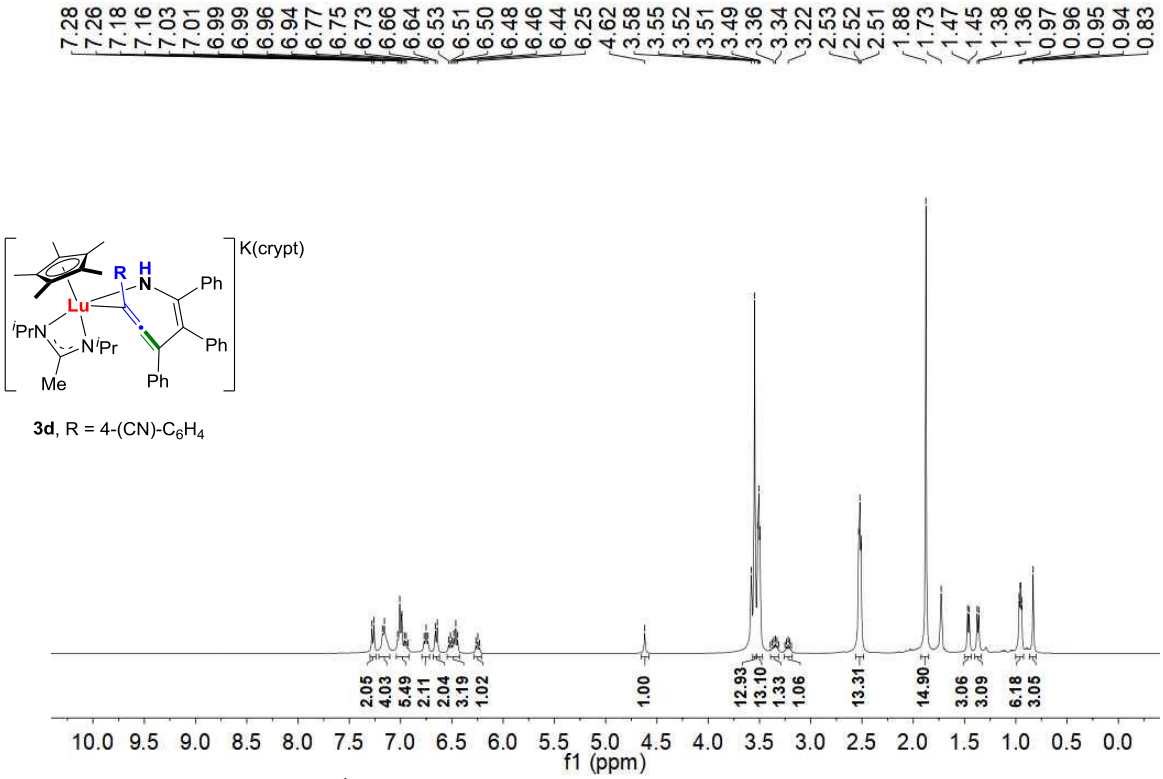



**Figure S7.** $^{1}$H NMR spectrum of **3d** (25 °C, 400 MHz, THF-$d_8$).

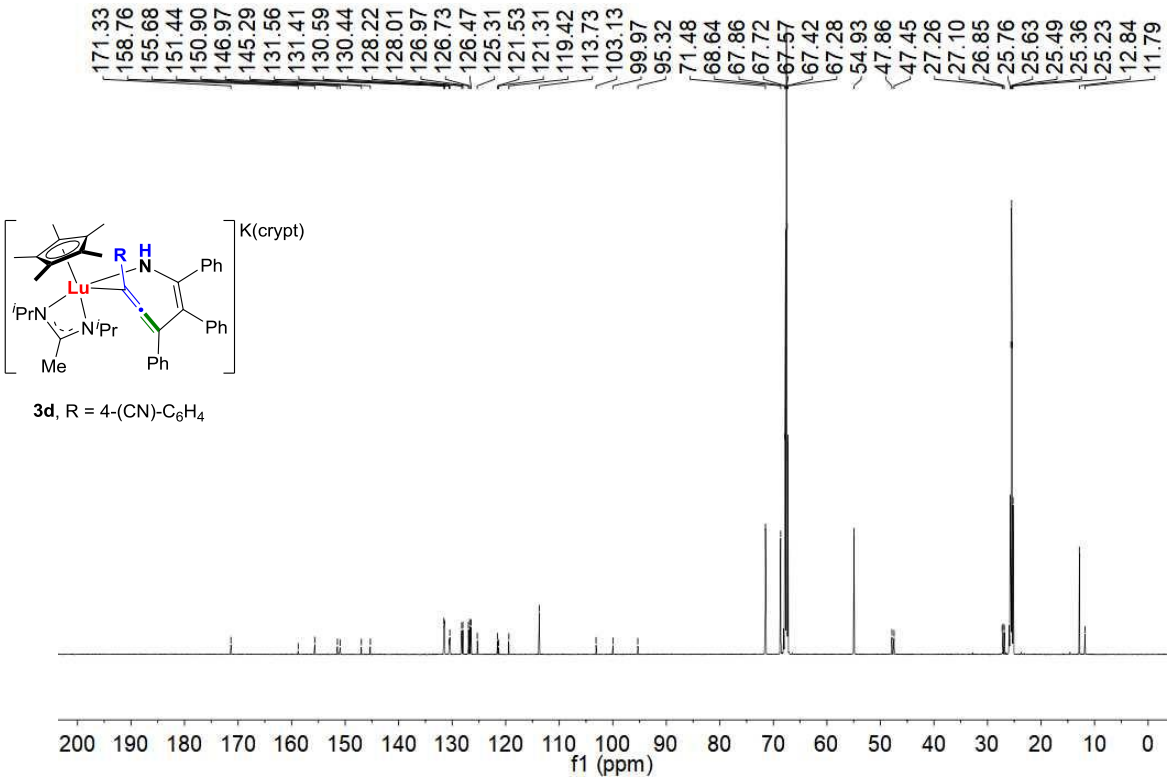



**Figure S8**. $^{13}$C NMR spectrum of **3d** (25 °C, 151 MHz, THF-$d_8$).

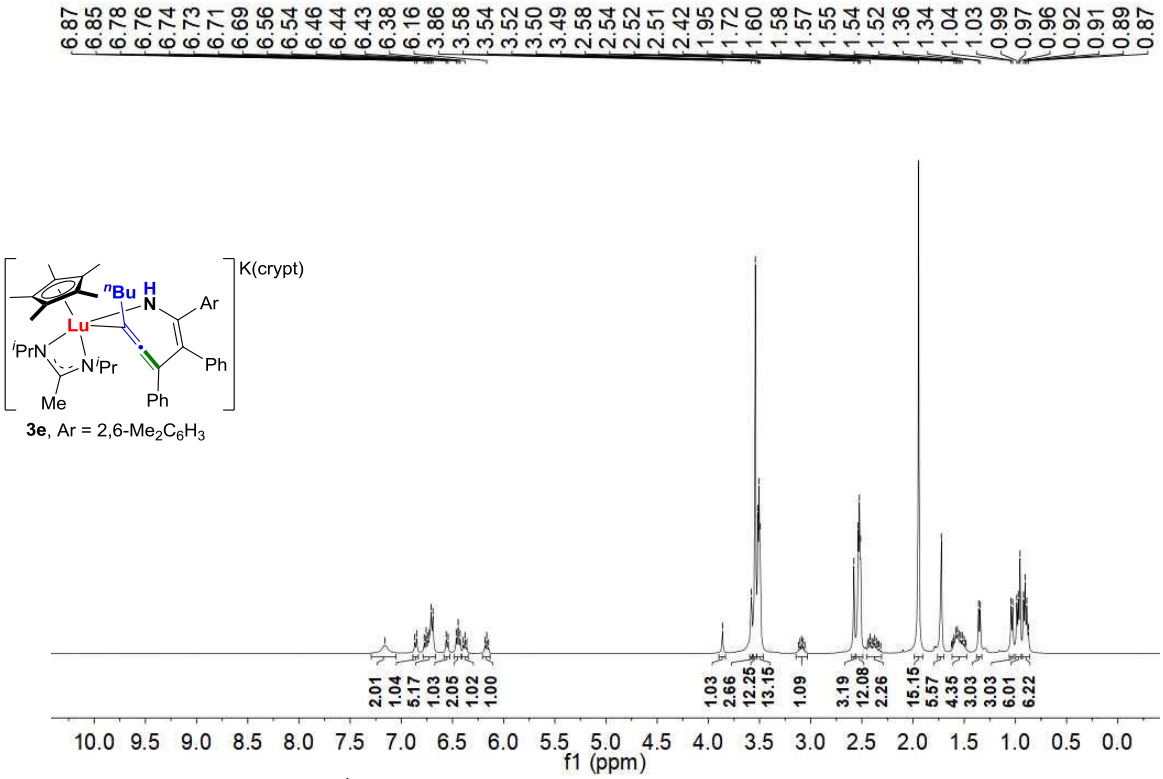



**Figure S9.** $^{1}$H NMR spectrum of **3e** (25 °C, 400 MHz, THF-$d_8$).

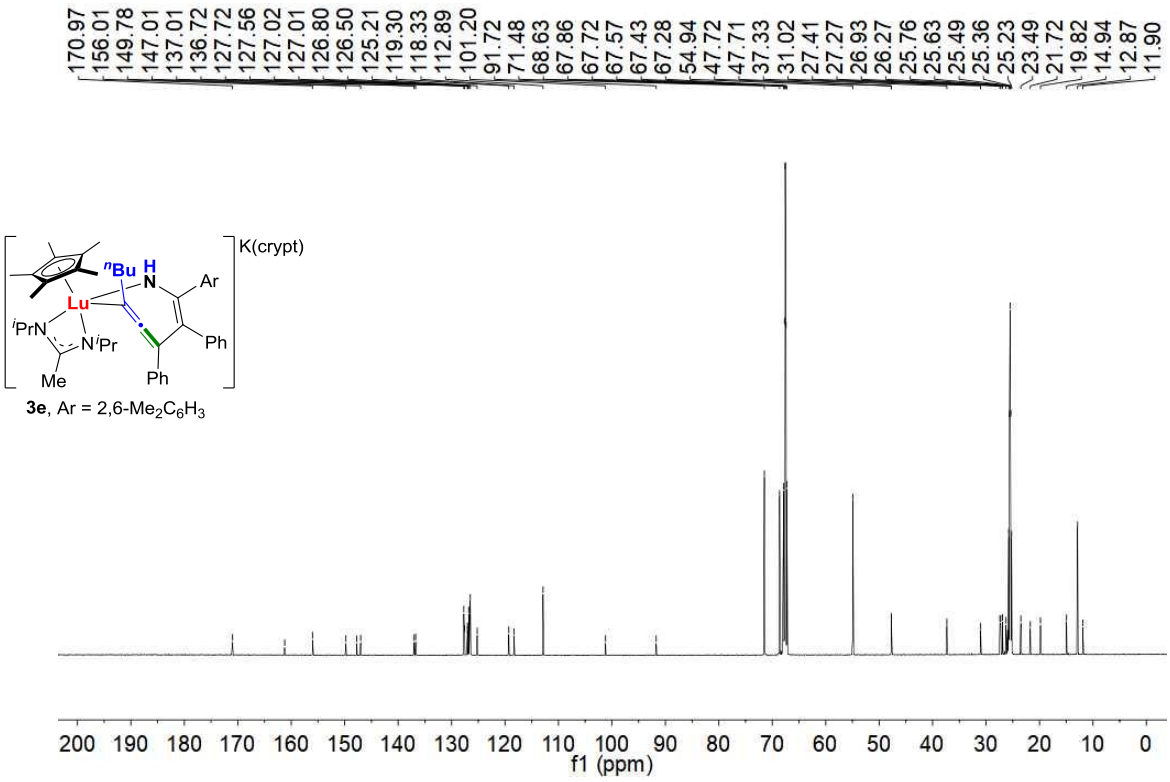



**Figure S10**. $^{13}$C NMR spectrum of **3e** (25 °C, 151 MHz, THF-$d_8$).

### 3) X-ray Crystallographic Studies

The single crystals of **3a·THF**, **3b**, **3c·THF**, **3d** and **3f** suitable for X-ray analysis were obtained as described in the experimental details. Data collections were performed on a XtaLAB PRO 007HF(Mo): Kappa single diffractometer at 180 K. Using Olex2,[2] the structures were solved with Superflip[3] structure solution program using Charge Flipping or ShelXS-97[4] structure solution program using Direct Methods and refined with the ShelXL[5] refinement package using Least Squares minimization. Refinement was performed on $F^2$ anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method. The hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre with supplementary publication numbers: CCDC 2288512 (**3a·THF**), CCDC 2288515 (**3b**), CCDC 2288513 (**3c·THF**), CCDC 2288514 (**3d**), CCDC 2288516 (**3f**).

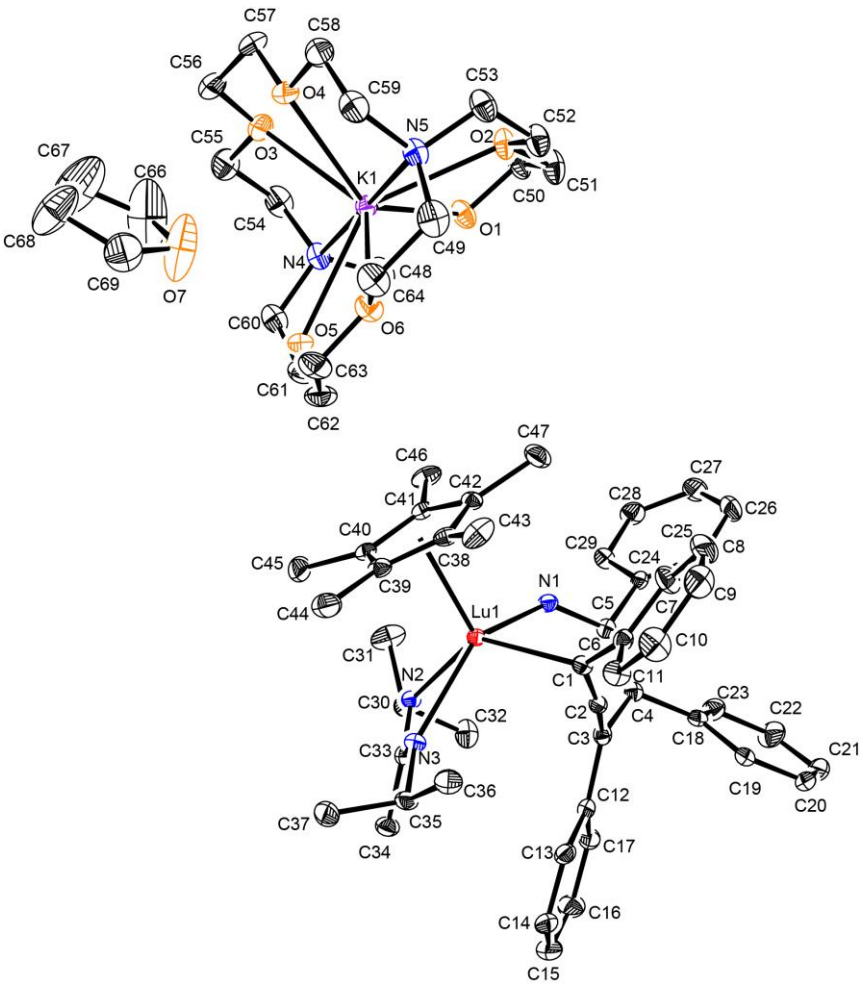



**Figure S11.** ORTEP drawing of **3a·THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

**Table 1 Crystal data and structure refinement for 3a·THF.**

| | |
|---|---|
| Identification code | **3a·THF** |
| Empirical formula | $C_{69}H_{97}KLuN_5O_7$ |
| Formula weight | 1322.58 |
| Temperature/K | 180.00(10) |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 10.14485(19) |
| b/Å | 24.5981(7) |
| c/Å | 27.0702(6) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 6755.2(3) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.300 |
| μ/mm$^{-1}$ | 1.577 |
| F(000) | 2768.0 |
| Crystal size/mm$^3$ | 0.15 × 0.13 × 0.12 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.288 to 52.044 |
| Index ranges | -11 ≤ h ≤ 12, -30 ≤ k ≤ 28, -33 ≤ l ≤ 30 |
| Reflections collected | 61247 |
| Independent reflections | 13286 [$R_{int}$ = 0.0510, $R_{sigma}$ = 0.0474] |
| Data/restraints/parameters | 13286/1/762 |
| Goodness-of-fit on F$^2$ | 0.981 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0251, $wR_2$ = 0.0502 |
| Final R indexes [all data] | $R_1$ = 0.0311, $wR_2$ = 0.0516 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.35/-0.44 |
| Flack parameter | -0.015(3) |

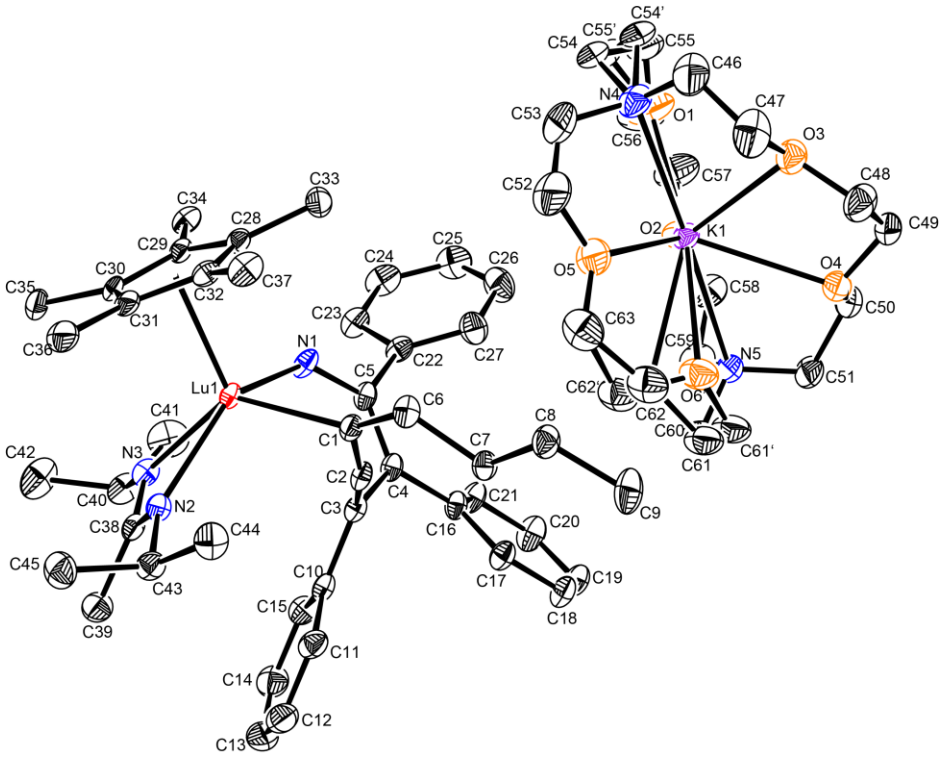



**Figure S12.** ORTEP drawing of **3b** with 30% thermal ellipsoids. H atoms are omitted for clarity.

**Table 2 Crystal data and structure refinement for 3b.**

| | |
|---|---|
| Identification code | **3b** |
| Empirical formula | $C_{63}H_{93}KLuN_5O_6$ |
| Formula weight | 1230.49 |
| Temperature/K | 180.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 10.2216(4) |
| b/Å | 35.5765(11) |
| c/Å | 17.2539(5) |
| α/° | 90 |
| β/° | 100.557(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 6168.2(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.325 |
| μ/mm$^{-1}$ | 1.720 |
| F(000) | 2576.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.316 to 54.968 |
| Index ranges | $-13 \le h \le 12$, $-44 \le k \le 46$, $-18 \le l \le 22$ |
| Reflections collected | 48971 |
| Independent reflections | 14109 [$R_{int}$ = 0.0586, $R_{sigma}$ = 0.0612] |
| Data/restraints/parameters | 14109/184/743 |

| | |
|---|---|
| Goodness-of-fit on $F^2$ | 1.054 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0355, $wR_2$ = 0.0762 |
| Final R indexes [all data] | $R_1$ = 0.0484, $wR_2$ = 0.0802 |
| Largest diff. peak/hole / e $Å^{-3}$ | 1.25/-0.76 |

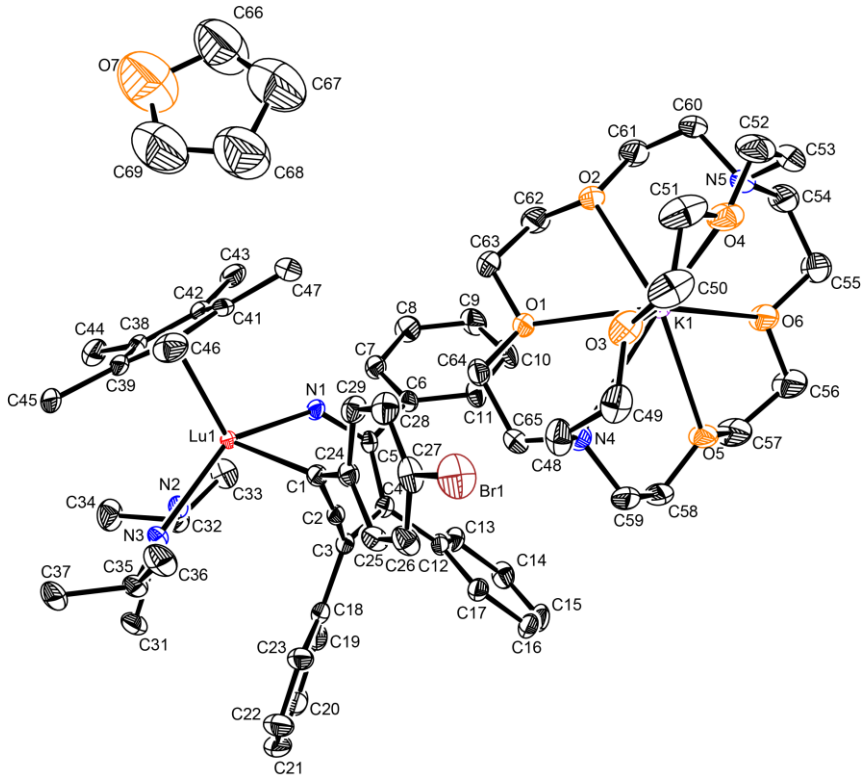



**Figure S13.** ORTEP drawing of **3c·THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

**Table 3 Crystal data and structure refinement for 3c·THF.**

| | |
|---|---|
| Identification code | **3c·THF** |
| Empirical formula | $C_{69}H_{96}BrKLuN_5O_7$ |
| Formula weight | 1401.48 |
| Temperature/K | 180.00(10) |
| Crystal system | triclinic |
| Space group | P1 |
| a/Å | 10.3921(2) |
| b/Å | 13.6701(3) |
| c/Å | 13.8088(3) |
| α/° | 78.741(2) |
| β/° | 72.513(2) |
| γ/° | 69.266(2) |
| Volume/$Å^3$ | 1741.15(7) |
| Z | 1 |
| $\rho_{calc}$g/$cm^3$ | 1.337 |
| μ/$mm^{-1}$ | 2.104 |

| | |
|---|---|
| F(000) | 726.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.65 to 54.97 |
| Index ranges | -13 ≤ h ≤ 13, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17 |
| Reflections collected | 36970 |
| Independent reflections | 14745 [$R_{int}$ = 0.0228, $R_{sigma}$ = 0.0275] |
| Data/restraints/parameters | 14745/73/768 |
| Goodness-of-fit on $F^2$ | 1.037 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0205, $wR_2$ = 0.0504 |
| Final R indexes [all data] | $R_1$ = 0.0205, $wR_2$ = 0.0505 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.75/-0.56 |
| Flack parameter | 0.746(5) |

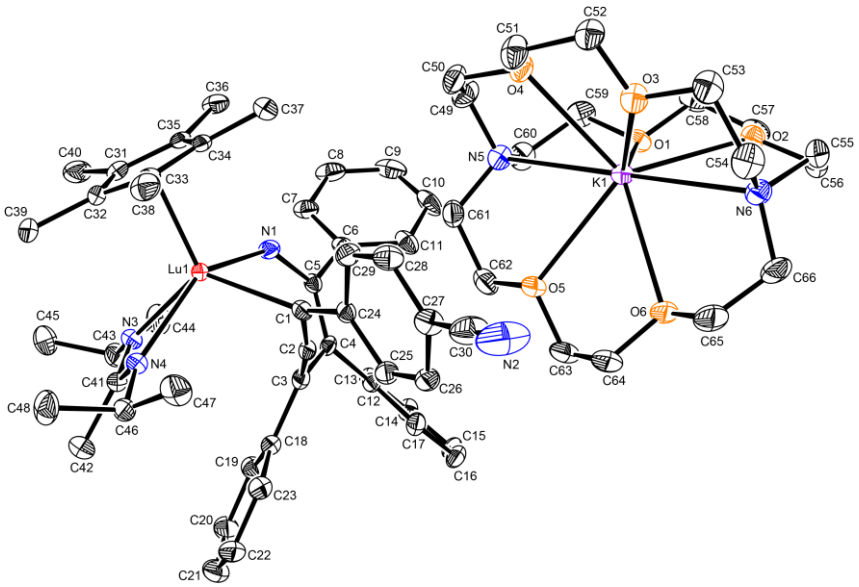



**Figure S14.** ORTEP drawing of **3d** with 30% thermal ellipsoids. H atoms are omitted for clarity.

**Table 4 Crystal data and structure refinement for 3f.**

| | |
|---|---|
| Identification code | **3f** |
| Empirical formula | $C_{66}H_{88}KLuN_6O_6$ |
| Formula weight | 1275.49 |
| Temperature/K | 179.99(10) |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 10.4772(4) |
| b/Å | 24.6064(10) |
| c/Å | 24.7943(9) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 6392.1(4) |

| | |
|---|---|
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.325 |
| μ/mm$^{-1}$ | 1.663 |
| F(000) | 2656.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.09 to 54.968 |
| Index ranges | -13 ≤ h ≤ 12, -31 ≤ k ≤ 31, -32 ≤ l ≤ 27 |
| Reflections collected | 47964 |
| Independent reflections | 14451 [$R_{int}$ = 0.0449, $R_{sigma}$ = 0.0493] |
| Data/restraints/parameters | 14451/30/731 |
| Goodness-of-fit on F$^2$ | 1.043 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0339, w$R_2$ = 0.0690 |
| Final R indexes [all data] | $R_1$ = 0.0390, w$R_2$ = 0.0703 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.48/-1.20 |
| Flack parameter | -0.008(4) |

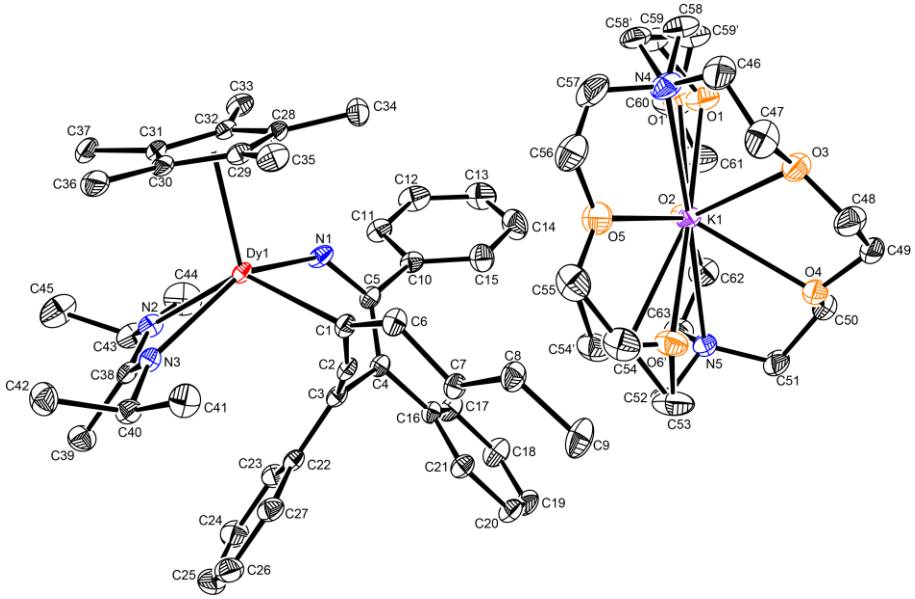



**Figure S15.** ORTEP drawing of **3f** with 30% thermal ellipsoids. H atoms are omitted for clarity.

**Table 5 Crystal data and structure refinement for 3f.**

| | |
|---|---|
| Identification code | **3f** |
| Empirical formula | $C_{63}H_{93}DyKN_5O_6$ |
| Formula weight | 1218.02 |
| Temperature/K | 179.99(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 10.2598(2) |
| b/Å | 35.6923(7) |
| c/Å | 17.2714(5) |
| α/° | 90 |

| | |
|---|---|
| β/° | 100.088(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 6226.9(3) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.299 |
| μ/mm$^{-1}$ | 1.319 |
| F(000) | 2556.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.19 to 54.968 |
| Index ranges | -13 ≤ h ≤ 13, -46 ≤ k ≤ 46, -22 ≤ l ≤ 22 |
| Reflections collected | 53034 |
| Independent reflections | 14237 [$R_{int}$ = 0.0286, $R_{sigma}$ = 0.0315] |
| Data/restraints/parameters | 14237/222/743 |
| Goodness-of-fit on F$^2$ | 1.036 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0304, w$R_2$ = 0.0619 |
| Final R indexes [all data] | $R_1$ = 0.03898, w$R_2$ = 0.0645 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.56/-0.46 |

**4) Details of DFT Calculations**

All calculations were carried out with GAUSSIAN 16 program package.[6] The structures were optimized at PBE0-D3[7,8]/MWB60[9] (for Lu)/6-31G(d,p)[10] (for other elements) level in gas phase. The effect of solvent was examined by performing single-point self-consistent reaction field (SCRF) calculations based on the solvation model density (SMD)[11] for gas-phase optimized structures. THF was used as the solvent, and solvation free energies ($\Delta G_{sol}$) were calculated by adding the solvation energies to the computed gas phase relative free energies ($\Delta G_{gas}$). Solvation free energies ($\Delta G_{sol}$) were calculated at PBE0-D3/MWB28[9] (for Lu)/6-311+G(d,p)[12] (for other elements) level. Harmonic frequency calculations were performed at the same level for every structure to confirm it as a local minimum and to derive the thermochemical corrections for enthalpies and free energies. The intrinsic reaction coordinate (IRC) analysis was carried out throughout the pathways to confirm that all stationary points are smoothly connected to each other. All enthalpies and the Gibbs free energies in the text were given in Hartree. All distances were given in Å. The PIO analysis was performed by the combination of the program package from Github (https://github.com/jxzhangcc/PIO) and the NBO analysis.[13]

**2a**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.811806
Thermal correction to Gibbs Free Energy= 0.681103
Sum of electronic and thermal Enthalpies= -1716.144980
Sum of electronic and thermal Free Energies= -1716.275684
298 K, in THF
Sum of electronic and thermal Free Energies = -2912.934950

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 2.213748 | -1.866251 | 1.064266 |
| 2 | 7 | 0 | 2.563110 | 0.253360 | 1.722301 |
| 3 | 6 | 0 | -1.980045 | 0.255919 | 0.130747 |
| 4 | 6 | 0 | -1.678849 | -1.218112 | -0.126711 |
| 5 | 6 | 0 | 2.035792 | -3.281960 | 1.307550 |
| 6 | 1 | 0 | 2.890077 | -3.696691 | 1.871500 |
| 7 | 6 | 0 | 0.755120 | -3.531932 | 2.112252 |
| 8 | 1 | 0 | 0.775185 | -2.998163 | 3.069148 |
| 9 | 1 | 0 | 0.615156 | -4.600064 | 2.319337 |
| 10 | 1 | 0 | -0.099925 | -3.168904 | 1.531988 |
| 11 | 6 | 0 | 1.951840 | -4.012936 | -0.028709 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 1 | 0 | 1.111871 | -3.602586 | -0.600584 |
| 13 | 1 | 0 | 1.786224 | -5.085903 | 0.123591 |
| 14 | 1 | 0 | 2.873378 | -3.880245 | -0.602340 |
| 15 | 6 | 0 | 2.732585 | -1.045753 | 1.970365 |
| 16 | 6 | 0 | 3.469725 | -1.577365 | 3.182209 |
| 17 | 1 | 0 | 4.028268 | -0.798826 | 3.702602 |
| 18 | 1 | 0 | 4.167865 | -2.362886 | 2.879459 |
| 19 | 1 | 0 | 2.764528 | -2.025400 | 3.889583 |
| 20 | 6 | 0 | 3.040448 | 1.277418 | 2.623288 |
| 21 | 1 | 0 | 4.071882 | 1.062545 | 2.958521 |
| 22 | 6 | 0 | 2.157925 | 1.388552 | 3.872050 |
| 23 | 1 | 0 | 1.123228 | 1.583201 | 3.573800 |
| 24 | 1 | 0 | 2.490441 | 2.200087 | 4.530961 |
| 25 | 1 | 0 | 2.161235 | 0.457695 | 4.447602 |
| 26 | 6 | 0 | 3.087019 | 2.612193 | 1.886246 |
| 27 | 1 | 0 | 3.776433 | 2.557249 | 1.041068 |
| 28 | 1 | 0 | 3.415093 | 3.418998 | 2.551605 |
| 29 | 1 | 0 | 2.096551 | 2.872167 | 1.498747 |
| 30 | 6 | 0 | 3.083957 | 0.740103 | -1.827596 |
| 31 | 6 | 0 | 1.925667 | 1.507592 | -2.128062 |
| 32 | 6 | 0 | 0.972891 | 0.633553 | -2.723889 |
| 33 | 6 | 0 | 1.546944 | -0.665384 | -2.800928 |
| 34 | 6 | 0 | 2.849663 | -0.599847 | -2.242974 |
| 35 | 6 | 0 | 4.392736 | 1.232105 | -1.289368 |
| 36 | 1 | 0 | 4.370924 | 2.311688 | -1.114677 |
| 37 | 1 | 0 | 5.209254 | 1.036235 | -1.998486 |
| 38 | 1 | 0 | 4.661995 | 0.747421 | -0.342741 |
| 39 | 6 | 0 | 1.770584 | 2.985122 | -1.921946 |
| 40 | 1 | 0 | 0.730236 | 3.265377 | -1.735463 |
| 41 | 1 | 0 | 2.116228 | 3.555339 | -2.795779 |
| 42 | 1 | 0 | 2.346173 | 3.335137 | -1.058755 |
| 43 | 6 | 0 | -0.387907 | 0.987783 | -3.240260 |
| 44 | 1 | 0 | -1.168361 | 0.375265 | -2.772825 |
| 45 | 1 | 0 | -0.455090 | 0.836008 | -4.326339 |
| 46 | 1 | 0 | -0.627792 | 2.034563 | -3.038390 |
| 47 | 6 | 0 | 0.873626 | -1.856617 | -3.408805 |
| 48 | 1 | 0 | -0.137484 | -1.980282 | -3.007835 |
| 49 | 1 | 0 | 1.416824 | -2.780221 | -3.187754 |
| 50 | 1 | 0 | 0.802932 | -1.765219 | -4.501817 |
| 51 | 6 | 0 | 3.873142 | -1.690515 | -2.166889 |
| 52 | 1 | 0 | 4.213902 | -1.859464 | -1.138501 |
| 53 | 1 | 0 | 4.758520 | -1.447231 | -2.771334 |
| 54 | 1 | 0 | 3.474647 | -2.638687 | -2.537762 |
| 55 | 71 | 0 | 1.161113 | -0.184945 | -0.213878 |
| 56 | 6 | 0 | -0.914017 | 1.090212 | 0.286801 |
| 57 | 7 | 0 | -0.532590 | -1.622283 | -0.499185 |
| 58 | 6 | 0 | -2.758489 | -2.244053 | 0.133735 |
| 59 | 6 | 0 | -2.745072 | -3.426554 | -0.615620 |
| 60 | 6 | 0 | -3.701321 | -2.123335 | 1.160999 |
| 61 | 6 | 0 | -3.657602 | -4.444183 | -0.368042 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -1.977283 | -3.522255 | -1.378851 |
| 63 | 6 | 0 | -4.602376 | -3.151849 | 1.428401 |
| 64 | 1 | 0 | -3.728499 | -1.216858 | 1.757970 |
| 65 | 6 | 0 | -4.592633 | -4.312279 | 0.659564 |
| 66 | 1 | 0 | -3.637514 | -5.348937 | -0.971905 |
| 67 | 1 | 0 | -5.319009 | -3.041638 | 2.239149 |
| 68 | 1 | 0 | -5.304111 | -5.109832 | 0.860778 |
| 69 | 6 | 0 | -3.393669 | 0.719333 | 0.080164 |
| 70 | 6 | 0 | -4.230552 | 0.324511 | -0.974605 |
| 71 | 6 | 0 | -3.931670 | 1.572849 | 1.054607 |
| 72 | 6 | 0 | -5.545131 | 0.770896 | -1.058675 |
| 73 | 1 | 0 | -3.835460 | -0.345537 | -1.733971 |
| 74 | 6 | 0 | -5.247125 | 2.016627 | 0.976064 |
| 75 | 1 | 0 | -3.295714 | 1.891929 | 1.875004 |
| 76 | 6 | 0 | -6.062567 | 1.619107 | -0.081990 |
| 77 | 1 | 0 | -6.170024 | 0.451122 | -1.889330 |
| 78 | 1 | 0 | -5.637588 | 2.679034 | 1.745200 |
| 79 | 1 | 0 | -7.091239 | 1.965560 | -0.143671 |
| 80 | 6 | 0 | -1.089212 | 2.540761 | 0.393037 |
| 81 | 6 | 0 | -0.573457 | 3.259193 | 1.487563 |
| 82 | 6 | 0 | -1.705613 | 3.296973 | -0.626081 |
| 83 | 6 | 0 | -0.663174 | 4.644964 | 1.562859 |
| 84 | 1 | 0 | -0.102401 | 2.702658 | 2.292313 |
| 85 | 6 | 0 | -1.777410 | 4.683440 | -0.561638 |
| 86 | 1 | 0 | -2.138141 | 2.768693 | -1.470416 |
| 87 | 6 | 0 | -1.256615 | 5.372831 | 0.533024 |
| 88 | 1 | 0 | -0.255400 | 5.160641 | 2.429921 |
| 89 | 1 | 0 | -2.254760 | 5.231223 | -1.371522 |
| 90 | 1 | 0 | -1.313108 | 6.457128 | 0.582426 |

---

**Phenylacetylene**
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.117731
Thermal correction to Gibbs Free Energy = 0.079962
Sum of electronic and thermal Enthalpies = -307.912910
Sum of electronic and thermal Free Energies = -307.950678
298 K, in THF
Sum of electronic and thermal Free Energies = -308.024913

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.508305 | 1.205620 | 0.000037 |
| 2 | 6 | 0 | 0.119367 | 1.210323 | 0.000003 |
| 3 | 6 | 0 | -0.590523 | -0.000002 | -0.000014 |
| 4 | 6 | 0 | 0.119376 | -1.210326 | 0.000003 |
| 5 | 6 | 0 | 1.508311 | -1.205614 | 0.000037 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 2.206425 | 0.000006 | 0.000054 |
| 7 | 1 | 0 | 2.048817 | 2.147609 | 0.000050 |
| 8 | 1 | 0 | -0.430370 | 2.146084 | -0.000010 |
| 9 | 1 | 0 | -0.430360 | -2.146088 | -0.000010 |
| 10 | 1 | 0 | 2.048832 | -2.147598 | 0.000050 |
| 11 | 1 | 0 | 3.292454 | 0.000007 | 0.000080 |
| 12 | 6 | 0 | -2.017225 | -0.000012 | -0.000048 |
| 13 | 6 | 0 | -3.226758 | -0.000013 | -0.000079 |
| 14 | 1 | 0 | -4.293042 | 0.000095 | -0.000113 |

**TS1**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.927702
Thermal correction to Gibbs Free Energy = 0.783443
Sum of electronic and thermal Enthalpies = -2024.050884
Sum of electronic and thermal Free Energies = -2024.195143
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.920830

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | -0.564369 | -1.168383 | -0.128162 |
| 2 | 7 | 0 | 1.225458 | -0.694533 | -1.630056 |
| 3 | 1 | 0 | 0.123219 | 0.099279 | -1.778463 |
| 4 | 7 | 0 | 0.519815 | -2.000954 | 1.792733 |
| 5 | 7 | 0 | -1.444447 | -0.938983 | 2.047128 |
| 6 | 6 | 0 | 0.613842 | 0.984066 | 0.474723 |
| 7 | 6 | 0 | 1.826552 | 1.115747 | -0.138005 |
| 8 | 6 | 0 | 2.145269 | 0.073471 | -1.153064 |
| 9 | 6 | 0 | 0.181875 | 1.933764 | 1.497397 |
| 10 | 6 | 0 | -0.803006 | 2.904870 | 1.235026 |
| 11 | 1 | 0 | -1.196990 | 2.986009 | 0.226658 |
| 12 | 6 | 0 | -1.277405 | 3.741932 | 2.238647 |
| 13 | 1 | 0 | -2.042257 | 4.477082 | 1.997430 |
| 14 | 6 | 0 | -0.787996 | 3.644678 | 3.540502 |
| 15 | 1 | 0 | -1.165054 | 4.296014 | 4.324612 |
| 16 | 6 | 0 | 0.202225 | 2.702260 | 3.814652 |
| 17 | 1 | 0 | 0.612601 | 2.619690 | 4.819213 |
| 18 | 6 | 0 | 0.681043 | 1.866878 | 2.811708 |
| 19 | 1 | 0 | 1.460093 | 1.144549 | 3.034096 |
| 20 | 6 | 0 | 2.779207 | 2.206785 | 0.213207 |
| 21 | 6 | 0 | 2.453950 | 3.541388 | -0.064155 |
| 22 | 1 | 0 | 1.510496 | 3.751965 | -0.559780 |
| 23 | 6 | 0 | 3.308567 | 4.579183 | 0.295314 |
| 24 | 1 | 0 | 3.031873 | 5.606721 | 0.071358 |
| 25 | 6 | 0 | 4.511403 | 4.305451 | 0.942720 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | 5.180132 | 5.115049 | 1.224372 |
| 27 | 6 | 0 | 4.846077 | 2.983900 | 1.230823 |
| 28 | 1 | 0 | 5.779899 | 2.757272 | 1.740099 |
| 29 | 6 | 0 | 3.989804 | 1.948425 | 0.870399 |
| 30 | 1 | 0 | 4.259979 | 0.919936 | 1.091989 |
| 31 | 6 | 0 | 3.555626 | -0.132691 | -1.629294 |
| 32 | 6 | 0 | 4.366269 | 0.911507 | -2.087717 |
| 33 | 1 | 0 | 3.992666 | 1.930147 | -2.065074 |
| 34 | 6 | 0 | 5.644027 | 0.654568 | -2.578763 |
| 35 | 1 | 0 | 6.254730 | 1.477926 | -2.941026 |
| 36 | 6 | 0 | 6.141812 | -0.645521 | -2.599100 |
| 37 | 1 | 0 | 7.144631 | -0.842406 | -2.970297 |
| 38 | 6 | 0 | 5.341515 | -1.693539 | -2.146073 |
| 39 | 1 | 0 | 5.717017 | -2.713859 | -2.163232 |
| 40 | 6 | 0 | 4.056832 | -1.438486 | -1.681062 |
| 41 | 1 | 0 | 3.411075 | -2.249247 | -1.357493 |
| 42 | 6 | 0 | 1.787809 | -2.531231 | 2.246680 |
| 43 | 1 | 0 | 1.699503 | -2.916985 | 3.276363 |
| 44 | 6 | 0 | 2.190685 | -3.702314 | 1.355768 |
| 45 | 1 | 0 | 1.472873 | -4.520880 | 1.433629 |
| 46 | 1 | 0 | 3.184725 | -4.078196 | 1.622877 |
| 47 | 1 | 0 | 2.215427 | -3.375310 | 0.310941 |
| 48 | 6 | 0 | 2.897392 | -1.476101 | 2.222388 |
| 49 | 1 | 0 | 3.034077 | -1.113757 | 1.199752 |
| 50 | 1 | 0 | 3.848347 | -1.892787 | 2.576207 |
| 51 | 1 | 0 | 2.648911 | -0.609751 | 2.841406 |
| 52 | 6 | 0 | -0.332566 | -1.391206 | 2.618767 |
| 53 | 6 | 0 | -0.046063 | -1.221650 | 4.095320 |
| 54 | 1 | 0 | 1.021532 | -1.104230 | 4.286971 |
| 55 | 1 | 0 | -0.391039 | -2.102310 | 4.649024 |
| 56 | 1 | 0 | -0.558138 | -0.342914 | 4.490070 |
| 57 | 6 | 0 | -2.398562 | -0.088318 | 2.728774 |
| 58 | 1 | 0 | -1.877312 | 0.723772 | 3.263286 |
| 59 | 6 | 0 | -3.279642 | 0.570342 | 1.670930 |
| 60 | 1 | 0 | -2.665417 | 1.113346 | 0.947710 |
| 61 | 1 | 0 | -3.977080 | 1.284019 | 2.122533 |
| 62 | 1 | 0 | -3.856624 | -0.191975 | 1.135595 |
| 63 | 6 | 0 | -3.277176 | -0.845996 | 3.729699 |
| 64 | 1 | 0 | -3.859123 | -1.615037 | 3.211891 |
| 65 | 1 | 0 | -3.976586 | -0.161837 | 4.225355 |
| 66 | 1 | 0 | -2.684647 | -1.339686 | 4.505066 |
| 67 | 6 | 0 | -2.641200 | -2.130630 | -1.543272 |
| 68 | 6 | 0 | -2.618363 | -2.943782 | -0.379251 |
| 69 | 6 | 0 | -1.439169 | -3.732718 | -0.410655 |
| 70 | 6 | 0 | -0.723287 | -3.405542 | -1.592444 |
| 71 | 6 | 0 | -1.463843 | -2.414897 | -2.293698 |
| 72 | 6 | 0 | -3.775725 | -1.258534 | -1.985482 |
| 73 | 1 | 0 | -4.341089 | -0.868335 | -1.131621 |
| 74 | 1 | 0 | -4.487209 | -1.810934 | -2.615291 |
| 75 | 1 | 0 | -3.420958 | -0.398196 | -2.559476 |

| | | | | | |
|---|---|---|---|---|---|
| 76 | 6 | 0 | -3.694198 | -3.098532 | 0.647672 |
| 77 | 1 | 0 | -3.276926 | -3.093592 | 1.659716 |
| 78 | 1 | 0 | -4.239443 | -4.044946 | 0.516928 |
| 79 | 1 | 0 | -4.432889 | -2.293299 | 0.592106 |
| 80 | 6 | 0 | -1.121978 | -4.789430 | 0.600974 |
| 81 | 1 | 0 | -0.255402 | -5.384010 | 0.297818 |
| 82 | 1 | 0 | -1.965677 | -5.482467 | 0.720825 |
| 83 | 1 | 0 | -0.903434 | -4.361492 | 1.587141 |
| 84 | 6 | 0 | 0.558135 | -4.002256 | -2.088313 |
| 85 | 1 | 0 | 1.016516 | -4.655848 | -1.339714 |
| 86 | 1 | 0 | 1.276586 | -3.211539 | -2.337408 |
| 87 | 1 | 0 | 0.397359 | -4.602353 | -2.994516 |
| 88 | 6 | 0 | -1.093838 | -1.872001 | -3.638573 |
| 89 | 1 | 0 | -1.634213 | -0.947098 | -3.858594 |
| 90 | 1 | 0 | -1.319899 | -2.592407 | -4.437965 |
| 91 | 1 | 0 | -0.023471 | -1.642653 | -3.679876 |
| 92 | 6 | 0 | -0.980116 | 0.825750 | -1.791311 |
| 93 | 6 | 0 | -1.825696 | 1.695325 | -1.985537 |
| 94 | 6 | 0 | -2.810450 | 2.708075 | -2.139735 |
| 95 | 6 | 0 | -2.527325 | 3.887169 | -2.852371 |
| 96 | 6 | 0 | -4.084398 | 2.563590 | -1.559577 |
| 97 | 6 | 0 | -3.488160 | 4.882069 | -2.981910 |
| 98 | 1 | 0 | -1.543610 | 4.006368 | -3.295950 |
| 99 | 6 | 0 | -5.037152 | 3.565099 | -1.692818 |
| 100 | 1 | 0 | -4.305576 | 1.658187 | -1.003684 |
| 101 | 6 | 0 | -4.747450 | 4.728449 | -2.404368 |
| 102 | 1 | 0 | -3.250539 | 5.786847 | -3.535701 |
| 103 | 1 | 0 | -6.014481 | 3.436540 | -1.234739 |
| 104 | 1 | 0 | -5.495697 | 5.509873 | -2.505560 |

**IM1**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.933873
Thermal correction to Gibbs Free Energy = 0.786995
Sum of electronic and thermal Enthalpies = -2024.097578
Sum of electronic and thermal Free Energies = -2024.244456
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.970725

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | -1.411020 | -0.473449 | 0.170894 |
| 2 | 7 | 0 | 0.312827 | -0.631527 | 1.840143 |
| 3 | 1 | 0 | 0.386286 | -1.382889 | 2.519881 |
| 4 | 7 | 0 | -2.189535 | 1.569516 | 1.219548 |
| 5 | 7 | 0 | -2.702484 | 1.179795 | -0.930670 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 0.541643 | 1.072153 | -0.285270 |
| 7 | 6 | 0 | 1.601873 | 0.949185 | 0.573386 |
| 8 | 6 | 0 | 1.463076 | -0.066125 | 1.618301 |
| 9 | 6 | 0 | 0.536476 | 2.035358 | -1.378665 |
| 10 | 6 | 0 | 0.596758 | 1.609524 | -2.720915 |
| 11 | 1 | 0 | 0.721193 | 0.548296 | -2.916646 |
| 12 | 6 | 0 | 0.495136 | 2.518792 | -3.766188 |
| 13 | 1 | 0 | 0.548474 | 2.155731 | -4.790240 |
| 14 | 6 | 0 | 0.312023 | 3.879473 | -3.517205 |
| 15 | 1 | 0 | 0.217636 | 4.585269 | -4.338283 |
| 16 | 6 | 0 | 0.260689 | 4.316954 | -2.195456 |
| 17 | 1 | 0 | 0.135953 | 5.375545 | -1.976330 |
| 18 | 6 | 0 | 0.386211 | 3.414915 | -1.143921 |
| 19 | 1 | 0 | 0.376948 | 3.770500 | -0.119543 |
| 20 | 6 | 0 | 2.840380 | 1.774030 | 0.529148 |
| 21 | 6 | 0 | 3.530456 | 1.992224 | -0.672588 |
| 22 | 1 | 0 | 3.151696 | 1.542197 | -1.584685 |
| 23 | 6 | 0 | 4.673207 | 2.783952 | -0.712558 |
| 24 | 1 | 0 | 5.187552 | 2.932588 | -1.658845 |
| 25 | 6 | 0 | 5.158320 | 3.382795 | 0.448128 |
| 26 | 1 | 0 | 6.052669 | 3.999903 | 0.416566 |
| 27 | 6 | 0 | 4.479970 | 3.185960 | 1.648755 |
| 28 | 1 | 0 | 4.840567 | 3.652957 | 2.562247 |
| 29 | 6 | 0 | 3.336296 | 2.395437 | 1.685241 |
| 30 | 1 | 0 | 2.811904 | 2.252127 | 2.626750 |
| 31 | 6 | 0 | 2.642062 | -0.531294 | 2.402355 |
| 32 | 6 | 0 | 3.814720 | -0.934216 | 1.755346 |
| 33 | 1 | 0 | 3.875231 | -0.864357 | 0.673865 |
| 34 | 6 | 0 | 4.880948 | -1.438145 | 2.490798 |
| 35 | 1 | 0 | 5.781243 | -1.762568 | 1.976413 |
| 36 | 6 | 0 | 4.799185 | -1.524526 | 3.879665 |
| 37 | 1 | 0 | 5.639288 | -1.908530 | 4.452342 |
| 38 | 6 | 0 | 3.637120 | -1.118732 | 4.531005 |
| 39 | 1 | 0 | 3.567614 | -1.180460 | 5.613847 |
| 40 | 6 | 0 | 2.560623 | -0.633577 | 3.794629 |
| 41 | 1 | 0 | 1.649903 | -0.313158 | 4.295288 |
| 42 | 6 | 0 | -2.038206 | 2.381052 | 2.407342 |
| 43 | 1 | 0 | -2.887058 | 3.080530 | 2.513328 |
| 44 | 6 | 0 | -2.043442 | 1.470506 | 3.631860 |
| 45 | 1 | 0 | -2.968551 | 0.893643 | 3.685800 |
| 46 | 1 | 0 | -1.933324 | 2.049044 | 4.556495 |
| 47 | 1 | 0 | -1.206382 | 0.767703 | 3.555825 |
| 48 | 6 | 0 | -0.742108 | 3.200017 | 2.410903 |
| 49 | 1 | 0 | 0.108658 | 2.532771 | 2.243998 |
| 50 | 1 | 0 | -0.605769 | 3.723838 | 3.365202 |
| 51 | 1 | 0 | -0.731168 | 3.947727 | 1.613742 |
| 52 | 6 | 0 | -2.627876 | 2.062692 | 0.066294 |
| 53 | 6 | 0 | -3.012699 | 3.516011 | -0.115100 |
| 54 | 1 | 0 | -2.552137 | 4.160201 | 0.633378 |
| 55 | 1 | 0 | -4.098993 | 3.629682 | -0.033025 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 1 | 0 | -2.706005 | 3.869702 | -1.102278 |
| 57 | 6 | 0 | -2.953812 | 1.566024 | -2.305053 |
| 58 | 1 | 0 | -2.299642 | 2.408469 | -2.592079 |
| 59 | 6 | 0 | -2.588118 | 0.387771 | -3.203535 |
| 60 | 1 | 0 | -1.565777 | 0.051907 | -3.013087 |
| 61 | 1 | 0 | -2.672344 | 0.657640 | -4.262213 |
| 62 | 1 | 0 | -3.258289 | -0.456145 | -3.006941 |
| 63 | 6 | 0 | -4.408108 | 1.968666 | -2.579378 |
| 64 | 1 | 0 | -5.077409 | 1.136086 | -2.339084 |
| 65 | 1 | 0 | -4.543210 | 2.220248 | -3.638521 |
| 66 | 1 | 0 | -4.722007 | 2.833861 | -1.990183 |
| 67 | 6 | 0 | -2.693975 | -2.804555 | -0.333665 |
| 68 | 6 | 0 | -3.733936 | -1.916481 | 0.041837 |
| 69 | 6 | 0 | -3.573396 | -1.600031 | 1.414831 |
| 70 | 6 | 0 | -2.437587 | -2.302332 | 1.897940 |
| 71 | 6 | 0 | -1.885284 | -3.039218 | 0.813988 |
| 72 | 6 | 0 | -2.526517 | -3.476430 | -1.661375 |
| 73 | 1 | 0 | -2.994830 | -2.899520 | -2.465576 |
| 74 | 1 | 0 | -2.981053 | -4.477835 | -1.669185 |
| 75 | 1 | 0 | -1.468460 | -3.577221 | -1.919502 |
| 76 | 6 | 0 | -4.894193 | -1.462669 | -0.785900 |
| 77 | 1 | 0 | -5.026606 | -0.378017 | -0.716885 |
| 78 | 1 | 0 | -5.830852 | -1.935417 | -0.455623 |
| 79 | 1 | 0 | -4.762619 | -1.713254 | -1.842648 |
| 80 | 6 | 0 | -4.534876 | -0.769808 | 2.207687 |
| 81 | 1 | 0 | -4.329998 | -0.843479 | 3.280717 |
| 82 | 1 | 0 | -5.568985 | -1.105517 | 2.050888 |
| 83 | 1 | 0 | -4.486373 | 0.291140 | 1.932189 |
| 84 | 6 | 0 | -1.996401 | -2.363525 | 3.329422 |
| 85 | 1 | 0 | -1.888621 | -1.372159 | 3.782180 |
| 86 | 1 | 0 | -1.035901 | -2.880602 | 3.430806 |
| 87 | 1 | 0 | -2.714034 | -2.921916 | 3.946524 |
| 88 | 6 | 0 | -0.710256 | -3.967474 | 0.859607 |
| 89 | 1 | 0 | -0.092555 | -3.858143 | -0.037662 |
| 90 | 1 | 0 | -1.019229 | -5.019936 | 0.935572 |
| 91 | 1 | 0 | -0.060997 | -3.761267 | 1.717702 |
| 92 | 6 | 0 | 0.127635 | -1.528490 | -1.388634 |
| 93 | 6 | 0 | 1.126946 | -1.983951 | -1.958442 |
| 94 | 6 | 0 | 2.347544 | -2.407632 | -2.552470 |
| 95 | 6 | 0 | 2.433250 | -3.576258 | -3.331696 |
| 96 | 6 | 0 | 3.524054 | -1.654113 | -2.363940 |
| 97 | 6 | 0 | 3.641094 | -3.972193 | -3.894117 |
| 98 | 1 | 0 | 1.533544 | -4.165411 | -3.483114 |
| 99 | 6 | 0 | 4.728449 | -2.055731 | -2.926892 |
| 100 | 1 | 0 | 3.466525 | -0.746373 | -1.770371 |
| 101 | 6 | 0 | 4.796421 | -3.217450 | -3.695792 |
| 102 | 1 | 0 | 3.682152 | -4.879757 | -4.492106 |
| 103 | 1 | 0 | 5.620815 | -1.455446 | -2.765553 |
| 104 | 1 | 0 | 5.739437 | -3.530732 | -4.136189 |

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**TS1'a**
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.930558
Thermal correction to Gibbs Free Energy = 0.788557
Sum of electronic and thermal Enthalpies = -2024.051800
Sum of electronic and thermal Free Energies = -2024.193801
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.916119

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.957877 | -0.804216 | 1.145065 |
| 2 | 7 | 0 | 2.992577 | 0.635331 | -0.512125 |
| 3 | 7 | 0 | 2.177572 | 0.682511 | 1.591346 |
| 4 | 6 | 0 | -1.790165 | 0.112745 | 0.855049 |
| 5 | 6 | 0 | -1.378024 | 1.399981 | 0.169089 |
| 6 | 6 | 0 | -0.295939 | 1.351062 | -0.653378 |
| 7 | 6 | 0 | -3.259387 | -0.107719 | 1.121938 |
| 8 | 6 | 0 | -3.633909 | -0.978301 | 2.150544 |
| 9 | 1 | 0 | -2.839485 | -1.404543 | 2.757543 |
| 10 | 6 | 0 | -4.967972 | -1.307639 | 2.357723 |
| 11 | 1 | 0 | -5.241489 | -1.979885 | 3.168248 |
| 12 | 6 | 0 | -5.955419 | -0.786062 | 1.520798 |
| 13 | 1 | 0 | -6.998884 | -1.052858 | 1.671461 |
| 14 | 6 | 0 | -5.593506 | 0.073066 | 0.486596 |
| 15 | 1 | 0 | -6.352445 | 0.469967 | -0.182999 |
| 16 | 6 | 0 | -4.258573 | 0.418926 | 0.297171 |
| 17 | 1 | 0 | -3.982124 | 1.081442 | -0.517386 |
| 18 | 6 | 0 | 3.833382 | 1.151803 | -1.576295 |
| 19 | 1 | 0 | 3.819295 | 2.254230 | -1.576538 |
| 20 | 6 | 0 | 5.291189 | 0.693072 | -1.441214 |
| 21 | 1 | 0 | 5.707739 | 0.952642 | -0.463104 |
| 22 | 1 | 0 | 5.921750 | 1.149959 | -2.214028 |
| 23 | 1 | 0 | 5.359538 | -0.394076 | -1.547140 |
| 24 | 6 | 0 | 3.282966 | 0.730561 | -2.933776 |
| 25 | 1 | 0 | 3.165057 | -0.356366 | -2.982869 |
| 26 | 1 | 0 | 3.960299 | 1.036819 | -3.739001 |
| 27 | 1 | 0 | 2.317821 | 1.209467 | -3.114186 |
| 28 | 6 | 0 | 3.020885 | 1.195001 | 0.692470 |
| 29 | 6 | 0 | 3.921557 | 2.358285 | 1.058310 |
| 30 | 1 | 0 | 3.324210 | 3.199457 | 1.419898 |
| 31 | 1 | 0 | 4.512141 | 2.713016 | 0.216292 |
| 32 | 1 | 0 | 4.602626 | 2.069075 | 1.864833 |
| 33 | 6 | 0 | 2.078527 | 1.217014 | 2.932537 |
| 34 | 1 | 0 | 2.345655 | 2.285945 | 2.945219 |
| 35 | 6 | 0 | 3.026568 | 0.500700 | 3.898136 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | 2.742591 | -0.551434 | 3.984174 |
| 37 | 1 | 0 | 2.989594 | 0.950773 | 4.897779 |
| 38 | 1 | 0 | 4.060722 | 0.539728 | 3.540089 |
| 39 | 6 | 0 | 0.635514 | 1.120850 | 3.414037 |
| 40 | 1 | 0 | -0.017578 | 1.705895 | 2.761575 |
| 41 | 1 | 0 | 0.538421 | 1.491846 | 4.441076 |
| 42 | 1 | 0 | 0.281159 | 0.086142 | 3.374147 |
| 43 | 6 | 0 | 1.187544 | -3.366488 | -0.647911 |
| 44 | 6 | 0 | 0.715089 | -3.431042 | 0.687486 |
| 45 | 6 | 0 | 1.746751 | -2.960245 | 1.541982 |
| 46 | 6 | 0 | 2.871592 | -2.623124 | 0.741858 |
| 47 | 6 | 0 | 2.521427 | -2.870141 | -0.614251 |
| 48 | 6 | 0 | 0.492733 | -3.893459 | -1.866684 |
| 49 | 1 | 0 | -0.592603 | -3.917948 | -1.736619 |
| 50 | 1 | 0 | 0.821475 | -4.915489 | -2.103710 |
| 51 | 1 | 0 | 0.685770 | -3.274278 | -2.748400 |
| 52 | 6 | 0 | -0.594038 | -3.965507 | 1.174383 |
| 53 | 1 | 0 | -1.204809 | -3.156520 | 1.597632 |
| 54 | 1 | 0 | -0.439853 | -4.725847 | 1.951791 |
| 55 | 1 | 0 | -1.161514 | -4.437001 | 0.366462 |
| 56 | 6 | 0 | 1.635497 | -2.931235 | 3.034968 |
| 57 | 1 | 0 | 2.582734 | -2.653020 | 3.504975 |
| 58 | 1 | 0 | 1.358074 | -3.919772 | 3.425264 |
| 59 | 1 | 0 | 0.866322 | -2.229928 | 3.381832 |
| 60 | 6 | 0 | 4.211877 | -2.152613 | 1.216592 |
| 61 | 1 | 0 | 4.983904 | -2.923799 | 1.085688 |
| 62 | 1 | 0 | 4.187101 | -1.885123 | 2.276447 |
| 63 | 1 | 0 | 4.535566 | -1.261255 | 0.668486 |
| 64 | 6 | 0 | 3.459142 | -2.833168 | -1.778819 |
| 65 | 1 | 0 | 2.935738 | -2.631272 | -2.719927 |
| 66 | 1 | 0 | 3.981332 | -3.793083 | -1.906477 |
| 67 | 1 | 0 | 4.224203 | -2.062968 | -1.652863 |
| 68 | 71 | 0 | 1.053394 | -0.760043 | 0.144427 |
| 69 | 6 | 0 | -0.197354 | -0.268376 | -2.170456 |
| 70 | 6 | 0 | 0.319659 | 2.521886 | -1.258384 |
| 71 | 6 | 0 | 0.289600 | 2.771647 | -2.644916 |
| 72 | 6 | 0 | 1.042903 | 3.431515 | -0.458918 |
| 73 | 6 | 0 | 0.963267 | 3.857624 | -3.199210 |
| 74 | 1 | 0 | -0.290553 | 2.110947 | -3.283699 |
| 75 | 6 | 0 | 1.717562 | 4.507995 | -1.015049 |
| 76 | 1 | 0 | 1.055347 | 3.265433 | 0.614462 |
| 77 | 6 | 0 | 1.691825 | 4.729007 | -2.394334 |
| 78 | 1 | 0 | 0.915278 | 4.022534 | -4.273579 |
| 79 | 1 | 0 | 2.265634 | 5.188440 | -0.366426 |
| 80 | 1 | 0 | 2.222556 | 5.571583 | -2.829442 |
| 81 | 6 | 0 | -2.096531 | 2.648531 | 0.528348 |
| 82 | 6 | 0 | -2.513091 | 2.864552 | 1.852811 |
| 83 | 6 | 0 | -2.380030 | 3.652781 | -0.411325 |
| 84 | 6 | 0 | -3.162515 | 4.035956 | 2.225634 |
| 85 | 1 | 0 | -2.325524 | 2.093937 | 2.595475 |

| | | | | | |
|---|---|---|---|---|---|
| 86 | 6 | 0 | -3.034337 | 4.821846 | -0.040946 |
| 87 | 1 | 0 | -2.080216 | 3.506022 | -1.443493 |
| 88 | 6 | 0 | -3.427354 | 5.024677 | 1.280825 |
| 89 | 1 | 0 | -3.467938 | 4.173974 | 3.260162 |
| 90 | 1 | 0 | -3.240835 | 5.580094 | -0.792754 |
| 91 | 1 | 0 | -3.938429 | 5.939780 | 1.569316 |
| 92 | 6 | 0 | -1.173463 | -1.019838 | -2.365428 |
| 93 | 1 | 0 | 0.742586 | 0.065732 | -2.580658 |
| 94 | 6 | 0 | -2.452808 | -1.616971 | -2.285043 |
| 95 | 6 | 0 | -2.851072 | -2.367765 | -1.160636 |
| 96 | 6 | 0 | -3.367779 | -1.459654 | -3.346283 |
| 97 | 6 | 0 | -4.111731 | -2.942944 | -1.112250 |
| 98 | 1 | 0 | -2.181855 | -2.424982 | -0.309300 |
| 99 | 6 | 0 | -4.634432 | -2.023958 | -3.274575 |
| 100 | 1 | 0 | -3.069214 | -0.885284 | -4.218484 |
| 101 | 6 | 0 | -5.013864 | -2.774352 | -2.162355 |
| 102 | 1 | 0 | -4.407073 | -3.485993 | -0.218876 |
| 103 | 1 | 0 | -5.330848 | -1.878900 | -4.097148 |
| 104 | 1 | 0 | -6.008400 | -3.208447 | -2.106662 |

**IM1'a**
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.933461
Thermal correction to Gibbs Free Energy = 0.790281
Sum of electronic and thermal Enthalpies = -2024.115397
Sum of electronic and thermal Free Energies = -2024.258577
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.982742

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.345501 | -0.985088 | -0.936367 |
| 2 | 7 | 0 | -2.751788 | 1.746146 | 0.527263 |
| 3 | 7 | 0 | -1.759940 | 1.561565 | -1.478951 |
| 4 | 6 | 0 | 1.566192 | -0.865720 | -0.639706 |
| 5 | 6 | 0 | 2.225972 | 0.432567 | -0.161309 |
| 6 | 6 | 0 | 1.615596 | 1.299683 | 0.696121 |
| 7 | 6 | 0 | 2.509542 | -2.030429 | -0.790135 |
| 8 | 6 | 0 | 2.306386 | -2.959593 | -1.813983 |
| 9 | 1 | 0 | 1.487855 | -2.779166 | -2.506318 |
| 10 | 6 | 0 | 3.118024 | -4.082473 | -1.925650 |
| 11 | 1 | 0 | 2.956729 | -4.790410 | -2.735584 |
| 12 | 6 | 0 | 4.133764 | -4.305424 | -0.995372 |
| 13 | 1 | 0 | 4.763115 | -5.188867 | -1.073991 |
| 14 | 6 | 0 | 4.330882 | -3.393982 | 0.039320 |
| 15 | 1 | 0 | 5.102527 | -3.571239 | 0.784454 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 3.533608 | -2.257279 | 0.132812 |
| 17 | 1 | 0 | 3.674879 | -1.557197 | 0.952038 |
| 18 | 6 | 0 | -3.170625 | 2.483951 | 1.703887 |
| 19 | 1 | 0 | -2.496806 | 3.338831 | 1.891279 |
| 20 | 6 | 0 | -4.595592 | 3.029068 | 1.559229 |
| 21 | 1 | 0 | -4.697390 | 3.673378 | 0.679923 |
| 22 | 1 | 0 | -4.890115 | 3.606249 | 2.444384 |
| 23 | 1 | 0 | -5.299680 | 2.199083 | 1.442611 |
| 24 | 6 | 0 | -3.074010 | 1.575184 | 2.925106 |
| 25 | 1 | 0 | -3.779185 | 0.743238 | 2.829981 |
| 26 | 1 | 0 | -3.315018 | 2.125960 | 3.841781 |
| 27 | 1 | 0 | -2.070893 | 1.144711 | 3.008606 |
| 28 | 6 | 0 | -2.266077 | 2.364729 | -0.546889 |
| 29 | 6 | 0 | -2.180448 | 3.872090 | -0.675732 |
| 30 | 1 | 0 | -1.129520 | 4.181411 | -0.634772 |
| 31 | 1 | 0 | -2.714960 | 4.389318 | 0.119215 |
| 32 | 1 | 0 | -2.586259 | 4.204468 | -1.635155 |
| 33 | 6 | 0 | -1.224273 | 2.089110 | -2.716037 |
| 34 | 1 | 0 | -0.861338 | 3.120398 | -2.579086 |
| 35 | 6 | 0 | -2.303373 | 2.117711 | -3.801985 |
| 36 | 1 | 0 | -2.642247 | 1.098324 | -4.012789 |
| 37 | 1 | 0 | -1.923058 | 2.555834 | -4.732928 |
| 38 | 1 | 0 | -3.175690 | 2.695014 | -3.476649 |
| 39 | 6 | 0 | -0.026830 | 1.262883 | -3.167537 |
| 40 | 1 | 0 | 0.756896 | 1.287070 | -2.407083 |
| 41 | 1 | 0 | 0.373316 | 1.646564 | -4.113730 |
| 42 | 1 | 0 | -0.308930 | 0.213928 | -3.300285 |
| 43 | 6 | 0 | -3.098234 | -2.459677 | 0.632423 |
| 44 | 6 | 0 | -2.315716 | -2.848564 | -0.489988 |
| 45 | 6 | 0 | -2.753124 | -2.095740 | -1.614721 |
| 46 | 6 | 0 | -3.818682 | -1.254942 | -1.194680 |
| 47 | 6 | 0 | -4.030005 | -1.480714 | 0.190454 |
| 48 | 6 | 0 | -3.048985 | -3.046783 | 2.011393 |
| 49 | 1 | 0 | -2.077143 | -3.497882 | 2.228903 |
| 50 | 1 | 0 | -3.812304 | -3.825683 | 2.149580 |
| 51 | 1 | 0 | -3.215762 | -2.284157 | 2.779308 |
| 52 | 6 | 0 | -1.255123 | -3.905034 | -0.550332 |
| 53 | 1 | 0 | -0.278616 | -3.473715 | -0.803650 |
| 54 | 1 | 0 | -1.496595 | -4.656320 | -1.313924 |
| 55 | 1 | 0 | -1.158892 | -4.436054 | 0.401865 |
| 56 | 6 | 0 | -2.154083 | -2.213931 | -2.981836 |
| 57 | 1 | 0 | -2.494786 | -1.411897 | -3.644345 |
| 58 | 1 | 0 | -2.412316 | -3.168983 | -3.460828 |
| 59 | 1 | 0 | -1.060026 | -2.157145 | -2.922520 |
| 60 | 6 | 0 | -4.631544 | -0.313047 | -2.028070 |
| 61 | 1 | 0 | -5.686544 | -0.618544 | -2.061293 |
| 62 | 1 | 0 | -4.269092 | -0.275650 | -3.058535 |
| 63 | 1 | 0 | -4.594973 | 0.708781 | -1.631965 |
| 64 | 6 | 0 | -5.150102 | -0.888849 | 0.984443 |
| 65 | 1 | 0 | -4.984377 | -0.992975 | 2.061094 |

| | | | | | |
|---|---|---|---|---|---|
| 66 | 1 | 0 | -6.107623 | -1.380508 | 0.757675 |
| 67 | 1 | 0 | -5.269636 | 0.177003 | 0.766748 |
| 68 | 71 | 0 | -1.610503 | -0.314675 | -0.042006 |
| 69 | 6 | 0 | 0.327260 | 0.958156 | 1.333243 |
| 70 | 6 | 0 | 2.019792 | 2.717082 | 0.870406 |
| 71 | 6 | 0 | 1.941224 | 3.310086 | 2.138271 |
| 72 | 6 | 0 | 2.363310 | 3.533684 | -0.218349 |
| 73 | 6 | 0 | 2.238961 | 4.656761 | 2.322301 |
| 74 | 1 | 0 | 1.631777 | 2.696366 | 2.980420 |
| 75 | 6 | 0 | 2.648607 | 4.881849 | -0.037787 |
| 76 | 1 | 0 | 2.398403 | 3.096828 | -1.211570 |
| 77 | 6 | 0 | 2.596730 | 5.449766 | 1.234749 |
| 78 | 1 | 0 | 2.180735 | 5.090351 | 3.317660 |
| 79 | 1 | 0 | 2.907459 | 5.494887 | -0.897528 |
| 80 | 1 | 0 | 2.820716 | 6.504255 | 1.374255 |
| 81 | 6 | 0 | 3.529514 | 0.744990 | -0.787931 |
| 82 | 6 | 0 | 3.733672 | 0.530947 | -2.159498 |
| 83 | 6 | 0 | 4.607436 | 1.222779 | -0.027748 |
| 84 | 6 | 0 | 4.957932 | 0.817492 | -2.753285 |
| 85 | 1 | 0 | 2.916299 | 0.138832 | -2.758488 |
| 86 | 6 | 0 | 5.832335 | 1.504196 | -0.619609 |
| 87 | 1 | 0 | 4.466776 | 1.367202 | 1.039503 |
| 88 | 6 | 0 | 6.013487 | 1.308132 | -1.987868 |
| 89 | 1 | 0 | 5.089531 | 0.650628 | -3.819459 |
| 90 | 1 | 0 | 6.652320 | 1.873829 | -0.008811 |
| 91 | 1 | 0 | 6.972396 | 1.525833 | -2.451126 |
| 92 | 6 | 0 | -0.088566 | -0.175755 | 1.950821 |
| 93 | 1 | 0 | -0.431408 | 1.727022 | 1.122619 |
| 94 | 6 | 0 | 0.890028 | -1.129255 | 2.461142 |
| 95 | 6 | 0 | 0.766098 | -2.508069 | 2.209198 |
| 96 | 6 | 0 | 1.956939 | -0.724161 | 3.290089 |
| 97 | 6 | 0 | 1.673701 | -3.425871 | 2.719314 |
| 98 | 1 | 0 | -0.044953 | -2.840581 | 1.570321 |
| 99 | 6 | 0 | 2.850000 | -1.645524 | 3.825615 |
| 100 | 1 | 0 | 2.066968 | 0.334438 | 3.512498 |
| 101 | 6 | 0 | 2.719766 | -3.004737 | 3.540204 |
| 102 | 1 | 0 | 1.566375 | -4.478821 | 2.470381 |
| 103 | 1 | 0 | 3.659658 | -1.299929 | 4.465588 |
| 104 | 1 | 0 | 3.422515 | -3.724762 | 3.951549 |

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**TS1'b**
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.927345
Thermal correction to Gibbs Free Energy = 0.780324
Sum of electronic and thermal Enthalpies = -2024.041871
Sum of electronic and thermal Free Energies = -2024.188892
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.917683

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | 0.977094 | -0.807052 | -0.176371 |
| 2 | 1 | 0 | -0.147073 | 0.599631 | 1.169479 |
| 3 | 7 | 0 | 0.121939 | -2.302278 | -1.785419 |
| 4 | 7 | 0 | 1.833140 | -0.962500 | -2.366710 |
| 5 | 6 | 0 | -1.510225 | 0.918589 | -1.071218 |
| 6 | 6 | 0 | -2.178483 | 0.342071 | 0.160043 |
| 7 | 6 | 0 | -2.321430 | 1.718577 | -2.059597 |
| 8 | 6 | 0 | -1.753744 | 2.881663 | -2.593368 |
| 9 | 1 | 0 | -0.775434 | 3.177748 | -2.224672 |
| 10 | 6 | 0 | -2.411046 | 3.615247 | -3.573503 |
| 11 | 1 | 0 | -1.958543 | 4.524370 | -3.963561 |
| 12 | 6 | 0 | -3.644748 | 3.184412 | -4.063297 |
| 13 | 1 | 0 | -4.157876 | 3.752545 | -4.835645 |
| 14 | 6 | 0 | -4.210328 | 2.017768 | -3.556540 |
| 15 | 1 | 0 | -5.166883 | 1.666135 | -3.936435 |
| 16 | 6 | 0 | -3.560133 | 1.297332 | -2.556638 |
| 17 | 1 | 0 | -4.018772 | 0.396512 | -2.160330 |
| 18 | 6 | 0 | -3.623295 | 0.576239 | 0.423200 |
| 19 | 6 | 0 | -4.093584 | 1.884006 | 0.607743 |
| 20 | 1 | 0 | -3.390333 | 2.708685 | 0.530699 |
| 21 | 6 | 0 | -5.434975 | 2.131959 | 0.874105 |
| 22 | 1 | 0 | -5.775349 | 3.154996 | 1.014335 |
| 23 | 6 | 0 | -6.342107 | 1.076806 | 0.955174 |
| 24 | 1 | 0 | -7.392125 | 1.270203 | 1.159370 |
| 25 | 6 | 0 | -5.890256 | -0.227117 | 0.771284 |
| 26 | 1 | 0 | -6.587213 | -1.059438 | 0.833143 |
| 27 | 6 | 0 | -4.545383 | -0.474169 | 0.509991 |
| 28 | 1 | 0 | -4.200285 | -1.492214 | 0.360477 |
| 29 | 6 | 0 | -1.041548 | -3.122364 | -2.044527 |
| 30 | 1 | 0 | -0.875827 | -3.749995 | -2.938061 |
| 31 | 6 | 0 | -1.241279 | -4.066496 | -0.863980 |
| 32 | 1 | 0 | -0.371442 | -4.714514 | -0.731975 |
| 33 | 1 | 0 | -2.132180 | -4.690393 | -0.998170 |
| 34 | 1 | 0 | -1.364311 | -3.480459 | 0.053297 |
| 35 | 6 | 0 | -2.312682 | -2.297884 | -2.266021 |
| 36 | 1 | 0 | -2.525505 | -1.716554 | -1.364532 |
| 37 | 1 | 0 | -3.172127 | -2.945719 | -2.479268 |
| 38 | 1 | 0 | -2.202247 | -1.586621 | -3.088422 |
| 39 | 6 | 0 | 0.775772 | -1.666202 | -2.758601 |
| 40 | 6 | 0 | 0.294471 | -1.646411 | -4.190024 |
| 41 | 1 | 0 | -0.305802 | -0.740923 | -4.335755 |
| 42 | 1 | 0 | -0.331070 | -2.508768 | -4.425671 |
| 43 | 1 | 0 | 1.128407 | -1.616326 | -4.893783 |
| 44 | 6 | 0 | 2.423228 | 0.040470 | -3.233465 |
| 45 | 1 | 0 | 1.675247 | 0.438516 | -3.937165 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 6 | 0 | 2.877064 | 1.217060 | -2.371576 |
| 47 | 1 | 0 | 2.009199 | 1.656769 | -1.869565 |
| 48 | 1 | 0 | 3.366604 | 1.989940 | -2.975940 |
| 49 | 1 | 0 | 3.593732 | 0.872302 | -1.615209 |
| 50 | 6 | 0 | 3.596244 | -0.519464 | -4.042974 |
| 51 | 1 | 0 | 4.399273 | -0.837765 | -3.371196 |
| 52 | 1 | 0 | 3.999067 | 0.236977 | -4.727814 |
| 53 | 1 | 0 | 3.296159 | -1.391048 | -4.634271 |
| 54 | 6 | 0 | 3.196034 | -0.950082 | 1.329356 |
| 55 | 6 | 0 | 3.400037 | -1.937264 | 0.330232 |
| 56 | 6 | 0 | 2.472339 | -2.986846 | 0.545733 |
| 57 | 6 | 0 | 1.689565 | -2.657136 | 1.684003 |
| 58 | 6 | 0 | 2.135236 | -1.396128 | 2.172353 |
| 59 | 6 | 0 | 4.061760 | 0.247341 | 1.575128 |
| 60 | 1 | 0 | 4.477709 | 0.649225 | 0.644153 |
| 61 | 1 | 0 | 4.913247 | 0.000370 | 2.225175 |
| 62 | 1 | 0 | 3.502581 | 1.055193 | 2.053321 |
| 63 | 6 | 0 | 4.476886 | -1.966821 | -0.706494 |
| 64 | 1 | 0 | 4.083943 | -2.315007 | -1.666036 |
| 65 | 1 | 0 | 5.298031 | -2.636224 | -0.410967 |
| 66 | 1 | 0 | 4.912980 | -0.976147 | -0.869843 |
| 67 | 6 | 0 | 2.414323 | -4.239751 | -0.272549 |
| 68 | 1 | 0 | 1.762998 | -4.987089 | 0.190860 |
| 69 | 1 | 0 | 3.409712 | -4.692443 | -0.370506 |
| 70 | 1 | 0 | 2.032396 | -4.046957 | -1.282653 |
| 71 | 6 | 0 | 0.702679 | -3.551271 | 2.371175 |
| 72 | 1 | 0 | 0.222526 | -4.242448 | 1.672203 |
| 73 | 1 | 0 | -0.092827 | -2.983601 | 2.861103 |
| 74 | 1 | 0 | 1.190878 | -4.160039 | 3.145655 |
| 75 | 6 | 0 | 1.724520 | -0.761608 | 3.465046 |
| 76 | 1 | 0 | 1.757741 | 0.330370 | 3.405171 |
| 77 | 1 | 0 | 2.388125 | -1.071127 | 4.285651 |
| 78 | 1 | 0 | 0.704908 | -1.036955 | 3.747202 |
| 79 | 6 | 0 | 0.840839 | 1.451112 | 1.148759 |
| 80 | 6 | 0 | 1.418027 | 2.522825 | 1.303639 |
| 81 | 6 | 0 | 2.156700 | 3.730626 | 1.433296 |
| 82 | 6 | 0 | 1.795258 | 4.707844 | 2.376392 |
| 83 | 6 | 0 | 3.276359 | 3.966267 | 0.614826 |
| 84 | 6 | 0 | 2.530036 | 5.881277 | 2.494021 |
| 85 | 1 | 0 | 0.931789 | 4.530074 | 3.010122 |
| 86 | 6 | 0 | 4.007467 | 5.139997 | 0.742761 |
| 87 | 1 | 0 | 3.554255 | 3.214026 | -0.117100 |
| 88 | 6 | 0 | 3.639770 | 6.103815 | 1.680805 |
| 89 | 1 | 0 | 2.235132 | 6.627123 | 3.227831 |
| 90 | 1 | 0 | 4.870442 | 5.305050 | 0.102810 |
| 91 | 1 | 0 | 4.213521 | 7.021663 | 1.776734 |
| 92 | 7 | 0 | -0.271186 | 0.754048 | -1.286833 |
| 93 | 6 | 0 | -1.354426 | -0.234249 | 1.081160 |
| 94 | 6 | 0 | -1.857296 | -0.687857 | 2.384848 |
| 95 | 6 | 0 | -1.711084 | 0.136083 | 3.515824 |

| | | | | | |
|---|---|---|---|---|---|
| 96 | 6 | 0 | -2.447526 | -1.947503 | 2.578603 |
| 97 | 6 | 0 | -2.140932 | -0.277316 | 4.771525 |
| 98 | 1 | 0 | -1.247920 | 1.111348 | 3.391214 |
| 99 | 6 | 0 | -2.875547 | -2.362525 | 3.835986 |
| 100 | 1 | 0 | -2.556356 | -2.612101 | 1.726173 |
| 101 | 6 | 0 | -2.726305 | -1.530890 | 4.942930 |
| 102 | 1 | 0 | -2.015634 | 0.385339 | 5.624841 |
| 103 | 1 | 0 | -3.327042 | -3.345468 | 3.949751 |
| 104 | 1 | 0 | -3.058902 | -1.855125 | 5.925438 |

**IM1'b**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.933571
Thermal correction to Gibbs Free Energy = 0.783981
Sum of electronic and thermal Enthalpies = -2024.108322
Sum of electronic and thermal Free Energies = -2024.257911
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.986666

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | 1.739407 | 0.016323 | -0.395310 |
| 2 | 1 | 0 | -2.615382 | -0.842459 | 0.063987 |
| 3 | 7 | 0 | 3.251468 | 1.128061 | 1.112760 |
| 4 | 7 | 0 | 3.674251 | -1.002222 | 0.548388 |
| 5 | 6 | 0 | -1.034226 | 0.616621 | 1.327747 |
| 6 | 6 | 0 | -2.290366 | 1.115401 | 0.632602 |
| 7 | 6 | 0 | -1.247918 | -0.225824 | 2.556402 |
| 8 | 6 | 0 | -0.180399 | -0.975401 | 3.062337 |
| 9 | 1 | 0 | 0.771811 | -0.912670 | 2.543769 |
| 10 | 6 | 0 | -0.349139 | -1.792397 | 4.172375 |
| 11 | 1 | 0 | 0.486188 | -2.383158 | 4.540120 |
| 12 | 6 | 0 | -1.590853 | -1.868014 | 4.805895 |
| 13 | 1 | 0 | -1.725304 | -2.512358 | 5.671305 |
| 14 | 6 | 0 | -2.657754 | -1.116870 | 4.318943 |
| 15 | 1 | 0 | -3.628706 | -1.169527 | 4.805616 |
| 16 | 6 | 0 | -2.486887 | -0.304863 | 3.199975 |
| 17 | 1 | 0 | -3.324926 | 0.263354 | 2.806998 |
| 18 | 6 | 0 | -2.628355 | 2.544308 | 0.775516 |
| 19 | 6 | 0 | -3.954932 | 2.944182 | 1.002801 |
| 20 | 1 | 0 | -4.734896 | 2.188185 | 1.019966 |
| 21 | 6 | 0 | -4.273381 | 4.282510 | 1.199111 |
| 22 | 1 | 0 | -5.307843 | 4.568378 | 1.373272 |
| 23 | 6 | 0 | -3.272921 | 5.253578 | 1.180021 |
| 24 | 1 | 0 | -3.522400 | 6.300572 | 1.332234 |
| 25 | 6 | 0 | -1.950899 | 4.867462 | 0.971378 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | -1.159463 | 5.612718 | 0.960022 |
| 27 | 6 | 0 | -1.629252 | 3.528332 | 0.777236 |
| 28 | 1 | 0 | -0.603268 | 3.213950 | 0.618700 |
| 29 | 6 | 0 | 3.160735 | 2.229218 | 2.048252 |
| 30 | 1 | 0 | 4.161030 | 2.491563 | 2.439783 |
| 31 | 6 | 0 | 2.634714 | 3.449564 | 1.300330 |
| 32 | 1 | 0 | 3.308500 | 3.724590 | 0.484815 |
| 33 | 1 | 0 | 2.520239 | 4.308547 | 1.970894 |
| 34 | 1 | 0 | 1.656299 | 3.211171 | 0.869702 |
| 35 | 6 | 0 | 2.245006 | 1.909534 | 3.233946 |
| 36 | 1 | 0 | 1.252958 | 1.647291 | 2.853617 |
| 37 | 1 | 0 | 2.157678 | 2.766498 | 3.913052 |
| 38 | 1 | 0 | 2.618402 | 1.057484 | 3.811292 |
| 39 | 6 | 0 | 3.893334 | 0.001653 | 1.398344 |
| 40 | 6 | 0 | 4.763108 | -0.168978 | 2.627206 |
| 41 | 1 | 0 | 4.250192 | -0.803855 | 3.357986 |
| 42 | 1 | 0 | 4.983273 | 0.786454 | 3.104529 |
| 43 | 1 | 0 | 5.707242 | -0.658297 | 2.378122 |
| 44 | 6 | 0 | 4.349977 | -2.273871 | 0.686792 |
| 45 | 1 | 0 | 4.452873 | -2.551048 | 1.751394 |
| 46 | 6 | 0 | 3.518792 | -3.359436 | 0.013610 |
| 47 | 1 | 0 | 2.512940 | -3.405112 | 0.437820 |
| 48 | 1 | 0 | 4.001942 | -4.339115 | 0.106763 |
| 49 | 1 | 0 | 3.400517 | -3.130669 | -1.051611 |
| 50 | 6 | 0 | 5.756187 | -2.240370 | 0.074880 |
| 51 | 1 | 0 | 5.685181 | -2.050147 | -0.999968 |
| 52 | 1 | 0 | 6.276258 | -3.194647 | 0.224517 |
| 53 | 1 | 0 | 6.370899 | -1.444846 | 0.508863 |
| 54 | 6 | 0 | 1.800575 | -0.538815 | -3.018456 |
| 55 | 6 | 0 | 3.008939 | 0.160136 | -2.764196 |
| 56 | 6 | 0 | 2.679296 | 1.494930 | -2.400257 |
| 57 | 6 | 0 | 1.262833 | 1.623227 | -2.435992 |
| 58 | 6 | 0 | 0.719502 | 0.362518 | -2.807307 |
| 59 | 6 | 0 | 1.658276 | -1.952465 | -3.492001 |
| 60 | 1 | 0 | 2.574868 | -2.527479 | -3.324785 |
| 61 | 1 | 0 | 1.438271 | -1.997035 | -4.568003 |
| 62 | 1 | 0 | 0.852748 | -2.466159 | -2.957944 |
| 63 | 6 | 0 | 4.405372 | -0.350233 | -2.934233 |
| 64 | 1 | 0 | 5.056927 | -0.011355 | -2.121817 |
| 65 | 1 | 0 | 4.851651 | -0.006704 | -3.879026 |
| 66 | 1 | 0 | 4.435588 | -1.444249 | -2.941112 |
| 67 | 6 | 0 | 3.682906 | 2.576671 | -2.141166 |
| 68 | 1 | 0 | 3.192481 | 3.511121 | -1.854013 |
| 69 | 1 | 0 | 4.284807 | 2.787150 | -3.036330 |
| 70 | 1 | 0 | 4.373462 | 2.307911 | -1.333006 |
| 71 | 6 | 0 | 0.473732 | 2.871902 | -2.186389 |
| 72 | 1 | 0 | 0.981338 | 3.540839 | -1.483340 |
| 73 | 1 | 0 | -0.504822 | 2.642431 | -1.755514 |
| 74 | 1 | 0 | 0.303924 | 3.439680 | -3.111998 |
| 75 | 6 | 0 | -0.730476 | 0.035357 | -2.990179 |

| | | | | | |
|---|---|---|---|---|---|
| 76 | 1 | 0 | -0.958303 | -0.967876 | -2.615791 |
| 77 | 1 | 0 | -1.030239 | 0.079180 | -4.046669 |
| 78 | 1 | 0 | -1.371790 | 0.728035 | -2.438569 |
| 79 | 6 | 0 | 0.395487 | -1.975648 | -0.318331 |
| 80 | 6 | 0 | -0.604669 | -2.695516 | -0.227039 |
| 81 | 6 | 0 | -1.839152 | -3.388462 | -0.084044 |
| 82 | 6 | 0 | -2.483249 | -3.448104 | 1.168736 |
| 83 | 6 | 0 | -2.492690 | -3.959048 | -1.192819 |
| 84 | 6 | 0 | -3.731814 | -4.043631 | 1.296422 |
| 85 | 1 | 0 | -1.996279 | -2.997620 | 2.028382 |
| 86 | 6 | 0 | -3.740225 | -4.556276 | -1.055807 |
| 87 | 1 | 0 | -2.010163 | -3.904968 | -2.164145 |
| 88 | 6 | 0 | -4.370034 | -4.600937 | 0.187877 |
| 89 | 1 | 0 | -4.213952 | -4.061835 | 2.270819 |
| 90 | 1 | 0 | -4.230338 | -4.980435 | -1.928958 |
| 91 | 1 | 0 | -5.349590 | -5.060610 | 0.290844 |
| 92 | 7 | 0 | 0.093762 | 0.845903 | 0.822766 |
| 93 | 6 | 0 | -2.965056 | 0.180561 | -0.069852 |
| 94 | 6 | 0 | -4.054371 | 0.300328 | -1.040192 |
| 95 | 6 | 0 | -4.858405 | -0.829295 | -1.267888 |
| 96 | 6 | 0 | -4.298569 | 1.450452 | -1.808874 |
| 97 | 6 | 0 | -5.892570 | -0.797708 | -2.196152 |
| 98 | 1 | 0 | -4.655186 | -1.741158 | -0.710337 |
| 99 | 6 | 0 | -5.329907 | 1.477647 | -2.739224 |
| 100 | 1 | 0 | -3.661220 | 2.319394 | -1.681416 |
| 101 | 6 | 0 | -6.138992 | 0.358317 | -2.933605 |
| 102 | 1 | 0 | -6.500224 | -1.685868 | -2.351314 |
| 103 | 1 | 0 | -5.495692 | 2.377010 | -3.327201 |
| 104 | 1 | 0 | -6.942646 | 0.383148 | -3.665113 |

**TS2**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.931891
Thermal correction to Gibbs Free Energy = 0.789106
Sum of electronic and thermal Enthalpies = -2024.081933
Sum of electronic and thermal Free Energies = -2024.224719
298 K, in THF
Sum of electronic and thermal Free Energies = -3220.948425

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | 1.429424 | 0.057938 | -0.416870 |
| 2 | 6 | 0 | -0.576793 | -0.267927 | 0.924949 |
| 3 | 7 | 0 | 0.138326 | 2.018766 | -0.338389 |
| 4 | 6 | 0 | -1.047054 | 1.997564 | 0.258389 |
| 5 | 6 | 0 | -1.513023 | 0.816092 | 0.889744 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -1.853571 | 3.251325 | 0.264428 |
| 7 | 6 | 0 | -2.529066 | 3.668117 | 1.417709 |
| 8 | 6 | 0 | -3.230516 | 4.867743 | 1.434031 |
| 9 | 6 | 0 | -3.278556 | 5.670315 | 0.294976 |
| 10 | 6 | 0 | -2.615645 | 5.263562 | -0.860123 |
| 11 | 6 | 0 | -1.905612 | 4.066841 | -0.872450 |
| 12 | 7 | 0 | 2.696479 | -1.400218 | 0.988993 |
| 13 | 6 | 0 | 3.235549 | -0.408353 | 1.685662 |
| 14 | 6 | 0 | 4.268368 | -0.621338 | 2.773032 |
| 15 | 7 | 0 | 2.837359 | 0.814224 | 1.333530 |
| 16 | 6 | 0 | 3.054355 | 1.962660 | 2.177966 |
| 17 | 6 | 0 | 3.080614 | 3.230203 | 1.330681 |
| 18 | 6 | 0 | 1.528566 | 0.495270 | -3.036916 |
| 19 | 6 | 0 | 2.121907 | -0.789171 | -2.879160 |
| 20 | 6 | 0 | 3.381396 | -0.610370 | -2.243565 |
| 21 | 6 | 0 | 3.562449 | 0.776471 | -2.006372 |
| 22 | 6 | 0 | 2.424380 | 1.461869 | -2.504358 |
| 23 | 6 | 0 | 0.220156 | 0.772375 | -3.710450 |
| 24 | 6 | 0 | 1.546681 | -2.067342 | -3.411158 |
| 25 | 6 | 0 | 4.433738 | -1.640390 | -1.970611 |
| 26 | 6 | 0 | 4.802854 | 1.382826 | -1.427190 |
| 27 | 6 | 0 | 2.255178 | 2.948916 | -2.566553 |
| 28 | 6 | 0 | 2.983291 | -2.797403 | 1.234409 |
| 29 | 6 | 0 | 2.308731 | -3.612706 | 0.135193 |
| 30 | 6 | 0 | 2.471305 | -3.283326 | 2.594317 |
| 31 | 6 | 0 | 1.947493 | 2.059164 | 3.234117 |
| 32 | 1 | 0 | 1.207981 | 3.222088 | -2.731608 |
| 33 | 1 | 0 | 2.831534 | 3.390240 | -3.391762 |
| 34 | 1 | 0 | 2.584640 | 3.443144 | -1.645278 |
| 35 | 1 | 0 | 2.071383 | -2.942714 | -3.016618 |
| 36 | 1 | 0 | 1.612859 | -2.114757 | -4.507224 |
| 37 | 1 | 0 | 0.492185 | -2.176061 | -3.134701 |
| 38 | 1 | 0 | -0.475961 | -0.059767 | -3.569885 |
| 39 | 1 | 0 | 0.335861 | 0.940034 | -4.791194 |
| 40 | 1 | 0 | -0.265760 | 1.657692 | -3.286514 |
| 41 | 1 | 0 | 4.022132 | 1.899715 | 2.706064 |
| 42 | 1 | 0 | 4.072092 | -2.993004 | 1.178938 |
| 43 | 1 | 0 | 4.770410 | 2.475729 | -1.478116 |
| 44 | 1 | 0 | 5.698505 | 1.058764 | -1.975407 |
| 45 | 1 | 0 | 4.941766 | 1.106698 | -0.374587 |
| 46 | 1 | 0 | 4.639108 | -1.746389 | -0.898713 |
| 47 | 1 | 0 | 5.380360 | -1.370060 | -2.458944 |
| 48 | 1 | 0 | 4.147025 | -2.624828 | -2.351850 |
| 49 | 1 | 0 | 5.060696 | 0.127986 | 2.692068 |
| 50 | 1 | 0 | 4.722109 | -1.610936 | 2.703546 |
| 51 | 1 | 0 | 3.817101 | -0.520192 | 3.765667 |
| 52 | 1 | 0 | 3.879818 | 3.182211 | 0.586409 |
| 53 | 1 | 0 | 3.231021 | 4.119732 | 1.953029 |
| 54 | 1 | 0 | 2.125962 | 3.331688 | 0.805031 |
| 55 | 1 | 0 | 0.976194 | 2.111586 | 2.729607 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 1 | 0 | 2.068192 | 2.943349 | 3.872826 |
| 57 | 1 | 0 | 1.943110 | 1.169194 | 3.872349 |
| 58 | 1 | 0 | 1.225184 | -3.457765 | 0.180192 |
| 59 | 1 | 0 | 2.512486 | -4.683003 | 0.251639 |
| 60 | 1 | 0 | 2.652720 | -3.295353 | -0.850780 |
| 61 | 1 | 0 | 2.933312 | -2.752123 | 3.430340 |
| 62 | 1 | 0 | 2.675656 | -4.353632 | 2.722484 |
| 63 | 1 | 0 | 1.392311 | -3.127401 | 2.657601 |
| 64 | 1 | 0 | -2.493993 | 3.034360 | 2.298340 |
| 65 | 1 | 0 | -1.401947 | 3.738484 | -1.778567 |
| 66 | 1 | 0 | -3.744293 | 5.178177 | 2.340221 |
| 67 | 1 | 0 | -2.655383 | 5.876963 | -1.756798 |
| 68 | 1 | 0 | -3.831910 | 6.605862 | 0.307614 |
| 69 | 1 | 0 | 0.391637 | 2.952312 | -0.643201 |
| 70 | 6 | 0 | -0.703175 | -1.075103 | -0.853317 |
| 71 | 6 | 0 | -1.724866 | -1.551982 | -1.367325 |
| 72 | 6 | 0 | -2.929819 | -2.109497 | -1.874935 |
| 73 | 6 | 0 | -3.085774 | -2.402891 | -3.241016 |
| 74 | 6 | 0 | -3.999482 | -2.377173 | -0.999332 |
| 75 | 6 | 0 | -4.273670 | -2.946837 | -3.714606 |
| 76 | 1 | 0 | -2.262255 | -2.196225 | -3.918651 |
| 77 | 6 | 0 | -5.181696 | -2.920901 | -1.483466 |
| 78 | 1 | 0 | -3.892747 | -2.126757 | 0.052072 |
| 79 | 6 | 0 | -5.326797 | -3.210175 | -2.839986 |
| 80 | 1 | 0 | -4.378166 | -3.166416 | -4.774360 |
| 81 | 1 | 0 | -6.001135 | -3.105721 | -0.793614 |
| 82 | 1 | 0 | -6.255684 | -3.632961 | -3.214065 |
| 83 | 6 | 0 | -0.754042 | -1.345993 | 1.901382 |
| 84 | 6 | 0 | -1.148520 | -2.673795 | 1.662432 |
| 85 | 6 | 0 | -0.459146 | -1.005472 | 3.243903 |
| 86 | 6 | 0 | -1.260012 | -3.596238 | 2.701934 |
| 87 | 1 | 0 | -1.387390 | -2.971732 | 0.648400 |
| 88 | 6 | 0 | -0.582307 | -1.923228 | 4.275183 |
| 89 | 1 | 0 | -0.136275 | 0.010395 | 3.451346 |
| 90 | 6 | 0 | -0.987919 | -3.235916 | 4.017316 |
| 91 | 1 | 0 | -1.575509 | -4.611628 | 2.471244 |
| 92 | 1 | 0 | -0.351420 | -1.614150 | 5.292668 |
| 93 | 1 | 0 | -1.079388 | -3.958301 | 4.823880 |
| 94 | 6 | 0 | -2.968217 | 0.593984 | 1.072125 |
| 95 | 6 | 0 | -3.520685 | -0.019262 | 2.210855 |
| 96 | 6 | 0 | -3.855225 | 0.908949 | 0.025268 |
| 97 | 6 | 0 | -4.882094 | -0.298037 | 2.294200 |
| 98 | 1 | 0 | -2.871688 | -0.282927 | 3.038252 |
| 99 | 6 | 0 | -5.216985 | 0.645197 | 0.112746 |
| 100 | 1 | 0 | -3.452454 | 1.346485 | -0.883546 |
| 101 | 6 | 0 | -5.742177 | 0.034404 | 1.249280 |
| 102 | 1 | 0 | -5.272894 | -0.776261 | 3.189686 |
| 103 | 1 | 0 | -5.865888 | 0.892372 | -0.723901 |
| 104 | 1 | 0 | -6.804849 | -0.185315 | 1.317181 |

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**3a**
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.935255
Thermal correction to Gibbs Free Energy = 0.795281
Sum of electronic and thermal Enthalpies = -2024.167505
Sum of electronic and thermal Free Energies = -2024.307478
298 K, in THF
Sum of electronic and thermal Free Energies = -3221.028175

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | 1.233700 | -0.237033 | -0.499196 |
| 2 | 7 | 0 | -0.789253 | -1.223496 | -0.878460 |
| 3 | 1 | 0 | -0.776984 | -2.115362 | -1.359342 |
| 4 | 7 | 0 | 0.766205 | 1.329437 | -2.212835 |
| 5 | 7 | 0 | 2.074102 | 1.993580 | -0.516544 |
| 6 | 6 | 0 | 0.707529 | -0.340935 | 1.953348 |
| 7 | 6 | 0 | -0.306764 | 0.352694 | 1.603516 |
| 8 | 6 | 0 | -1.302546 | 0.978306 | 0.930594 |
| 9 | 6 | 0 | -2.380599 | 0.127466 | 0.353083 |
| 10 | 6 | 0 | -2.043647 | -0.967307 | -0.432073 |
| 11 | 6 | 0 | 1.115634 | -1.040496 | 3.153738 |
| 12 | 6 | 0 | 0.545815 | -2.287647 | 3.471289 |
| 13 | 1 | 0 | -0.231196 | -2.680496 | 2.821611 |
| 14 | 6 | 0 | 0.968881 | -3.006130 | 4.583263 |
| 15 | 1 | 0 | 0.511602 | -3.968456 | 4.802104 |
| 16 | 6 | 0 | 1.965949 | -2.501639 | 5.417652 |
| 17 | 1 | 0 | 2.297603 | -3.065717 | 6.285207 |
| 18 | 6 | 0 | 2.530670 | -1.262501 | 5.120304 |
| 19 | 1 | 0 | 3.307554 | -0.851921 | 5.761460 |
| 20 | 6 | 0 | 2.118152 | -0.543717 | 4.004221 |
| 21 | 1 | 0 | 2.577834 | 0.412237 | 3.772409 |
| 22 | 6 | 0 | -1.381020 | 2.450346 | 0.937624 |
| 23 | 6 | 0 | -0.490473 | 3.220338 | 1.708518 |
| 24 | 1 | 0 | 0.237066 | 2.704021 | 2.327031 |
| 25 | 6 | 0 | -0.525709 | 4.607702 | 1.695029 |
| 26 | 1 | 0 | 0.189310 | 5.164509 | 2.296660 |
| 27 | 6 | 0 | -1.472146 | 5.285583 | 0.924402 |
| 28 | 1 | 0 | -1.504096 | 6.371842 | 0.914338 |
| 29 | 6 | 0 | -2.383871 | 4.539928 | 0.180386 |
| 30 | 1 | 0 | -3.140233 | 5.043762 | -0.417095 |
| 31 | 6 | 0 | -2.343573 | 3.149000 | 0.188094 |
| 32 | 1 | 0 | -3.064138 | 2.588848 | -0.396169 |
| 33 | 6 | 0 | -3.762423 | 0.432658 | 0.749651 |
| 34 | 6 | 0 | -4.038722 | 0.929176 | 2.038736 |
| 35 | 1 | 0 | -3.211529 | 1.053012 | 2.732328 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | -5.331090 | 1.251859 | 2.433588 |
| 37 | 1 | 0 | -5.503400 | 1.626419 | 3.440349 |
| 38 | 6 | 0 | -6.402111 | 1.097035 | 1.554892 |
| 39 | 1 | 0 | -7.413006 | 1.351549 | 1.862912 |
| 40 | 6 | 0 | -6.148998 | 0.627456 | 0.266390 |
| 41 | 1 | 0 | -6.966107 | 0.519011 | -0.443682 |
| 42 | 6 | 0 | -4.855748 | 0.315657 | -0.132819 |
| 43 | 1 | 0 | -4.674336 | -0.018178 | -1.149900 |
| 44 | 6 | 0 | -3.052598 | -2.010593 | -0.784167 |
| 45 | 6 | 0 | -3.797568 | -2.663674 | 0.204482 |
| 46 | 1 | 0 | -3.680414 | -2.347785 | 1.236659 |
| 47 | 6 | 0 | -4.677534 | -3.687203 | -0.129296 |
| 48 | 1 | 0 | -5.245588 | -4.184401 | 0.652987 |
| 49 | 6 | 0 | -4.833148 | -4.076404 | -1.458735 |
| 50 | 1 | 0 | -5.524042 | -4.874366 | -1.718747 |
| 51 | 6 | 0 | -4.093200 | -3.437382 | -2.451223 |
| 52 | 1 | 0 | -4.208393 | -3.731286 | -3.491740 |
| 53 | 6 | 0 | -3.205382 | -2.419773 | -2.115018 |
| 54 | 1 | 0 | -2.628356 | -1.917466 | -2.887903 |
| 55 | 6 | 0 | -0.171777 | 1.505503 | -3.303295 |
| 56 | 1 | 0 | 0.191201 | 2.291327 | -3.990420 |
| 57 | 6 | 0 | -0.245281 | 0.205891 | -4.097591 |
| 58 | 1 | 0 | 0.734121 | -0.067880 | -4.496677 |
| 59 | 1 | 0 | -0.952612 | 0.293233 | -4.930088 |
| 60 | 1 | 0 | -0.583086 | -0.591865 | -3.427417 |
| 61 | 6 | 0 | -1.573169 | 1.891747 | -2.830785 |
| 62 | 1 | 0 | -1.938847 | 1.143350 | -2.119877 |
| 63 | 1 | 0 | -2.271006 | 1.949981 | -3.675646 |
| 64 | 1 | 0 | -1.574240 | 2.856732 | -2.319824 |
| 65 | 6 | 0 | 1.282314 | 2.348353 | -1.531564 |
| 66 | 6 | 0 | 0.932372 | 3.790365 | -1.814304 |
| 67 | 1 | 0 | 0.531304 | 3.920462 | -2.820403 |
| 68 | 1 | 0 | 1.793251 | 4.450124 | -1.696040 |
| 69 | 1 | 0 | 0.167865 | 4.111170 | -1.097070 |
| 70 | 6 | 0 | 2.729283 | 2.988387 | 0.306184 |
| 71 | 1 | 0 | 2.049252 | 3.830233 | 0.518163 |
| 72 | 6 | 0 | 3.100348 | 2.359870 | 1.644437 |
| 73 | 1 | 0 | 2.211787 | 1.958949 | 2.135655 |
| 74 | 1 | 0 | 3.582835 | 3.087825 | 2.306515 |
| 75 | 1 | 0 | 3.791576 | 1.523567 | 1.488051 |
| 76 | 6 | 0 | 3.994287 | 3.547449 | -0.358296 |
| 77 | 1 | 0 | 4.734264 | 2.750684 | -0.479245 |
| 78 | 1 | 0 | 4.440613 | 4.342675 | 0.251775 |
| 79 | 1 | 0 | 3.786466 | 3.957071 | -1.351474 |
| 80 | 6 | 0 | 3.286394 | -1.866294 | 0.029733 |
| 81 | 6 | 0 | 3.734686 | -1.031946 | -1.029042 |
| 82 | 6 | 0 | 2.992745 | -1.352654 | -2.194490 |
| 83 | 6 | 0 | 2.076056 | -2.384345 | -1.858781 |
| 84 | 6 | 0 | 2.252027 | -2.698482 | -0.481494 |
| 85 | 6 | 0 | 3.900528 | -1.934187 | 1.393854 |

| | | | | | |
|---|---|---|---|---|---|
| 86 | 1 | 0 | 4.099644 | -0.939070 | 1.806460 |
| 87 | 1 | 0 | 4.857925 | -2.473271 | 1.370935 |
| 88 | 1 | 0 | 3.251314 | -2.441370 | 2.110644 |
| 89 | 6 | 0 | 4.890963 | -0.083914 | -0.992187 |
| 90 | 1 | 0 | 4.699424 | 0.797320 | -1.611290 |
| 91 | 1 | 0 | 5.811631 | -0.558274 | -1.362956 |
| 92 | 1 | 0 | 5.096717 | 0.265949 | 0.024025 |
| 93 | 6 | 0 | 3.236799 | -0.755372 | -3.546698 |
| 94 | 1 | 0 | 2.657497 | -1.272574 | -4.317178 |
| 95 | 1 | 0 | 4.295371 | -0.834645 | -3.826913 |
| 96 | 1 | 0 | 2.960238 | 0.305279 | -3.580558 |
| 97 | 6 | 0 | 1.185009 | -3.120868 | -2.812428 |
| 98 | 1 | 0 | 0.368595 | -3.631859 | -2.290531 |
| 99 | 1 | 0 | 1.738549 | -3.898312 | -3.357305 |
| 100 | 1 | 0 | 0.734968 | -2.459108 | -3.558671 |
| 101 | 6 | 0 | 1.518613 | -3.770397 | 0.265437 |
| 102 | 1 | 0 | 1.618980 | -3.640067 | 1.346042 |
| 103 | 1 | 0 | 1.893973 | -4.772395 | 0.014994 |
| 104 | 1 | 0 | 0.445462 | -3.755813 | 0.043667 |

**3a'**

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.934630
Thermal correction to Gibbs Free Energy = 0.791634
Sum of electronic and thermal Enthalpies = -2024.146441
Sum of electronic and thermal Free Energies = -2024.289436
298 K, in THF
Sum of electronic and thermal Free Energies = -3221.015814

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 71 | 0 | -0.193483 | -1.055746 | -0.466969 |
| 2 | 6 | 0 | 0.203559 | 0.953003 | 1.097309 |
| 3 | 7 | 0 | 2.029372 | -0.826457 | -0.068881 |
| 4 | 6 | 0 | 2.427073 | 0.460951 | 0.111786 |
| 5 | 6 | 0 | 1.493388 | 1.423755 | 0.495191 |
| 6 | 6 | 0 | 3.887935 | 0.743565 | 0.024599 |
| 7 | 6 | 0 | 4.516641 | 1.587092 | 0.953548 |
| 8 | 6 | 0 | 5.891171 | 1.782311 | 0.924656 |
| 9 | 6 | 0 | 6.676851 | 1.133648 | -0.028515 |
| 10 | 6 | 0 | 6.069737 | 0.280069 | -0.945347 |
| 11 | 6 | 0 | 4.692356 | 0.080934 | -0.912416 |
| 12 | 7 | 0 | -1.945276 | -2.332417 | 0.549192 |
| 13 | 6 | 0 | -1.203244 | -3.431503 | 0.625156 |
| 14 | 6 | 0 | -1.715904 | -4.747281 | 1.170133 |
| 15 | 7 | 0 | 0.038671 | -3.310045 | 0.156323 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 1.074414 | -4.252356 | 0.523863 |
| 17 | 6 | 0 | 2.111154 | -4.361201 | -0.589624 |
| 18 | 6 | 0 | -0.382997 | 0.416387 | -2.688764 |
| 19 | 6 | 0 | -1.686254 | -0.142106 | -2.558992 |
| 20 | 6 | 0 | -1.579825 | -1.546258 | -2.737548 |
| 21 | 6 | 0 | -0.215968 | -1.853543 | -2.999335 |
| 22 | 6 | 0 | 0.522401 | -0.639569 | -2.982405 |
| 23 | 6 | 0 | -0.081177 | 1.883471 | -2.686363 |
| 24 | 6 | 0 | -2.937100 | 0.674641 | -2.445420 |
| 25 | 6 | 0 | -2.685037 | -2.557225 | -2.763910 |
| 26 | 6 | 0 | 0.282591 | -3.210304 | -3.385826 |
| 27 | 6 | 0 | 1.967133 | -0.477657 | -3.331471 |
| 28 | 6 | 0 | -3.342385 | -2.311314 | 0.938790 |
| 29 | 6 | 0 | -3.976753 | -1.032651 | 0.409559 |
| 30 | 6 | 0 | -3.533467 | -2.386334 | 2.457001 |
| 31 | 6 | 0 | 1.723474 | -3.831584 | 1.845948 |
| 32 | 1 | 0 | 2.418898 | 0.350669 | -2.778509 |
| 33 | 1 | 0 | 2.103133 | -0.277029 | -4.403380 |
| 34 | 1 | 0 | 2.540808 | -1.378450 | -3.090178 |
| 35 | 1 | 0 | -3.825365 | 0.083681 | -2.689605 |
| 36 | 1 | 0 | -2.904830 | 1.516280 | -3.148012 |
| 37 | 1 | 0 | -3.085342 | 1.105303 | -1.451743 |
| 38 | 1 | 0 | -0.541408 | 2.392832 | -1.834519 |
| 39 | 1 | 0 | -0.452697 | 2.363827 | -3.603124 |
| 40 | 1 | 0 | 0.991871 | 2.076136 | -2.625626 |
| 41 | 1 | 0 | 0.655302 | -5.262196 | 0.666118 |
| 42 | 1 | 0 | -3.883250 | -3.160036 | 0.480679 |
| 43 | 1 | 0 | 1.371755 | -3.276166 | -3.314421 |
| 44 | 1 | 0 | 0.007957 | -3.456186 | -4.421956 |
| 45 | 1 | 0 | -0.136447 | -3.988931 | -2.739717 |
| 46 | 1 | 0 | -2.580017 | -3.302074 | -1.965863 |
| 47 | 1 | 0 | -2.702670 | -3.099583 | -3.718646 |
| 48 | 1 | 0 | -3.663905 | -2.086113 | -2.637420 |
| 49 | 1 | 0 | -1.370315 | -5.575463 | 0.545784 |
| 50 | 1 | 0 | -2.805267 | -4.772935 | 1.204214 |
| 51 | 1 | 0 | -1.338051 | -4.915101 | 2.184217 |
| 52 | 1 | 0 | 1.675372 | -4.812385 | -1.484357 |
| 53 | 1 | 0 | 2.964563 | -4.970770 | -0.272476 |
| 54 | 1 | 0 | 2.477751 | -3.368552 | -0.868181 |
| 55 | 1 | 0 | 2.147623 | -2.827640 | 1.749433 |
| 56 | 1 | 0 | 2.512712 | -4.531438 | 2.147779 |
| 57 | 1 | 0 | 0.978326 | -3.780646 | 2.646598 |
| 58 | 1 | 0 | -3.429028 | -0.158077 | 0.778524 |
| 59 | 1 | 0 | -5.021954 | -0.945790 | 0.725201 |
| 60 | 1 | 0 | -3.940520 | -1.005417 | -0.679497 |
| 61 | 1 | 0 | -3.091009 | -3.288391 | 2.888201 |
| 62 | 1 | 0 | -4.599719 | -2.372810 | 2.713533 |
| 63 | 1 | 0 | -3.046238 | -1.530740 | 2.928919 |
| 64 | 1 | 0 | 3.904556 | 2.084635 | 1.699258 |
| 65 | 1 | 0 | 4.220482 | -0.583394 | -1.630050 |

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|---|---|---|---|---|---|
| 66 | 1 | 0 | 6.354660 | 2.439890 | 1.655812 |
| 67 | 1 | 0 | 6.670020 | -0.235140 | -1.691495 |
| 68 | 1 | 0 | 7.752900 | 1.286667 | -0.049316 |
| 69 | 1 | 0 | 2.803956 | -1.476564 | -0.036259 |
| 70 | 6 | 0 | -0.979866 | 1.643342 | 0.792218 |
| 71 | 6 | 0 | -2.023621 | 2.258249 | 0.572771 |
| 72 | 6 | 0 | -3.196860 | 2.992179 | 0.315753 |
| 73 | 6 | 0 | -4.375354 | 2.780921 | 1.066816 |
| 74 | 6 | 0 | -3.239971 | 3.958091 | -0.715934 |
| 75 | 6 | 0 | -5.531838 | 3.496941 | 0.793391 |
| 76 | 1 | 0 | -4.362586 | 2.040830 | 1.861657 |
| 77 | 6 | 0 | -4.403275 | 4.665795 | -0.978331 |
| 78 | 1 | 0 | -2.341963 | 4.134454 | -1.300313 |
| 79 | 6 | 0 | -5.560830 | 4.444903 | -0.229967 |
| 80 | 1 | 0 | -6.424720 | 3.310962 | 1.386188 |
| 81 | 1 | 0 | -4.407598 | 5.401503 | -1.779405 |
| 82 | 1 | 0 | -6.469606 | 5.001582 | -0.441300 |
| 83 | 6 | 0 | 0.234061 | 0.257078 | 2.404618 |
| 84 | 6 | 0 | -0.939065 | 0.079417 | 3.168655 |
| 85 | 6 | 0 | 1.427991 | -0.247859 | 2.963498 |
| 86 | 6 | 0 | -0.923277 | -0.567585 | 4.397204 |
| 87 | 1 | 0 | -1.870354 | 0.486376 | 2.784649 |
| 88 | 6 | 0 | 1.437287 | -0.899140 | 4.191165 |
| 89 | 1 | 0 | 2.358577 | -0.112823 | 2.426210 |
| 90 | 6 | 0 | 0.264524 | -1.075205 | 4.922426 |
| 91 | 1 | 0 | -1.852757 | -0.670704 | 4.953850 |
| 92 | 1 | 0 | 2.381784 | -1.273944 | 4.580398 |
| 93 | 1 | 0 | 0.276247 | -1.586170 | 5.881565 |
| 94 | 6 | 0 | 1.720138 | 2.864566 | 0.358427 |
| 95 | 6 | 0 | 1.128570 | 3.776959 | 1.255796 |
| 96 | 6 | 0 | 2.500527 | 3.412011 | -0.680837 |
| 97 | 6 | 0 | 1.334321 | 5.145516 | 1.139715 |
| 98 | 1 | 0 | 0.503291 | 3.390595 | 2.054676 |
| 99 | 6 | 0 | 2.715235 | 4.779513 | -0.788700 |
| 100 | 1 | 0 | 2.941147 | 2.742054 | -1.413409 |
| 101 | 6 | 0 | 2.133946 | 5.662344 | 0.120726 |
| 102 | 1 | 0 | 0.863011 | 5.816807 | 1.854179 |
| 103 | 1 | 0 | 3.326844 | 5.160739 | -1.603621 |
| 104 | 1 | 0 | 2.287537 | 6.734377 | 0.027059 |

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