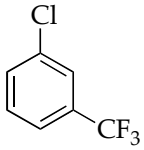
Regioselective Lithium Diisopropylamide-Mediated Ortholithiation of 1-Chloro-3-(trifluoromethyl)benzene: Role of Autocatalysis, Lithium Chloride Catalysis, and Reversibility

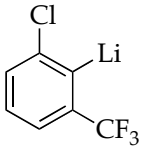
Alexander C. Hoepker, Lekha Gupta, Yun Ma, Marc F. Faggin, and David B. Collum*

Contribution from the Department of Chemistry and Chemical Biology
Baker Laboratory, Cornell University, Ithaca, New York 14853-1301

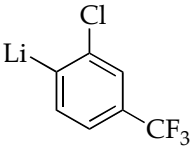
**Chart 1**



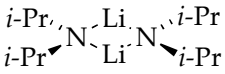

**1**




**2**




**3**




**4**

**Part 1: Experimental Procedures:**

Synthesis of deuterated 3-chlorobenzotrifluoride derivatives:

**2-Deutero-1-chloro-3-(trifluoromethyl)benzene (1-2-*d*).**
Using a method published by Knochel,[ref 14] commercially available 2-bromo-1-chloro-3-(trifluoromethyl)benzene (4.86 g, 18.7 mmol, 1.0 equiv) was added via syringe to a 1.3 M THF solution of isopropylmagnesium chloride–LiCl complex (29.0 mL, 22.3 mmol, 1.2 equiv) in dry THF at 0 °C under argon. After the solution was stirred for 20 minutes, 10 equiv of deuterium oxide (3.7 mL) was added to the solution. The mixture was allowed to warm to room temperature, and the pH was adjusted to 1.0 with 2.0 M aqueous HCl solution to dissolve all salts. Organic and aqueous layers were separated, and the aqueous layer was washed with 3 x 20 mL $Et_2O$. The organic layers were combined, dried over granular $Na_2SO_4$ and distilled, and **1**-2-*d* was collected at 135 °C as a colorless liquid (3.69g, 14.2 mmol) in 76% yield. $^1$H NMR $\delta$ 7.52 (m, 2H), 7.43 (m, 1H); $^{13}$C NMR $\delta$ 135.2 (s), 132.6 (q, $^2J_{C\text{-}F}$ = 33 Hz), 132.1 (s), 130.2 (s), 125.5 (tq, $^2J_{C\text{-}D}$ = 26 Hz, $^2J_{C\text{-}F}$ = 4.0 Hz), 123.8 (q, $^2J_{C\text{-}F}$ = 272 Hz), 123.4 (q, $^2J_{C\text{-}F}$ = 4.0 Hz).

**4-Deutero-1-chloro-3-(trifluromethyl)benzene (1-6-*d*).** The compound was synthesized as above from commercially available 4-bromo-1-chloro-3-(trifluoromethyl)benzene, and **1**-6-*d* was collected at 135 °C as a colorless liquid (3.9g, 15.0 mmol) in 80% yield. $^1$H NMR $\delta$ 7.62 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H); $^{13}$C NMR $\delta$ 135.0 (s), 132.5 (q, $^2J_{C\text{-}F}$ = 33 Hz), 131.9 (t, $^2J_{C\text{-}D}$ = 26 Hz), 130.2 (s), 125.8 (q, $^2J_{C\text{-}F}$ = 4.0 Hz), 123.6 (q, $^2J_{C\text{-}F}$ = 4.0 Hz), 123.5 (q, $^2J_{C\text{-}F}$ = 272 Hz).

**2,6-Dideutero-1-chloro-3-(trifluoromethyl)benzene (1-2,6-$d_2$).** A 2.5 M solution of *n*-BuLi in hexane (14.8 mL, 37.0 mmol) was added via syringe pump to a solution of dry diisopropylamine (5.7 mL, 40.7 mmol) and $Et_3N{\cdot}HCl$ (0.25 g, 1.85 mmol, 0.050 equiv) in 100 mL of dry THF at –78 °C under argon. After the solution was stirred for 20 minutes, **1** (5.0 mL, 37.0 mmol, 1 equiv) was added to the in situ generated LDA solution. After stirring at –78 °C for 30 min, *d*-MeOH (1.51 mL, 37.0 mmol, 1 equiv) was added. The process of sequential *n*-BuLi and *d*-MeOH addition of 1.0 equiv was repeated three more times. A final amount of *d*-MeOH (15 mL, 10 equiv) was added to fully quench the reaction. After the mixture was allowed to warm to room temperature, the pH was adjusted to 1.0 with 2.0 M HCl solution to dissolve all salts. Organic and aqueous layer were separated, and the aqueous layer was washed with 3 x 20 mL $Et_2O$. The organic layers were combined and dried over granular $Na_2SO_4$ and distilled, and **1**-2,6-$d_2$ was collected at 135 °C as a colorless liquid (3.74 g, 18.2 mmol) in 49% yield. $^1$H NMR $\delta$ 7.52 (m, 1H), 7.43 (m, 1H); $^{13}$C NMR $\delta$ 135.3 (s), 132.6 (q, $^2J_{C\text{-}F}$ = 33 Hz), 131.9 (t, $^2J_{C\text{-}D}$ = 26 Hz), 130.2 (s), 125.8 (tq, $^2J_{C\text{-}D}$ = 26 Hz, $^2J_{C\text{-}F}$ = 4.0 Hz), 123.8 (q, $^2J_{C\text{-}F}$ = 272 Hz), 123.5 (q, $^2J_{C\text{-}F}$ = 4.0 Hz).

**Part 2: NMR Spectroscopic Studies**

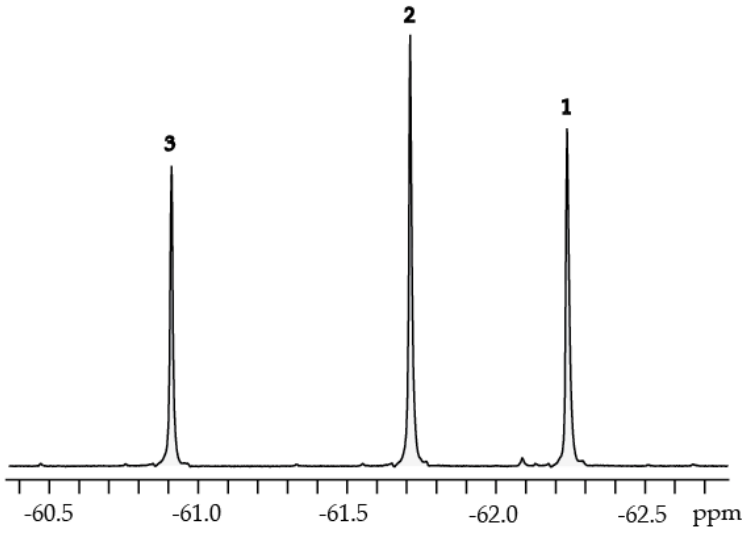



**Figure 1.** $^{19}F$ NMR spectrum of LDA (0.10 M) with **1** (0.050 M) in 12.2 M THF after aging for 10 minutes at - 90 °C: $\delta$ -60.90 (s) , -61.70 (s), -62.23 (s).

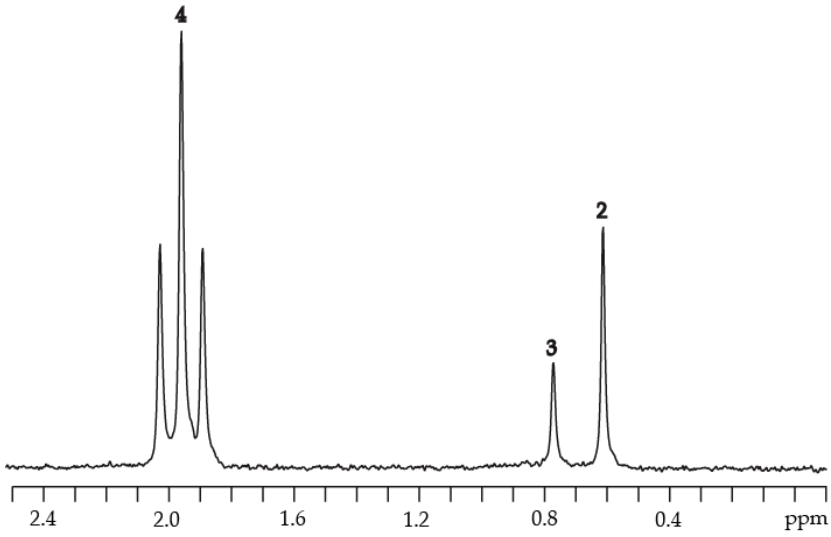



**Figure 2.** $^{6}Li$ NMR spectrum of [$^{6}Li$,$^{15}N$]LDA (0.10 M) and **1** (0.050 M) in neat THF recorded at -90 °C: $\delta$ 1.96 (t, $^{2}J_{Li\text{-}N}$ = 5.0 Hz) , 0.77 (s), 0.61 (s).

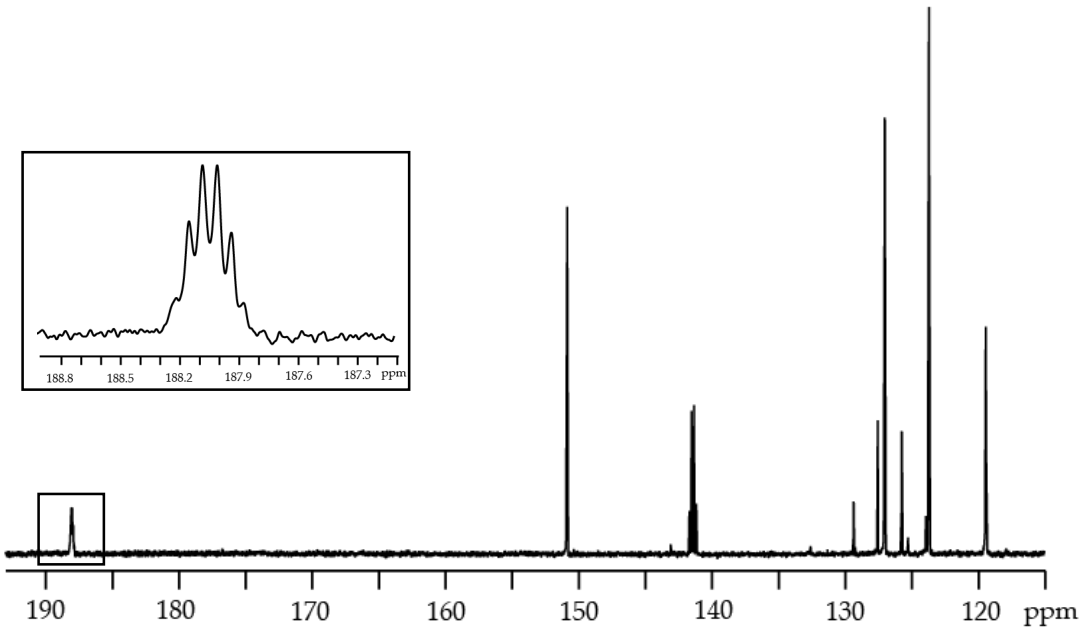



**Figure 3.** $^{13}C\{^{1}H\}$ NMR spectrum of **2** generated from **1** (0.20 M) with [$^{6}$Li]LDA (0.30 M) in 12.2 M THF-$d_8$ at -105 °C: $\delta$ 188.05 (m), 150.87 (s), 141.45 (q, $^{2}J_{C\text{-}F}$ = 26.6 Hz), 127.04 (s), 126.67 (q, $^{2}J_{C\text{-}F}$ = 272.0 Hz), 123.73 (s), 119.45 (q, $^{2}J_{C\text{-}F}$ = 3.9 Hz).

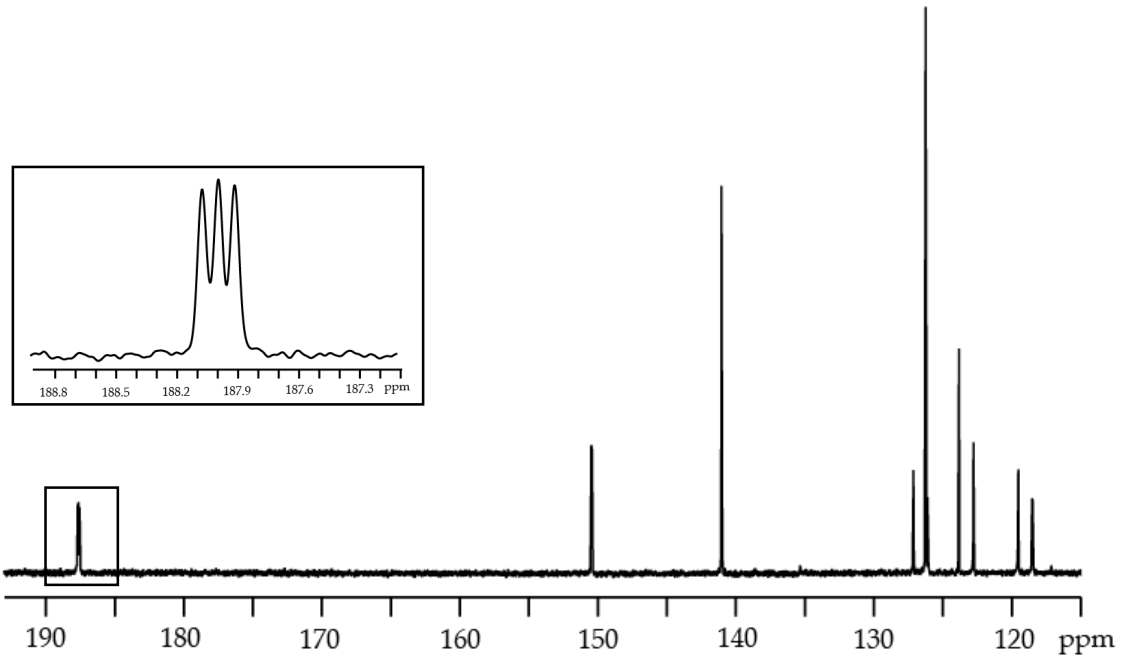



**Figure 4.** $^{13}C\{^{19}F\}$ NMR spectrum of **2** generated from **1** (0.20 M) with [$^{6}$Li]LDA (0.30 M) in 12.2 M THF-$d_8$ at -105 °C: $\delta$ 188.05 (t, $^{2}J_{C\text{-}Li}$ = 11.4 Hz), 150.87 (dm, $^{2}J_{C\text{-}H}$ = 10.8 Hz), 141.45 (d, $^{2}J_{C\text{-}H}$ = 8.6 Hz), 127.04 (dd, $^{2}J_{C\text{-}H}$ = 78.7 Hz, $^{2}J_{C\text{-}H}$ = 6.5 Hz), 126.67 (m), 123.73 (d, $^{2}J_{C\text{-}H}$ = 159.0 Hz), 119.45 (dd, $^{2}J_{C\text{-}H}$ = 155.8 Hz, $^{2}J_{C\text{-}H}$ = 6.2 Hz).

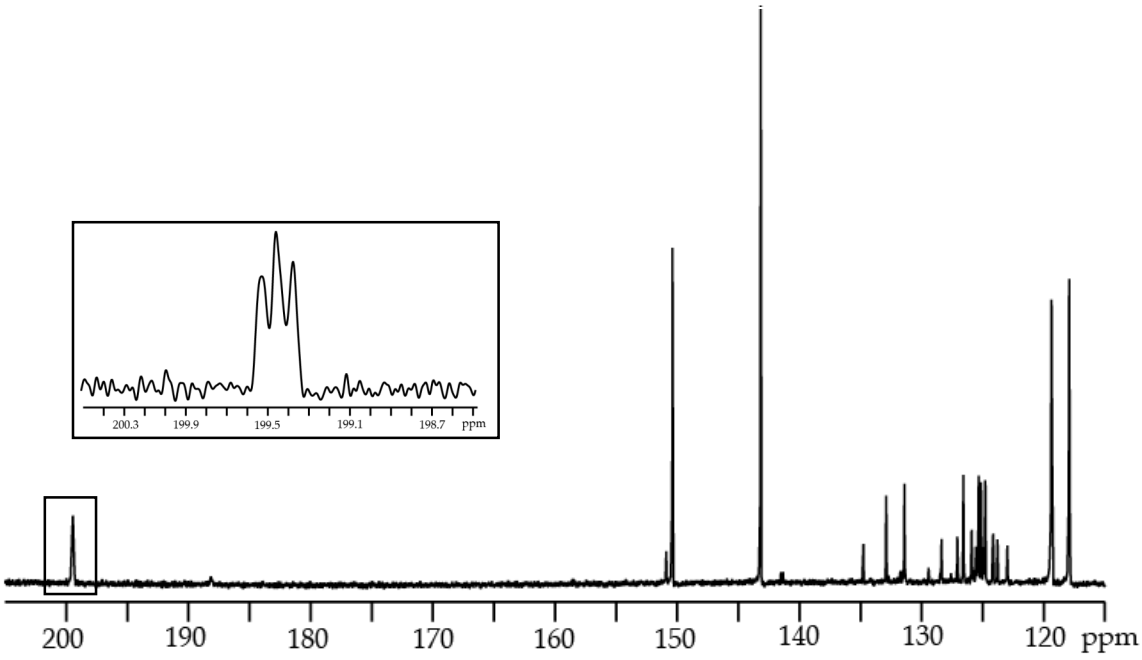



**Figure 5.** $^{13}C\{^{19}F\}$ NMR spectrum of **3** generated from **1** (0.15 M) with [$^{6}$Li,$^{15}$N]LiTMP (0.20 M) in 12.2 M THF-$d_8$ at -90 °C: $\delta$ 199.52 (t, $^{2}J_{C\text{-}Li}$ = 11.0 Hz), 150.40 (s), 143.17 (s), 125.68 (q, $^{2}J_{C\text{-}F}$ = 270.5 Hz), 125.23 (q, $^{2}J_{C\text{-}F}$ = 30.8 Hz), 119.36 (m), 117.91 (m).

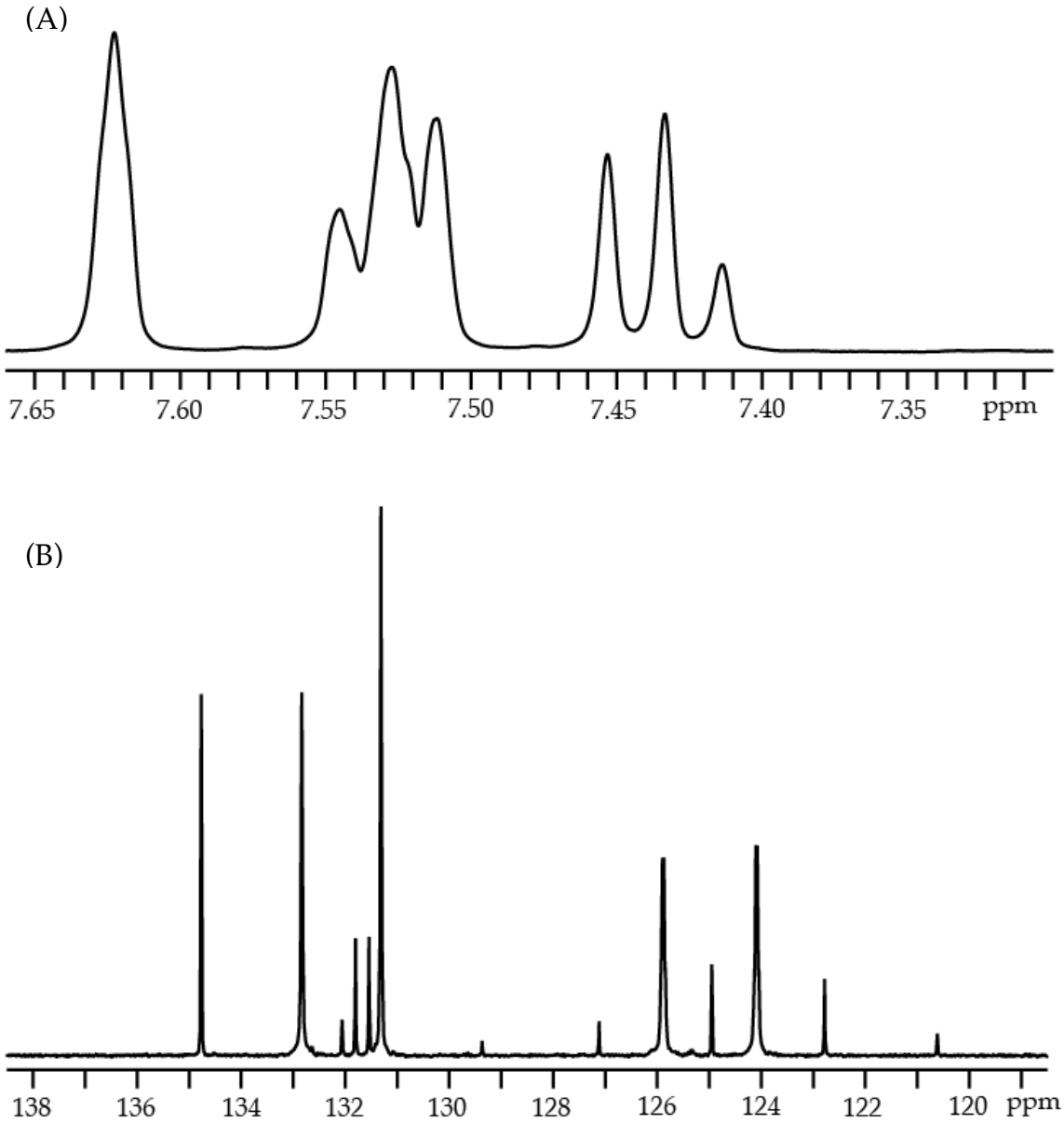



**Figure 6.** $^{1}$H and $^{13}$C NMR spectra of **1** in $CDCl_3$ and THF-$d_8$, respectively: (A) $^{1}$H NMR $\delta$ 7.62 (s, 1H), 7.52 (m, 2H), 7.43 (m, 1H); (B) $^{13}$C NMR $\delta$ 134.8 (s), 132.8 (s), 131.7 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 131.3 (s), 125.9 (q, $^{2}J_{C\text{-}F}$ = 3.8 Hz), 124.1 (q, $^{2}J_{C\text{-}F}$ = 2.5 Hz), 123.9 (q, $^{2}J_{C\text{-}F}$ = 273 Hz).

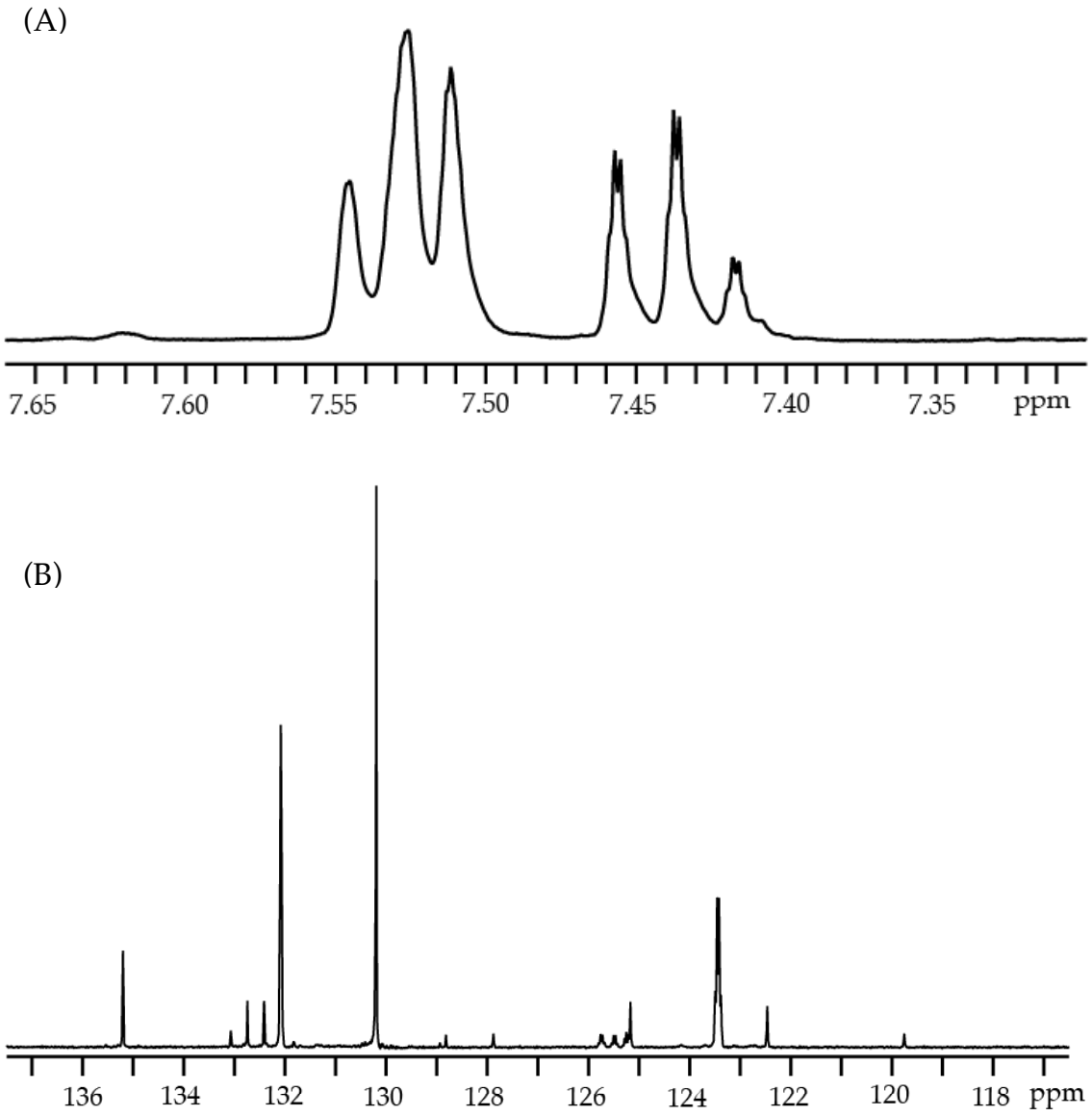



**Figure 7.** $^{1}$H and $^{13}$C NMR spectra of **1**-2-$d_1$ in $CDCl_3$. The compound was prepared as described in Part 1 using the Grignard method: (A) $^{1}$H NMR $\delta$ 7.52 (m, 2H), 7.43 (m, 1H); (B) $^{13}$C NMR $\delta$ 135.2 (s), 132.6 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 132.1 (s), 130.2 (s), 125.5 (tq, $^{2}J_{C\text{-}D}$ = 26 Hz, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 123.8 (q, $^{2}J_{C\text{-}F}$ = 272 Hz), 123.4 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz).

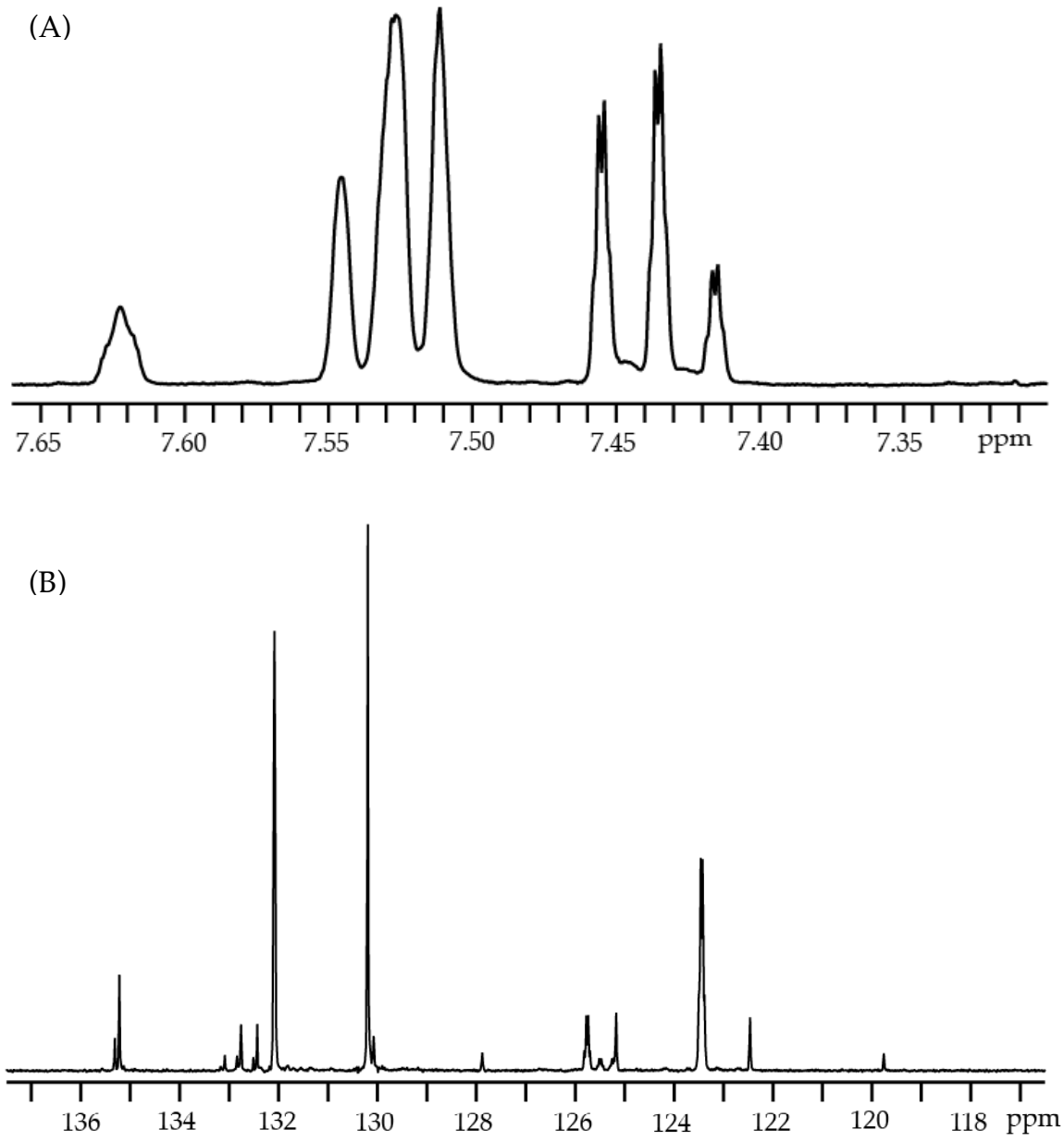



**Figure 8.** $^{1}$H and $^{13}$C NMR spectra of **1**-2-$d_1$ in $CDCl_3$. The compound was prepared as described in Part 1 using an LDA-mediated ortholithiation: (A) $^{1}$H NMR $\delta$ 7.62 (s, 0.2 H*), 7.52 (m, 2H), 7.43 (m, 1H); (B) $^{13}$C NMR $\delta$ 135.2 (s), 135.2 (s)*, 132.6 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 132.1 (s), 130.2 (s), 125.5 (tq, $^{2}J_{C\text{-}D}$ = 26 Hz, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 125.8 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz)*, 123.8 (q, $^{2}J_{C\text{-}F}$ = 272 Hz), 123.4 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz).

*proton resonance at position 2 of remaining **1**.

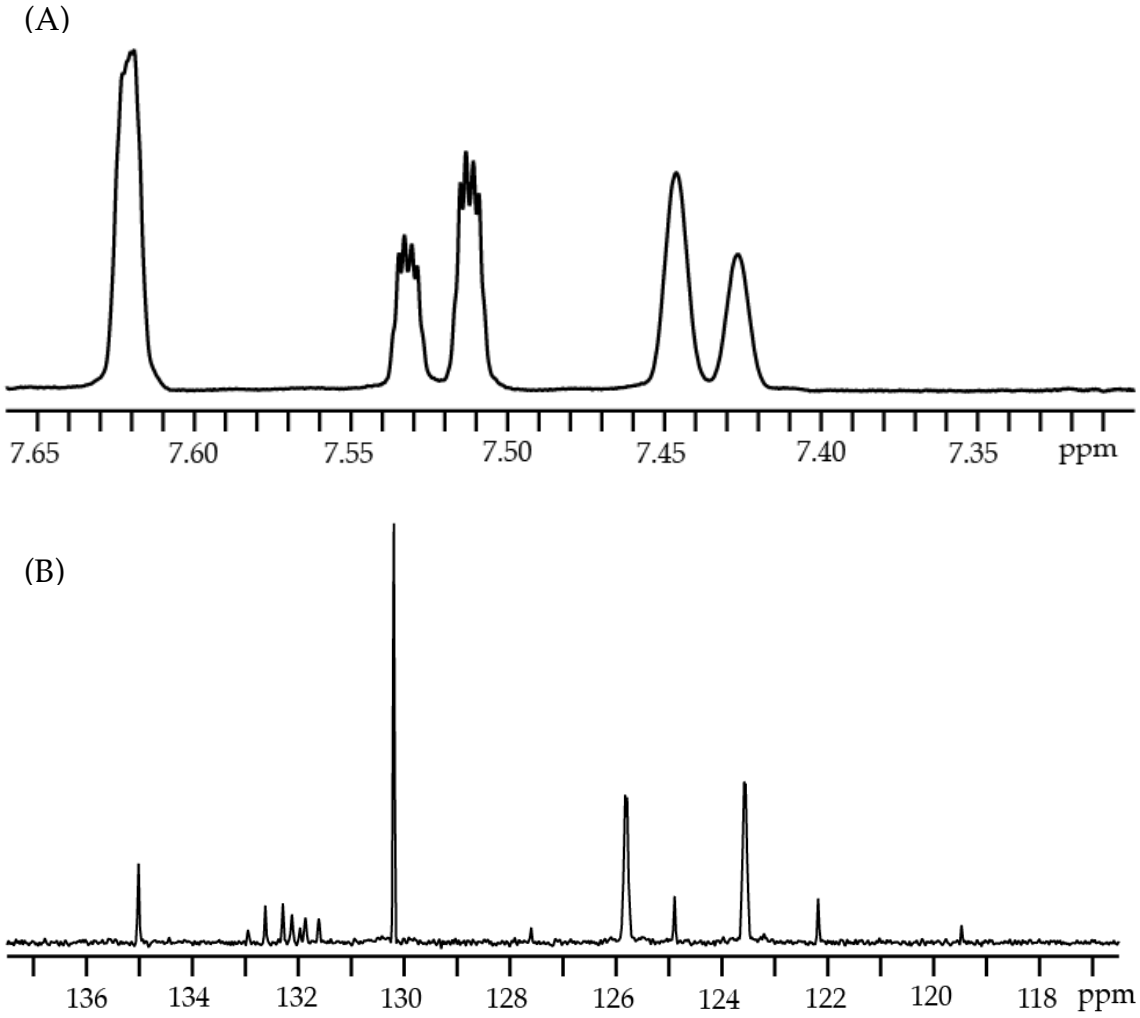



**Figure 9.** $^{1}$H and $^{13}$C NMR spectra of **1**-6-$d_1$ in $CDCl_3$. The compound was prepared as described in Part 1 using the Grignard method: (A) $^{1}$H NMR $\delta$ 7.62 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H); (B) $^{13}$C NMR $\delta$ 135.0 (s), 132.5 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 131.9 (t, $^{2}J_{C\text{-}D}$ = 26 Hz), 130.2 (s), 125.8 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 123.6 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 123.5 (q, $^{2}J_{C\text{-}F}$ = 272 Hz).

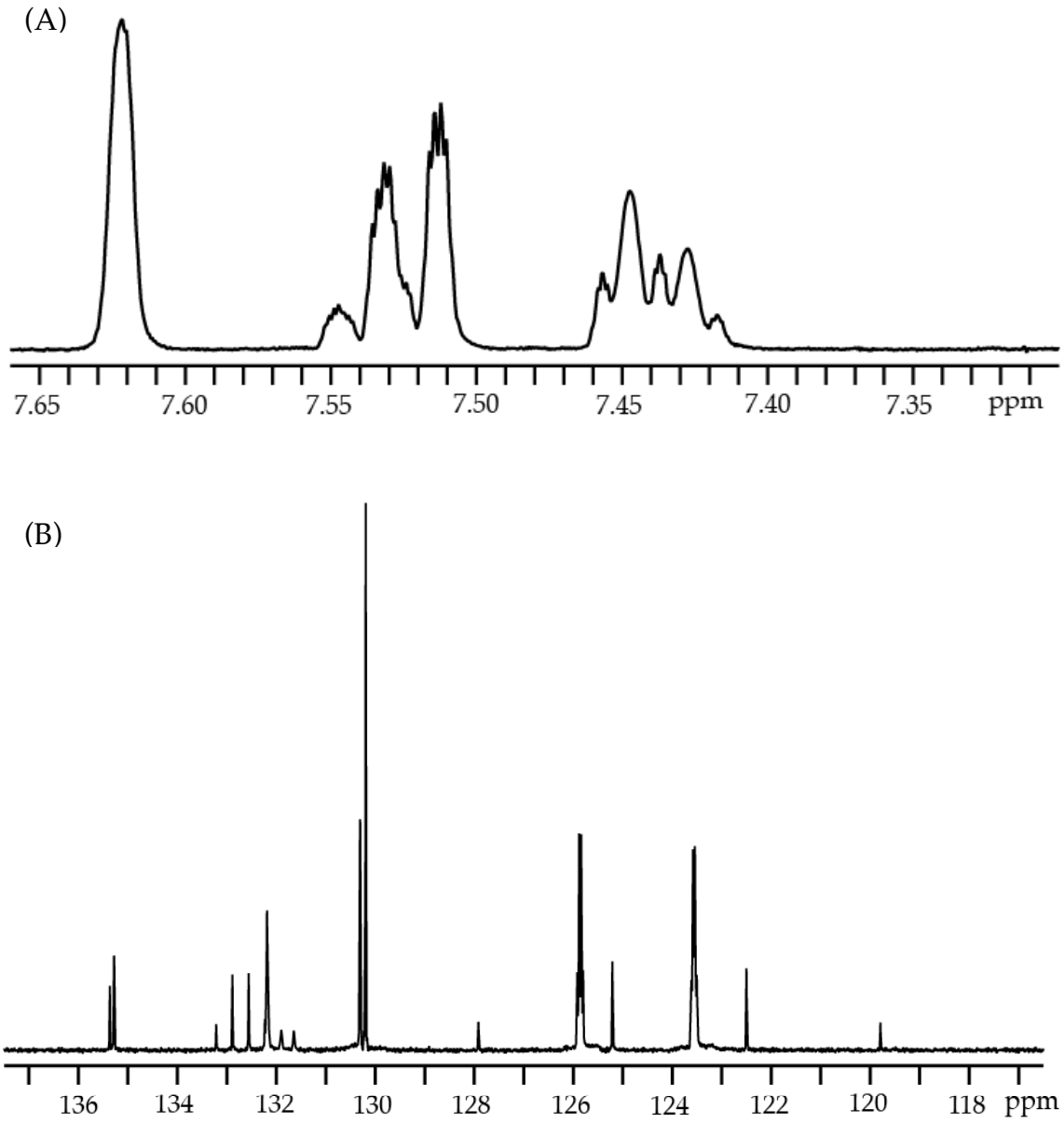



**Figure 10.** $^{1}$H and $^{13}$C NMR spectra of **1**-6-$d_1$ in $CDCl_3$. The compound was prepared as described in Part 1 using LiTMP: (A) $^{1}$H NMR $\delta$ 7.62 (s, 1H), 7.52 (m, 2H), 7.43 (m, 1H)*; (B) $^{13}$C NMR $\delta$ 135.4 (s), 135.3 (s)*, 132.7 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 132.1 (s)*, 131.9 (t, $^{2}J_{C\text{-}D}$ = 26 Hz), 130.3 (s), 130.2 (s)*, 125.9 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 123.9 (q, $^{2}J_{C\text{-}F}$ = 272 Hz), 123.6 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz).

* additional resonances are due to **1**-2-*d*.

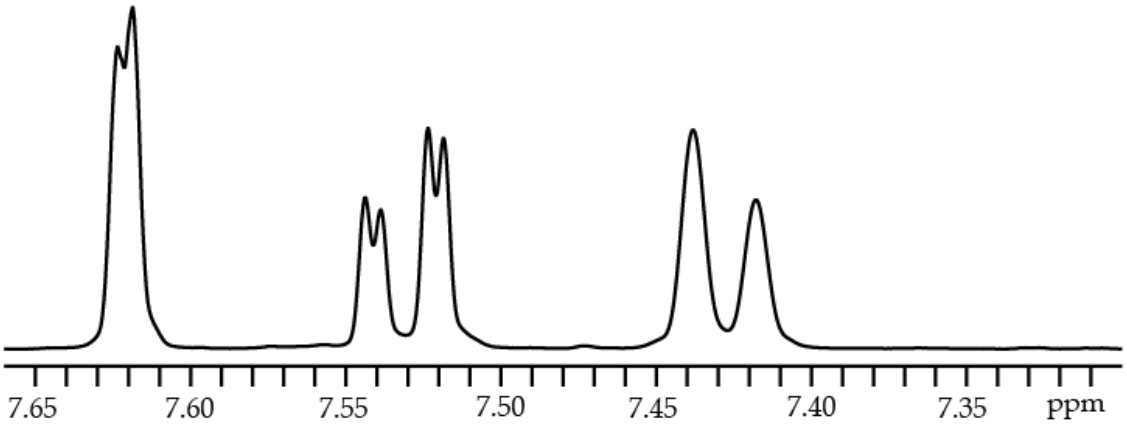



**Figure 11.** $^1$H NMR spectra of **1-**6-$d_1$ in $CDCl_3$. The compound was prepared as described in Part 1 using the Grignard method: $^1$H NMR $\delta$ 7.62 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H).

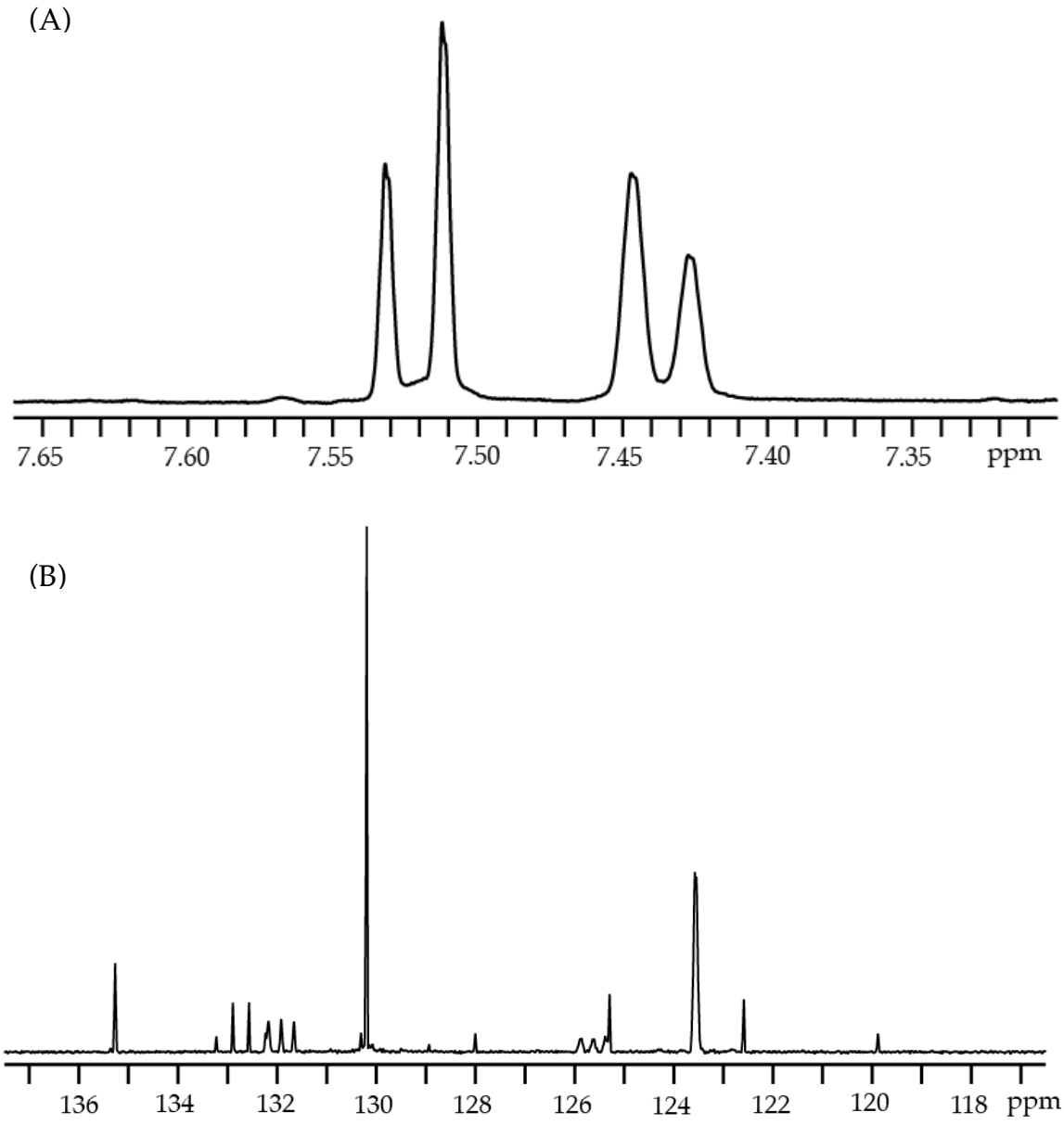



**Figure 12.** $^{1}$H and $^{13}$C NMR spectra of **1**-2,6-$d_2$ in $CDCl_3$. The compound was prepared as described in Part 1: (A) $^{1}$H NMR $\delta$ 7.52 (m, 1H), 7.43 (m, 1H); (B) $^{13}$C NMR $\delta$ 135.3 (s), 132.6 (q, $^{2}J_{C\text{-}F}$ = 33 Hz), 131.9 (t, $^{2}J_{C\text{-}D}$ = 26 Hz), 130.2 (s), 125.8 (tq, $^{2}J_{C\text{-}D}$ = 26 Hz, $^{2}J_{C\text{-}F}$ = 4.0 Hz), 123.8 (q, $^{2}J_{C\text{-}F}$ = 272 Hz), 123.5 (q, $^{2}J_{C\text{-}F}$ = 4.0 Hz).

**Part 3: Rate Studies**

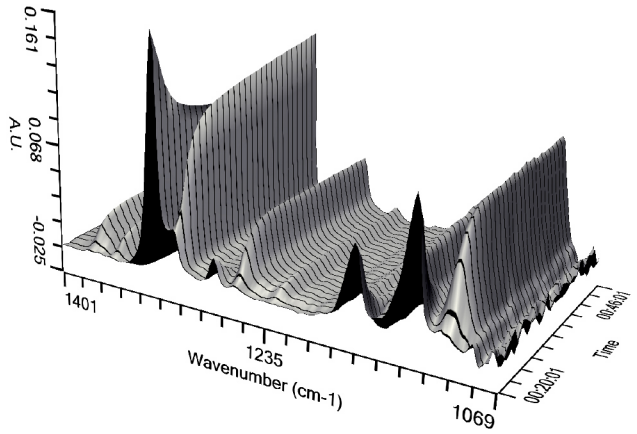



**Figure 13.** Representative in situ IR trace for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) in THF at -78 °C. Compounds **1**, **2**, and **3** exhibit the IR absorptions listed for the four possible isotopomers. The IR spectra were deconvoluted using ConcIRT®. Deconvolution of the product absorbances was not possible.

**1**: 1428 $cm^{-1}$, 1325 $cm^{-1}$, 1276 $cm^{-1}$, 1171 $cm^{-1}$, 1131 $cm^{-1}$
**2**: 1378 $cm^{-1}$, 1306 $cm^{-1}$, 1260 $cm^{-1}$, 1140 $cm^{-1}$, 1104 $cm^{-1}$
**3**: 1378 $cm^{-1}$, 1324 $cm^{-1}$, 1258 $cm^{-1}$, 1154 $cm^{-1}$, 1109 $cm^{-1}$

**1**-2-$d_1$: 1325 $cm^{-1}$, 1215 $cm^{-1}$, 1170 $cm^{-1}$, 1132 $cm^{-1}$
**2+3**: 1322 $cm^{-1}$, 1245 $cm^{-1}$, 1176 $cm^{-1}$, 1140 $cm^{-1}$, 1108 $cm^{-1}$

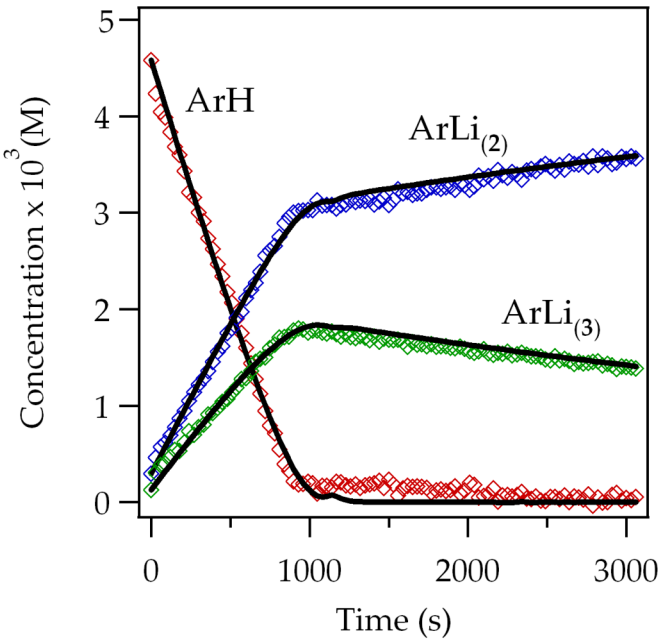
**1**-6-$d_1$: 1401 $cm^{-1}$, 1326 $cm^{-1}$, 1173 $cm^{-1}$, 1131 $cm^{-1}$
**2+3**: 1378$cm^{-1}$, 1329 $cm^{-1}$, 1299 $cm^{-1}$, 1260 $cm^{-1}$, 1146 $cm^{-1}$, 1121 $cm^{-1}$, 1104 $cm^{-1}$

**1**-2,6-$d_2$: 1383 $cm^{-1}$, 1324 $cm^{-1}$, 1181 $cm^{-1}$, 1161 $cm^{-1}$, 1131 $cm^{-1}$
**2+3**: 1322 $cm^{-1}$, 1297 $cm^{-1}$, 1260 $cm^{-1}$, 1245 $cm^{-1}$, 1212 $cm^{-1}$, 1176 $cm^{-1}$,1108 $cm^{-1}$

**Figure 14.** Time-dependent concentrations measured by $^{19}F$ NMR spectroscopy using 0.05 M **4** (0.10 N) and **1** in 12.2 M THF at -65 °C. Legend: ArH = **1**; $A_2$ = LDA dimer **4**; $ArLi_{(2)}$ = **2**; $ArLi_{(2)}$ = **3**. The curves represent a parametric fit to eqs 22-28 in the manuscript. (A) 0.005 M **1**; (B) 0.010 M **1**. (C) 0.020 M **1**. (D) 0.050 M **1**.

**Figure 14 (continued).**

(A)

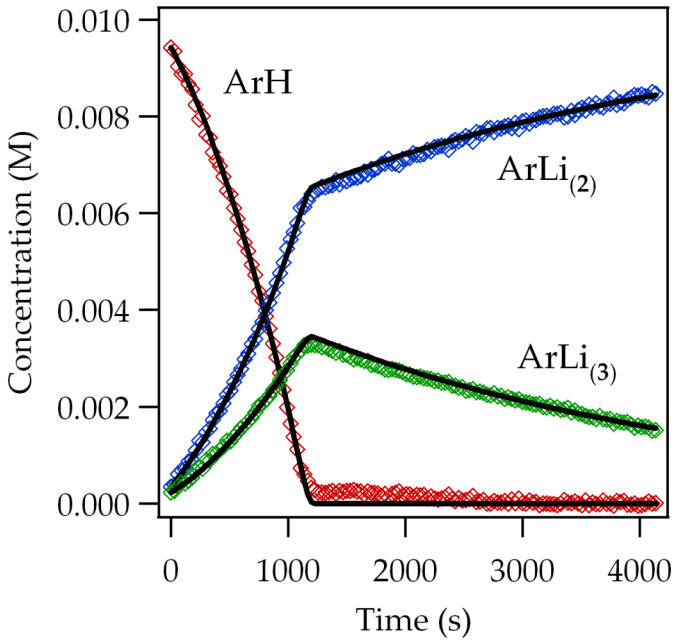



$k_1 = 0.000115 \pm 1e\text{-}006$
$k_{-1} = 1000k_1$
$k_2 = 0$
$k_{-2} = 0$
$k_3 = 220 \pm 20$
$k_4 = 150 \pm 13$
$k_5 = 0$
$k_6 = 0$
$k_7 = 0.0010 \pm 0.0008$
$k_{-7} = 0.30 \pm 0.002$

To simplify the curve fit, it was assumed that the effect of autocatalysis are negligible and the affiliated rate constants ($k_2$, $k_{-2}$, $k_5$, $k_6$) were set to zero.

**Figure 14 (continued).**

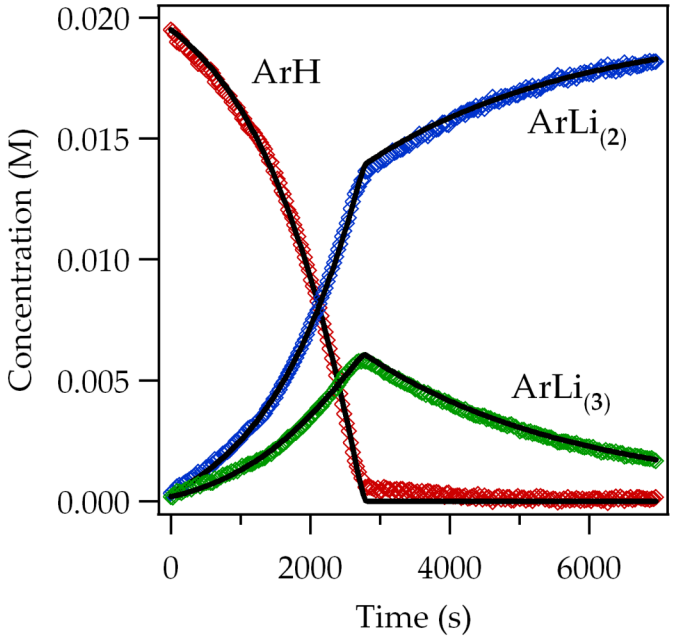
(B)




$k_1 = 0.00022 \pm 3e\text{-}005$
$k_{-1} = 1000k_1$
$k_2 = 0.020 \pm 0.0004$
$k_{-2} = 1000k_2$
$k_3 = 9.0 \pm 0.9$
$k_4 = 4.2 \pm 0.5$
$k_5 = 152 \pm 50$
$k_6 = 105 \pm 30$
$k_7 = 0.0001 \pm 0.0004$
$k_{-7} = 0.028 \pm 0.001$

**Figure 14 (continued).**

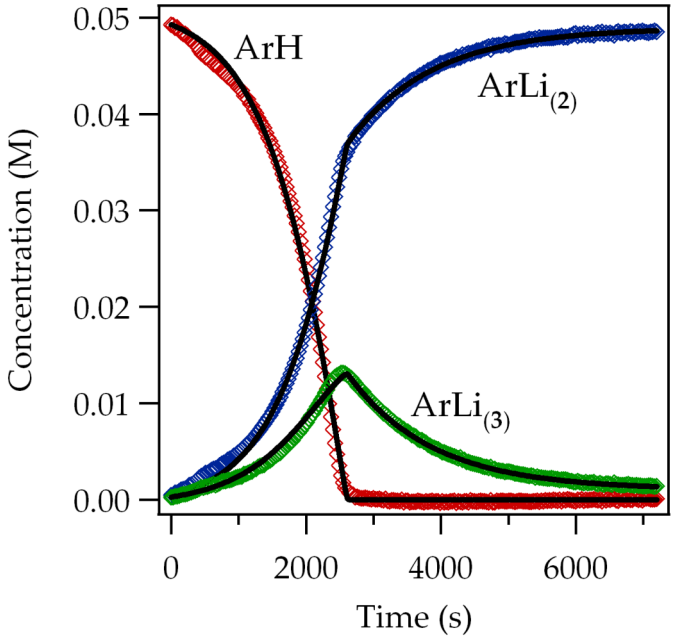
(C)




$k_1$ = 3.97e-005 ± 1e-006
$k_{-1}$ = 1000$k_1$
$k_2$ = 0.0123 ± 7e-005
$k_{-2}$ = 1000$k_2$
$k_3$ = 9.9 ± 0.9
$k_4$ = 4.5 ± 0.4
$k_5$ = 150 ± 20
$k_6$ = 92 ± 9
$k_7$ = 0.00021 ± 2e-005
$k_{-7}$ = 0.016 ± 0.0002

**Figure 14 (continued).**

(D)




$k_1$ = 3.6e-005 ± 1e-006
$k_{-1}$ = 1000$k_1$
$k_2$ = 0.023 ± 9e-005
$k_{-2}$ = 1000$k_2$
$k_3$ = 8.4 ± 1
$k_4$ = 6.1 ± 0.05
$k_5$ = 160 ± 4
$k_6$ = 90 ± 2
$k_7$ = 0.00033 ± 2e-005
$k_{-7}$ = 0.016 ± 0.0003

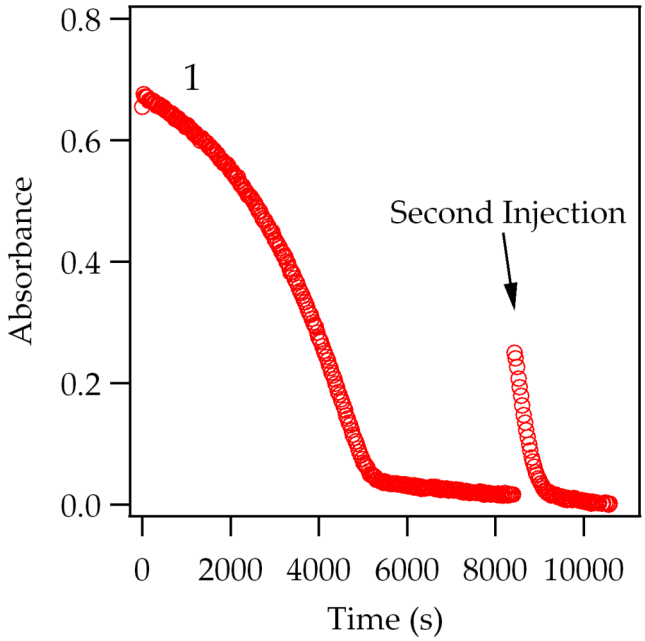



**Figure 15.** Representative plot showing absorbance of arene **1** vs time for the ortholithiation of **1** (0.010 M) with LDA (0.10 M) in THF (12.20 M) at –78 °C. After completion of the reaction a second aliquot of **1** (0.005) was injected.

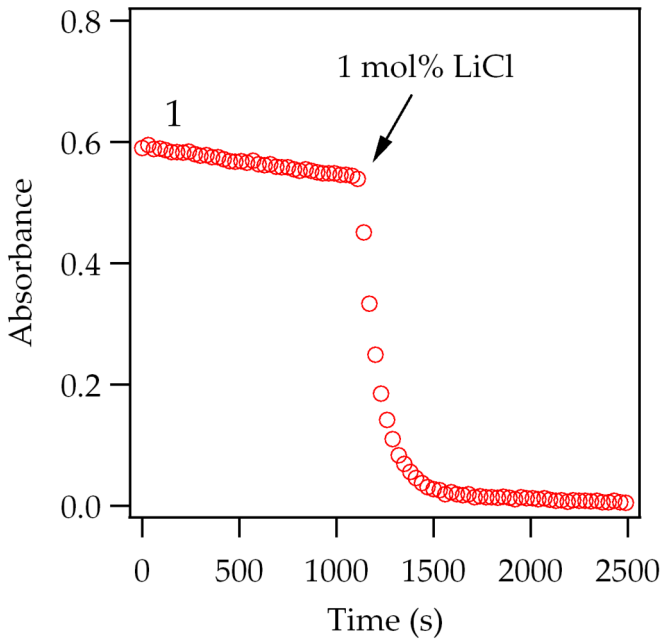



**Figure 16.** Ortholithiation of **1** (0.010 M) with LDA (0.10 M) in THF (12.2 M) at –78 °C monitored by IR spectroscopy (1325 $cm^{-1}$) with injection of 1.0 mol % LiCl.

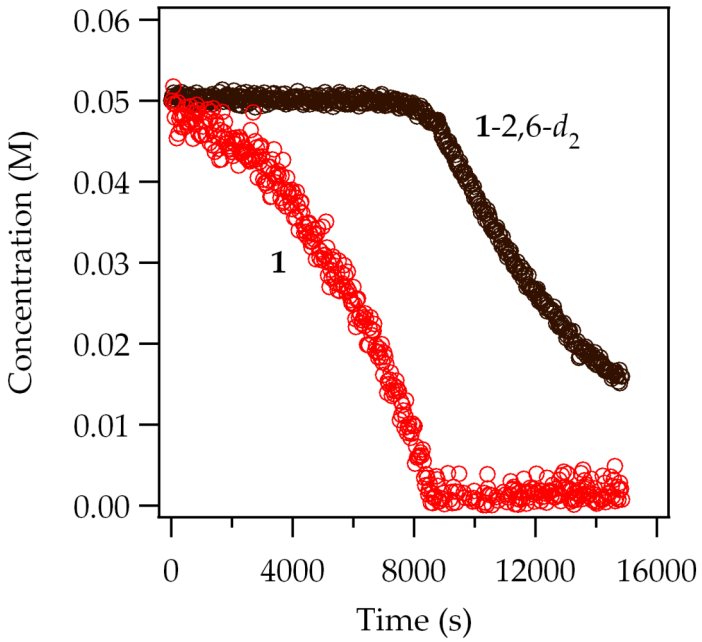



**Figure 17** Competitive ortholithiation of **1** (0.050 M) and **1**-2,6-$d_2$ (0.050 M) with LDA (0.10 M) in THF (12.2 M) at –78 °C monitored by IR spectroscopy.

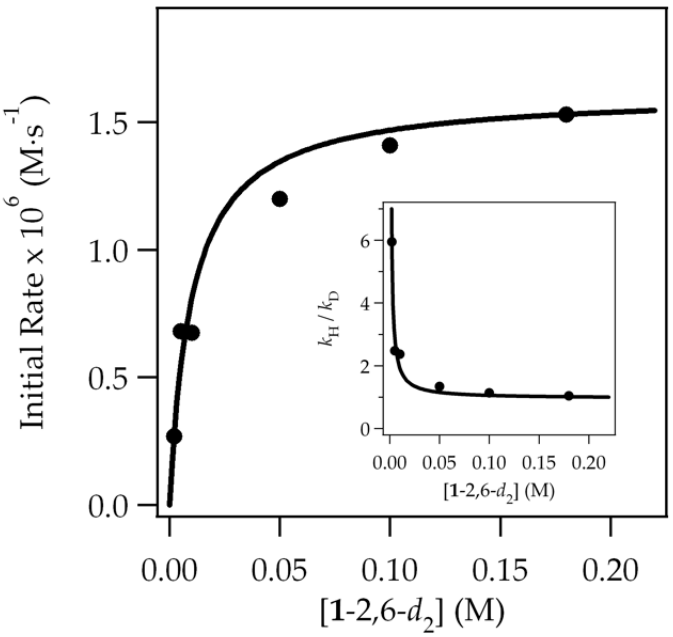



**Figure 18.** Plot of initial rate versus **1**-2,6-$d_2$ for the ortholithiation of **1**-2,6-$d_2$ by 0.10 M LDA in 12.2 M THF at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to a first-order saturation function: $-\Delta[ArH]/\Delta t\,|_{t=0} = (a[ArH])/(1 + b[ArH])$ where ArH is **1**-2,4-$d_2$. The ratio $a/b$ was constrained to 1.6 x$10^{-6}$ M·$s^{-1}$ to ensure saturation at the initial rate of **1** (1.6 x$10^{-6}$ M·$s^{-1}$). [$b$ = (2.62 $\pm$ 0.08) x $10^{-6}$]

| [**1**-2,6-$d_2$] (M) | -Δ[ArH]/Δt (M·$s^{-1}$) |
|---|---|
| 0.002 | 2.69 e-7 $\pm$ 2 e-8 |
| 0.005 | 6.46 e-7 $\pm$ 4 e-8 |
| 0.010 | 6.74 e-6 $\pm$ 1 e-7 |
| 0.050 | 1.96 e-6 $\pm$ 3 e-7 |
| 0.10 | 1.41 e-6 $\pm$ 6 e-7 |
| 0.18 | 1.53 e-6 $\pm$ 4 e-7 |
| 0.38 | 2.62 e-6 $\pm$ 2 e-7 |

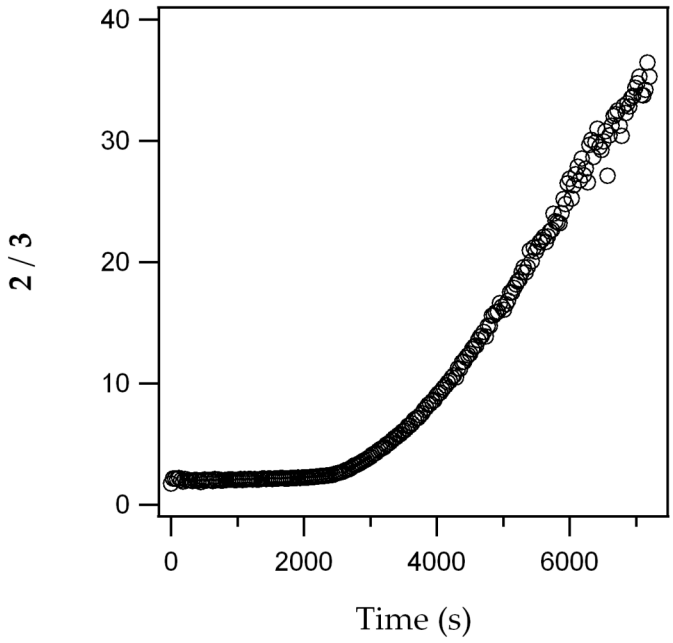



**Figure 19.** Plot of **2/3** versus time for the ortholithiation of **1** by LDA in THF (12.2 M) at -65 °C measured by $^{19}F$ NMR spectroscopy.

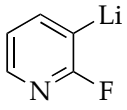
**Table 1.** Relative initial rates for the formation of **2** and **3** for the ortholithiation of **1**, **1**-2-*d*, **1**-6-*d*, and **1**-2,6-$d_2$ (0.050 M each) by LDA (0.10 M) in THF (12.2 M) at -78 °C measured by $^{19}$F NMR spectroscopy (A) in the absence of LiCl and (B) with 5 mol% LiCl.

| *No LiCl* | (**Δ2**/**Δ3**) |
|---|---|
| **1** | 1.65 |
| **1**-2-*d* | 0.057 |
| **1**-6-*d* | 34.0 |
| **1**-2,6-$d_2$ | 0.70 |

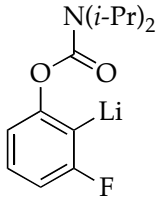
| *5 mol% LiCl* | (**Δ2**/**Δ3**) |
|---|---|
| **1** | 0.78 |
| **1**-2-*d* | 0.016 |
| **1**-6-*d* | 26.0 |
| **1**-2,6-$d_2$ | 0.30 |

**Table 2.** Table showing the relative initial rates for the formation of **2** and **3** with various lithium salts (0.020 M) for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) in 12.2 M THF at -90 °C measured by $^{19}$F NMR spectroscopy.

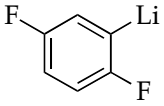
| Lithium salt | (Δ**2**/Δt)/(Δ**3**/Δt) |
|---|---|
| LiCl | 0.78 |
| **2** | 0.84 |
| **34** | 0.72 |
| **35** | 0.73 |
| **36** | 0.49 |




**34**




**35**




**36**

**Table 3.** Table showing regioselectivity at equilibrium for the ortholithiation of **1** by *sec*-BuLi (0.11 M) and *n*-BuLi (0.11 M) in 12.2 M THF at -90 °C measured by $^{19}F$ NMR spectroscopy.

| base | [**1**] (M) | (**2**/**3**) |
|---|---|---|
| *n*-BuLi (0.11 M) | 0.005 | 1.2 |
| | 0.020 | 2.4 |
| | 0.10 | 3.8 |
| *sec*-BuLi (0.11 M) | 0.005 | 0.15 |
| | 0.020 | 0.06 |
| | 0.10 | 0.05 |

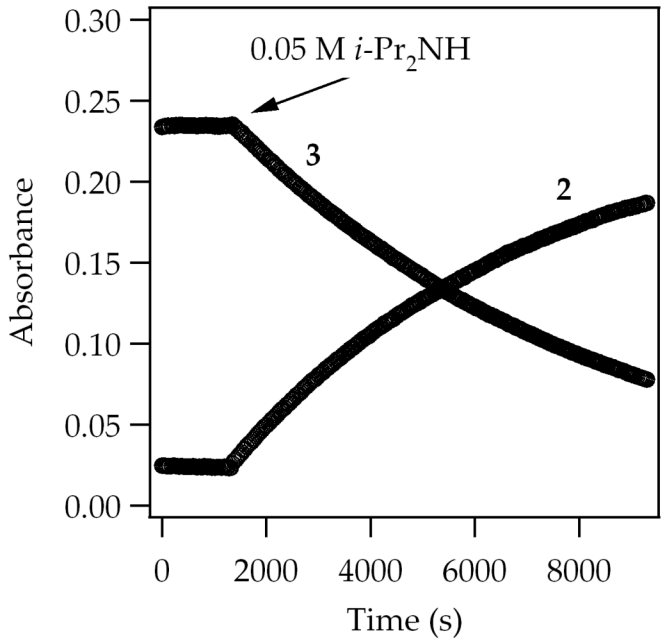



**Figure 20.** Representative IR plot for the equilibration of **3** (1151 $cm^{-1}$) to **2** (1306 $cm^{-1}$) was monitored by IR spectroscopy. Aryllithium **3** was generated by addition of LiTMP (0.050 M) to **1** (0.050 M) in 12.2 M THF at -78 °C. After **3** was produced quantitatively and no observable isomerization was detected, *i*-$Pr_2NH$ (0.050 M) was injected.

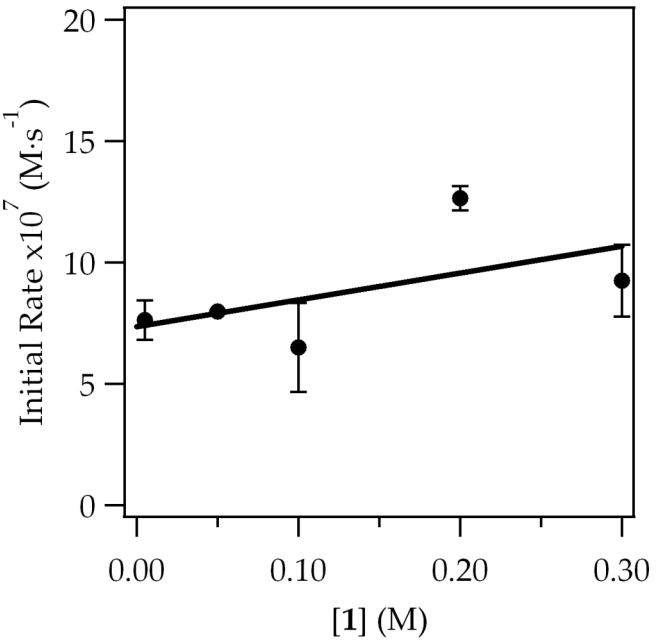



**Figure 21.** Plot of initial rate vs [**1**] (initial arene concentration) for the ortholithiation of **1** with LDA (0.10 M) in THF (12.2 M) at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to y = *a*[ArH] + *b*. [$a = (9 \pm 1) \times 10^{-7}$, $b = (7 \pm 8) \times 10^{-9}$]

| [**1**] (M) | y1 ($M \cdot s^{-1}$) | y2 ($M \cdot s^{-1}$) |
|---|---|---|
| 0.005 | 7.04 e-7 ± 4 e-9 | 8.20 e-7 ± 4 e-9 |
| 0.050 | 8.00 e-7 ± 2 e-8 | 7.94 e-7 ± 2 e-8 |
| 0.10 | 7.78 e-7 ± 2 e-8 | 5.21 e-7 ± 1 e-8 |
| 0.20 | 1.32 e-6 ± 6 e-8 | 1.23 e-6 ± 6 e-8 |
| 0.30 | 8.22 e-7 ± 1 e-7 | 1.03 e-6 ± 1 e-7 |

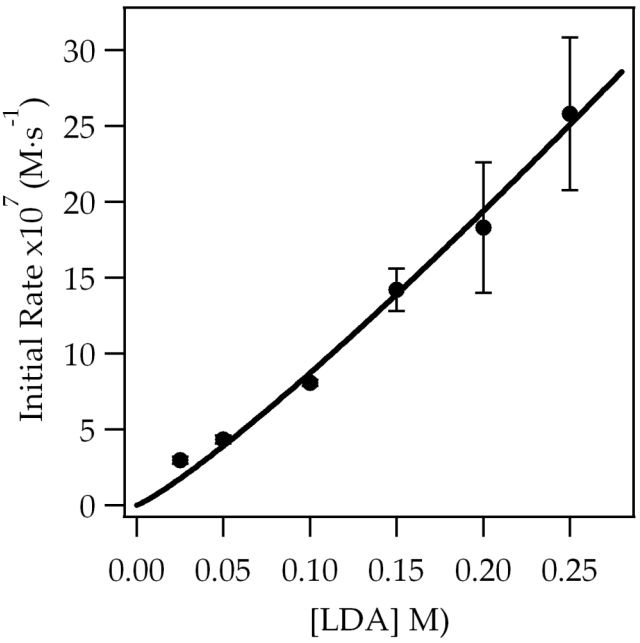



**Figure 22**. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.050 M) at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (1.2 \pm 0.2) \times 10^{-5}$, $n = (1.16 \pm 0.09)$]

| [LDA] (M) | y1 ($M \cdot s^{-1}$) | y2 ($M \cdot s^{-1}$) |
|---|---|---|
| 0.025 | 3.14 e-7 ± 4 e-8 | 2.81 e-7 ± 5 e-8 |
| 0.05 | 4.51 e-7 ± 6 e-8 | 4.13 e-6 ± 8 e-8 |
| 0.10 | 7.94 e-7 ± 3 e-8 | 8.20 e-7 ± 3 e-8 |
| 0.15 | 1.52 e-6 ± 3 e-7 | 1.32 e-6 ± 8 e-8 |
| 0.20 | 1.81 e-6 ± 2 e-7 | 1.20 e-6 ± 5 e-8 |
| 0.25 | 2.33 e-6 ± 3 e-7 | 2.37 e-6 ± 4 e-8 |

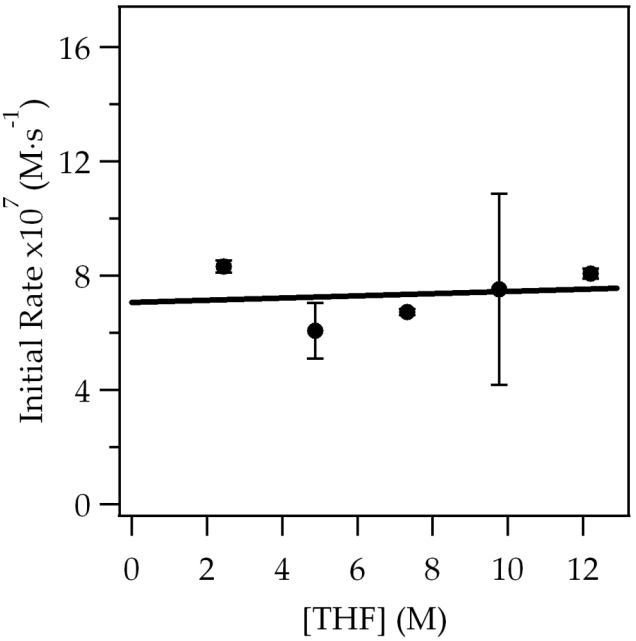



**Figure 23**. Plot of initial rate versus [THF] for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to y = *a*[THF] + *b*. [*a* = (7 ± 1) x $10^{-7}$, *b* = (3.9 ± 0.1) x $10^{-9}$]

| [THF] (M) | y1 ($M \cdot s^{-1}$) | y2 ($M \cdot s^{-1}$) |
|---|---|---|
| 2.44 | 8.18 e-7 ± 4 e-8 | 8.47 e-7 ± 5 e-8 |
| 4.88 | 5.39 e-7 ± 6 e-8 | 6.76 e-7 ± 4 e-8 |
| 7.32 | 6.65 e-7 ± 3 e-8 | 6.81 e-7 ± 3 e-8 |
| 9.77 | 9.89 e-7 ± 3 e-8 | 5.16 e-7 ± 1 e-8 |
| 12.2 | 7.94 e-7 ± 2 e-8 | 8.20 e-7 ± 5 e-8 |

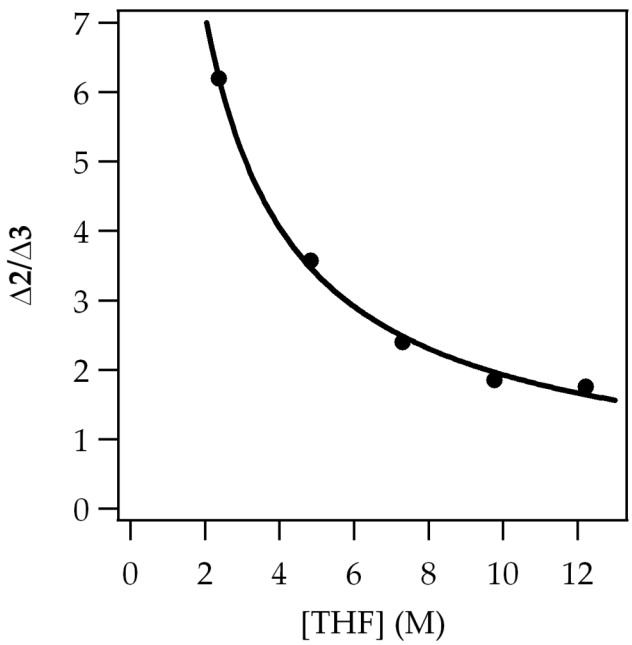



**Figure 24**. Ratio of relative initial rates of formation **2** and **3**, (Δ**2**/Δt)/(Δ**3**/Δt), versus [THF] for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at –65 °C measured by $^{19}$F NMR. The elevated temperature was used to shorten the duration of the experiments. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}]^n + b$. [$a = 12.5 \pm 0.8$, $n = -0.8 \pm 0.2$ and $b = 0.1 \pm 0.8$]

| [THF] (M) | (Δ**2**/Δt)/(Δ**3**/Δt) |
|---|---|
| 2.37 | 6.20 |
| 4.83 | 3.57 |
| 7.30 | 2.40 |
| 9.76 | 1.85 |
| 12.21 | 1.76 |

**Table 4**. Table of relative initial rate versus [LDA] for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at -65 °C measured by $^{19}F$ NMR. The relative initial rate is defined as $(\Delta \mathbf{2}/\Delta t)/(\Delta \mathbf{3}/\Delta t)$.

| [LDA] (M) | $(\Delta \mathbf{2}/\Delta t)/(\Delta \mathbf{3}/\Delta t)$ |
|---|---|
| 0.020 | 1.74 |
| 0.10 | 1.76 |
| 0.20 | 1.71 |

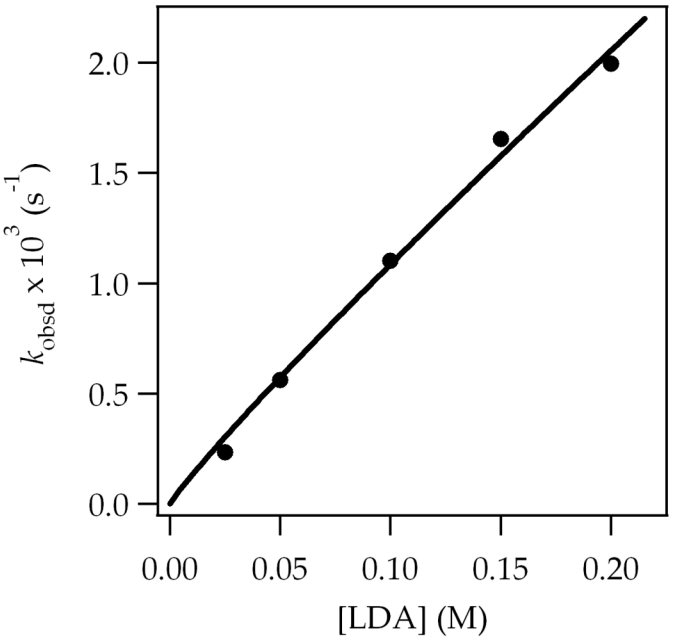



**Figure 25**. Plot of $k_{obsd}$ versus [LDA] in THF (12.2 M) for the ortholithiation of **1**-2,6-$d_2$ (0.002 M) –65 °C measured by $^{19}$F NMR spectroscopy. The curve depicts an unweighted least-squares fit to y = $k$[LDA]$^n$. [$k$ = (9 ± 1) x $10^{-3}$, $n$ = 0.92 ± 0.06]

| [LDA] (M) | y ($s^{-1}$) |
|---|---|
| 0.025 | 0.23 e-3 ± 2 e-6 |
| 0.050 | 0.58 e-3 ± 5 e-6 |
| 0.10 | 1.10 e-3 ± 5 e-6 |
| 0.15 | 1.68 e-3 ± 3 e-5 |
| 0.20 | 1.95 e-3 ± 2 e-5 |

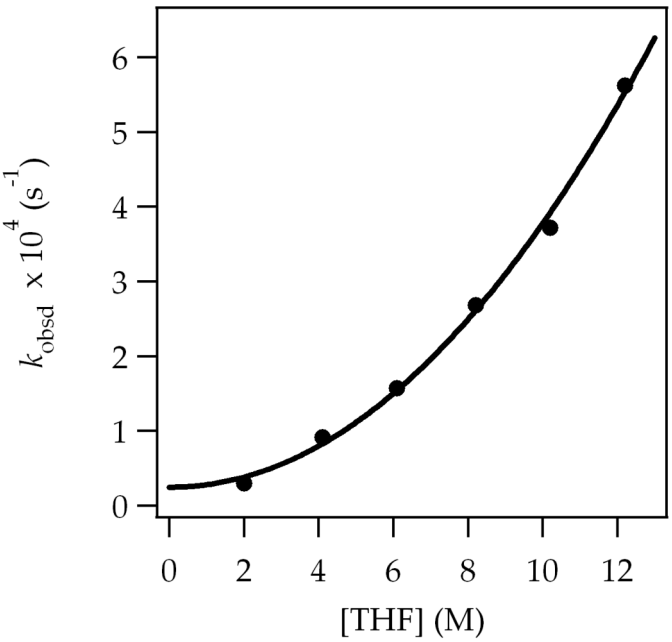



**Figure 26**. Plot of $k_{obsd}$ versus [THF] in hexanes for the ortholithiation of **1**-2,6-$d_2$ (0.002 M) by LDA (0.050 M) –65 °C measured by $^{19}$F NMR spectroscopy. The rates are not affected by medium effects as measured by the use of 2,6-dimethyltetrahydrofuran as a cosolvent. The curve depicts an unweighted least-squares fit to y = $k$[THF]$^n$ + $c$. [$k$ = (3 $\pm$ 1) x $10^{-6}$, $n$ = 2.0 $\pm$ 0.2, $c$ = (3 $\pm$ 1) x $10^{-5}$]

| [THF] (M) | y ($s^{-1}$) |
|---|---|
| 2.1 | 2.97 e-5 ± 5 e-7 |
| 4.1 | 9.15 e-5 ± 5 e-7 |
| 6.1 | 1.57 e-4 ± 7 e-7 |
| 8.2 | 2.68 e-4 ± 8 e-7 |
| 10.2 | 3.72 e-4 ± 1 e-6 |
| 12.2 | 5.62 e-4 ± 5 e-6 |

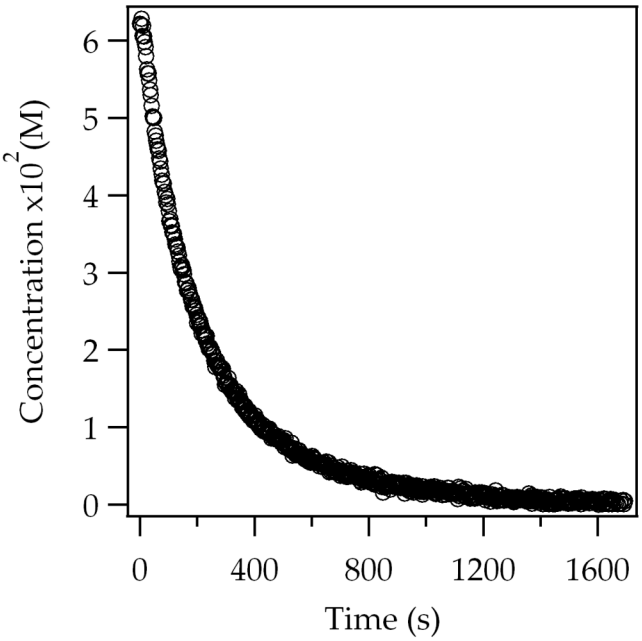



**Figure 27.** Representative plot of **1** (0.005 M) versus time for the ortholithiation by LDA (0.10 M) in 12.2 M THF in the presence of 5 mol% LiCl at -90 °C.

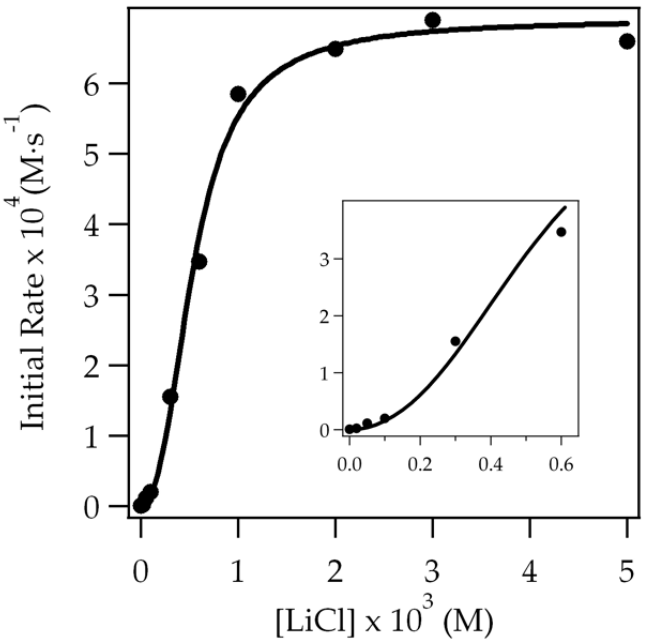



**Figure 28.** Plot of initial rate versus [LiCl] for the ortholithiation of **1** (0.074 M) by 0.10 M LDA in 12.2 M THF at –78 °C measured by IR spectroscopy. The inset is a magnified view of the data at low concentrations. The curve depicts an unweighted least-squares fit to eq 17. [ArH] = 0.074 M, $[A_2S_2]$ = 0.050 M, $c$ = 1.0 x $10^{-8}$. [$k_1$ = (1.5 ± 0.1) x $10^4$, $k_{-1}$ = (3.2 ± 0.4) x $10^6$, $k_2$ = 0.61 ± (6 x $10^{-4}$), $n$ = 2.0 ± 0.3]

| [LiCl] (mM) | (Δ[**1**]/Δt) (abs·s$^{-1}$) |
|---|---|
| 0.0 | 6.08 e-7 ± 4 e-7 |
| 0.02 | 2.37 e-6 ± 2 e-7 |
| 0.05 | 1.15 e-5 ± 9 e-7 |
| 0.10 | 1.99 e-5 ± 5 e-7 |
| 0.30 | 1.55 e-4 ± 4 e-6 |
| 0.60 | 3.47 e-4 ± 2 e-5 |
| 1.0 | 6.08 e-4 ± 1 e-5 |
| 2.0 | 6.49 e-4 ± 2 e-5 |
| 3.0 | 6.90 e-4 ± 2 e-5 |
| 5.0 | 6.602 e-4 ± 2 e-5 |

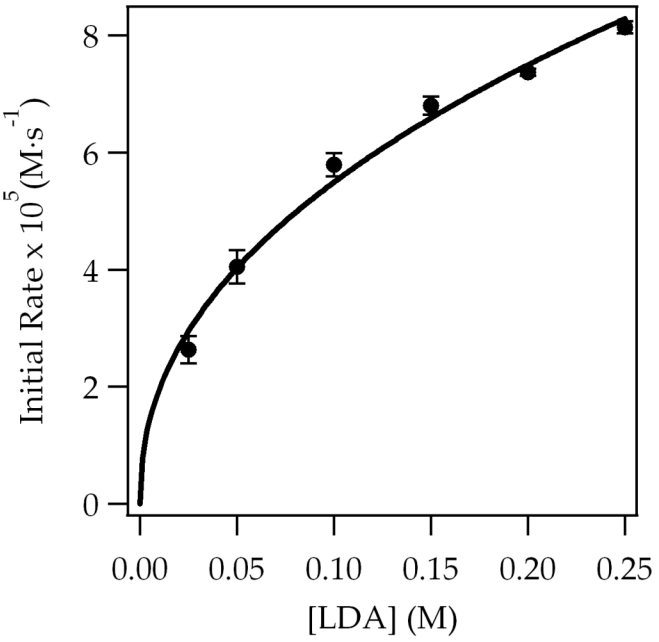



**Figure 29**. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.075 M) in the presence of 5 mol% LiCl at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\mathrm{LDA}]^n$. [$a = (154 \pm 9) \times 10^{-6}$, $n = 0.45 \pm 0.03$]

| [LDA] (M) | y1 ($M \cdot s^{-1}$) | y2 ($M \cdot s^{-1}$) |
|---|---|---|
| 0.025 | 2.60 e-5± 9 e-7 | 2.47 e-5 ± 8 e-7 |
| 0.050 | 5.35 e-5 ± 8 e-7 | 3.65 e-5 ± 9 e-7 |
| 0.10 | 6.08 e-5 ± 4 e-7 | 5.51 e-5 ± 3 e-7 |
| 0.15 | 6.58 e-5 ± 6 e-7 | 7.02 e-5 ± 2 e-6 |
| 0.20 | 7.28 e-5 ± 1 e-6 | 7.46 e-5 ± 1 e-6 |
| 0.25 | 8.29 e-5 ± 1 e-6 | 7.99 e-5 ± 1 e-6 |

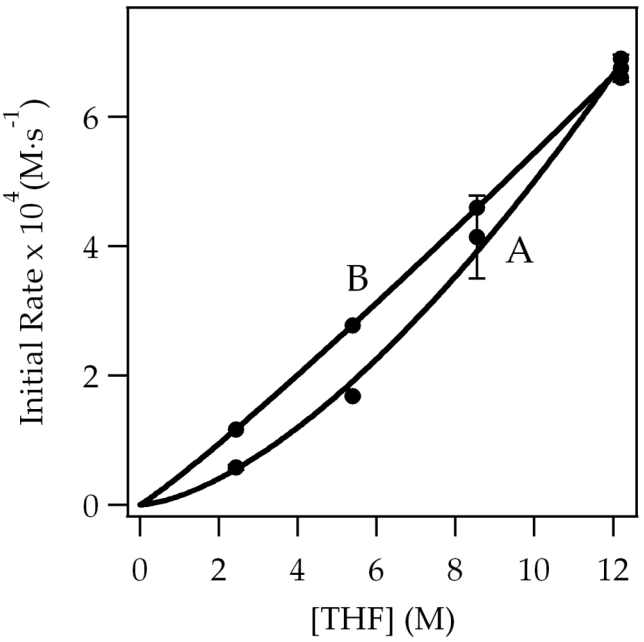



**Figure 30**. Plot of initial rate versus [THF] in hexanes (curve A) and 2,5-dimethyltetrahydrofuran (curve B) cosolvent for the ortholithiation of **1** (0.075 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at –78 °C. The data was measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[THF]^n + b$. Curve A: $a = (1.4 \pm 1.0) \times 10^{-5}$, $n = 1.6 \pm 0.3$, $b = (1.6 \pm 1) \times 10^{-5}$. Curve B: $a = (4.44 \pm 2.0) \times 10^{-5}$, $n = 1.1 \pm 0.1$, $b = (0.0 \pm 5) \times 10^{-5}$.

| [THF] (M) | y1 ($M \cdot s^{-1}$) | y2 ($M \cdot s^{-1}$) |
|---|---|---|
| 2.44 | 6.08 e-5 ± 8 e-7 | 5.5 e-5 ± 7 e-7 |
| 5.39 | 1.68 e-4 ± 3 e-6 | 1.67 e-4 ± 2 e-6 |
| 8.54 | 3.69 e-4 ± 1 e-5 | 3.40 e-4 ± 7 e-6 |
| 12.2 | 6.08 e-4 ± 4 e-6 | 5.51 e-4 ± 3 e-6 |

| [$Me_2$-THF] (M) | y ($M \cdot s^{-1}$) |
|---|---|
| 2.44 | 1.17 e-4 ± 4 e-6 |
| 5.39 | 2.77 e-4 ± 8 e-6 |
| 8.54 | 4.59 e-4 ± 2 e-5 |

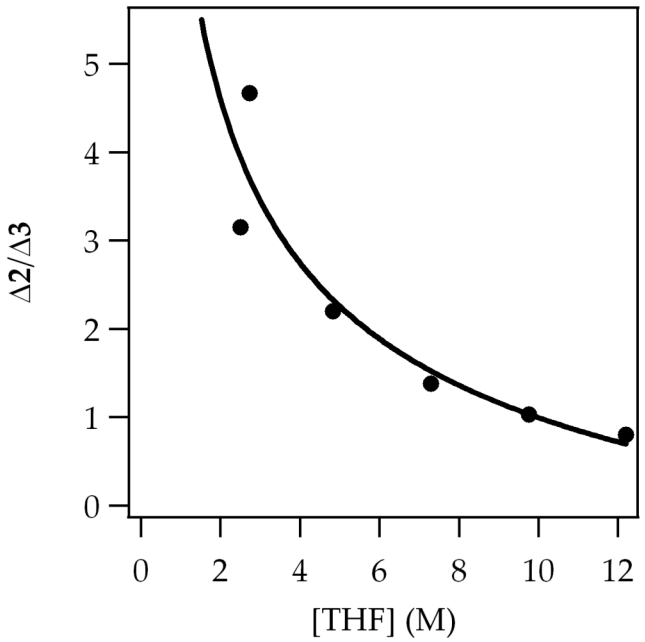



**Figure 31**. Plot of relative initial rate versus [THF] in 2,5-dimethyltetrahydrofuran cosolvent for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at –78 °C. The concentrations of **2** and **3** were monitored by $^{19}$F NMR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\mathrm{THF}]^n + b$. [$a = 9 \pm 6$, $n = -0.94 \pm 0.21$, $b = 0.0 \pm 0.3$]

| [THF] (M) | y1 | y2 |
|---|---|---|
| 2.50 | 3.15 | 4.30 |
| 4.83 | 2.20 | / |
| 7.30 | 1.38 | / |
| 9.76 | 1.03 | / |
| 12.2 | 0.78 | / |

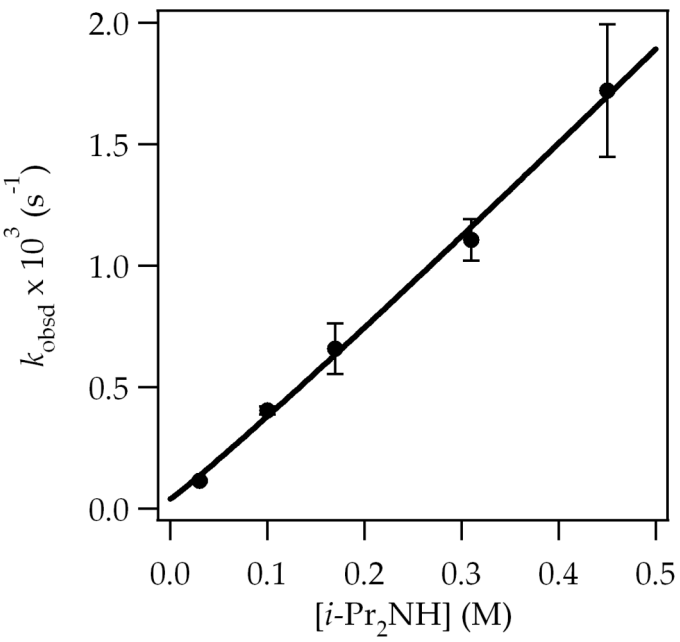



**Figure 32.** Plot of $k_{obsd}$ vs [$i$-$Pr_2NH$] for the isomerization of **3** (0.050 M) to **2** in 12.2 M THF at –78 °C measured by IR spectrocopy. The curve depicts an unweighted least-squares fit to $y = k[i\text{-}Pr_2NH]^n + c$. [$k = (3.8 \pm 0.3) \times 10^{-3}$, $n = 1.1 \pm 0.1$, $c = (2 \pm 1) \times 10^{-5}$]

| [$i$-$Pr_2NH$] (M) | y1 ($s^{-1}$) | y2 ($s^{-1}$) |
|---|---|---|
| 0.030 | 1.12 e-4 ± 4 e-6 | 1.18 e-4± 1 e-6 |
| 0.10 | 3.92 e-4 ± 3 e-6 | 4.15 e-4± 3 e-6 |
| 0.17 | 7.33 e-4 ± 5 e-6 | 5.86 e-4 ± 3 e-6 |
| 0.31 | 1.17 e-3 ± 7 e-6 | 1.05 e-3 ± 8 e-6 |
| 0.45 | 1.91 e-3± 2 e-5 | 1.53 e-3 ± 1 e-5 |

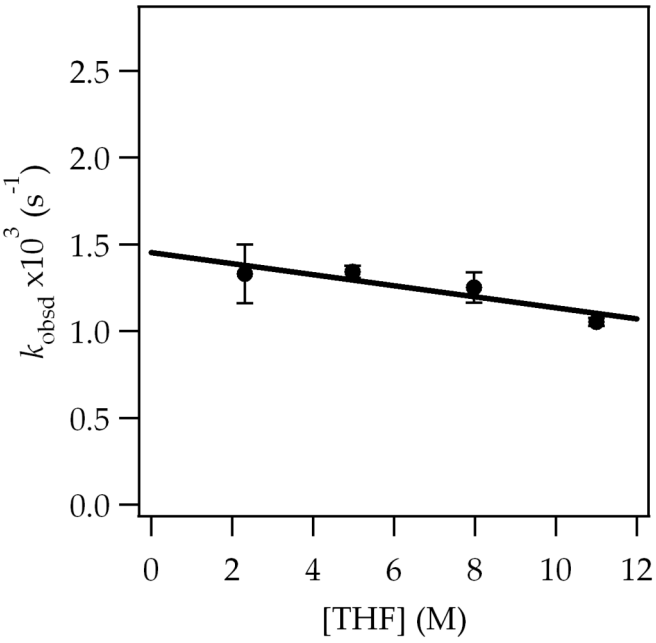



**Figure 33**. Plot of $k_{obsd}$ versus [THF] for the isomerization of **3** (0.050 M) to **2** in 12.2 M THF at –78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to y = *a*[THF]+b. [*a*= (1.45 ± 0.08) x $10^{-3}$, *b* = (3.2 ± 1.1) x $10^{-5}$]

| [THF] (M) | y1 ($s^{-1}$) | y2 ($s^{-1}$) |
|---|---|---|
| 2.31 | 1.21 e-3 ± 3 e-5 | 1.44 e-3 ± 2 e-5 |
| 4.97 | 1.32 e-3 ± 1 e-5 | 1.37 e-3 ± 2 e-5 |
| 7.98 | 1.31 e-3 ± 7 e-6 | 1.19 e-3 ± 1 e-5 |
| 11.0 | 1.04 e-3 ± 9 e-6 | 1.07 e-3 ± 8 e-6 |

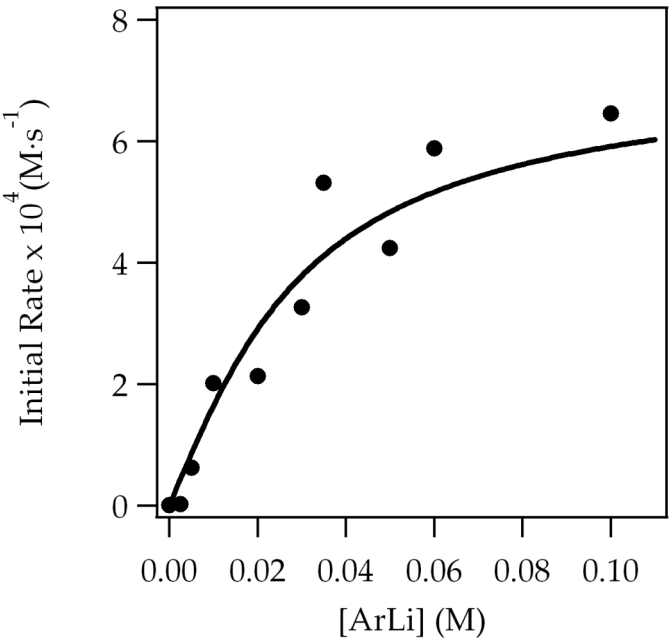



**Figure 34.** Plot of initial rate versus aryllithium **2**-6-*d* for the ortholithiation of **1** (0.075 M) by 0.10 M LDA in 12.2 M THF at –78 °C measured by IR spectroscopy. Aryllithium **2** was generated from **1**-6-*d* with one equivalent LDA at –40 °C prior to injection **1**. The curve depicts an unweighted least-squares fit a simple first-order saturation function: $-\Delta[ArH]/\Delta t\,|_{t=0} = (k_1 k_2 [A_2S_2][ArH])/(k_{-1} + k_2[ArH])$ where [ArH] = 0.075 M, $[A_2S_2]$ = 0.050 M. $k_2$ was constrained to the same value corresponding to lithium chloride saturation (see Figure 13). [$k_1$ = (0.18 $\pm$ 0.02); $k_{-1}$ = (1.97 $\pm$ 0.01) x $10^9$]

| [**2**-6-*d*] (M) | y (M·s$^{-1}$) |
|---|---|
| 0.0 | 0.006 e-4 $\pm$ 1 e-7 |
| 0.0025 | 0.026 e-4 $\pm$ 2 e-7 |
| 0.005 | 0.623 e-4 $\pm$ 7 e-7 |
| 0.010 | 2.02 e-4 $\pm$ 3 e-6 |
| 0.020 | 2.13 e-4 $\pm$ 4 e-6 |
| 0.030 | 3.27 e-4 $\pm$ 7 e-6 |
| 0.035 | 5.32 e-4 $\pm$ 8 e-6 |
| 0.050 | 4.24 e-4 $\pm$ 8 e-6 |
| 0.060 | 5.88 e-4 $\pm$ 1 e-5 |
| 0.10 | 6.46 e-4 $\pm$ 1 e-5 |

**Derivation.** Derivation of 2nd-order LiCl saturation curve (eq 17 in manuscript):

$$A_2S_2 + 2S \underset{k_{-1}[LiCl]^n}{\overset{k_1[LiCl]^n}{\rightleftharpoons}} 2AS_2$$

$$AS_2 + ArH \xrightarrow{k_2} \text{product}$$

The initial rate of consumption of ArH is defined as:

$$-\Delta[ArH]/\Delta t\big|_{t=0} = k_2[AS_2]_0[ArH]_0 \quad (1)$$

Applying the steady-state approximation to monomer $AS_2$ gives

$$\frac{d[AS_2]}{dt} = 2k_1[A_2S_2][LiCl]^n - 2k_{-1}[AS_2]^2[LiCl]^n - k_2[AS_2][ArH] = 0 \quad (2)$$

solving for $[AS_2]$ using the quadratic equation gives

$$[AS_2] = \frac{1}{4k_{-1}[LiCl]^n}\left(\sqrt{k_2^2[ArH]^2 + 16k_1k_{-1}[A_2S_2][LiCl]^{2n}} - k_2[ArH]\right) \quad (3)$$

Substituting eq 3 into eq 1 gives

$$-\Delta[ArH]/\Delta t\big|_{t=0} = \frac{k_2[ArH]}{4k_{-1}[LiCl]^n}\left(\sqrt{k_2^2[ArH]^2 + 16k_1k_{-1}[A_2S_2][LiCl]^{2n}} - k_2[ArH]\right) \quad (4)$$

where [ArH] and $[A_2S_2]$ are evaluated at $t$=0. To account for the LiCl-free pathway, we add a constant $c$ to eq 4 that reflects the initial rate without LiCl. The constant is determined experimentally rather than as an adjustable parameter.

$$-\Delta[ArH]/\Delta t\big|_{t=0} = \frac{k_2[ArH]}{4k_{-1}[LiCl]^n}\left(\sqrt{k_2^2[ArH]^2 + 16k_1k_{-1}[A_2S_2][LiCl]^{2n}} - k_2[ArH]\right) + c \quad (5)$$

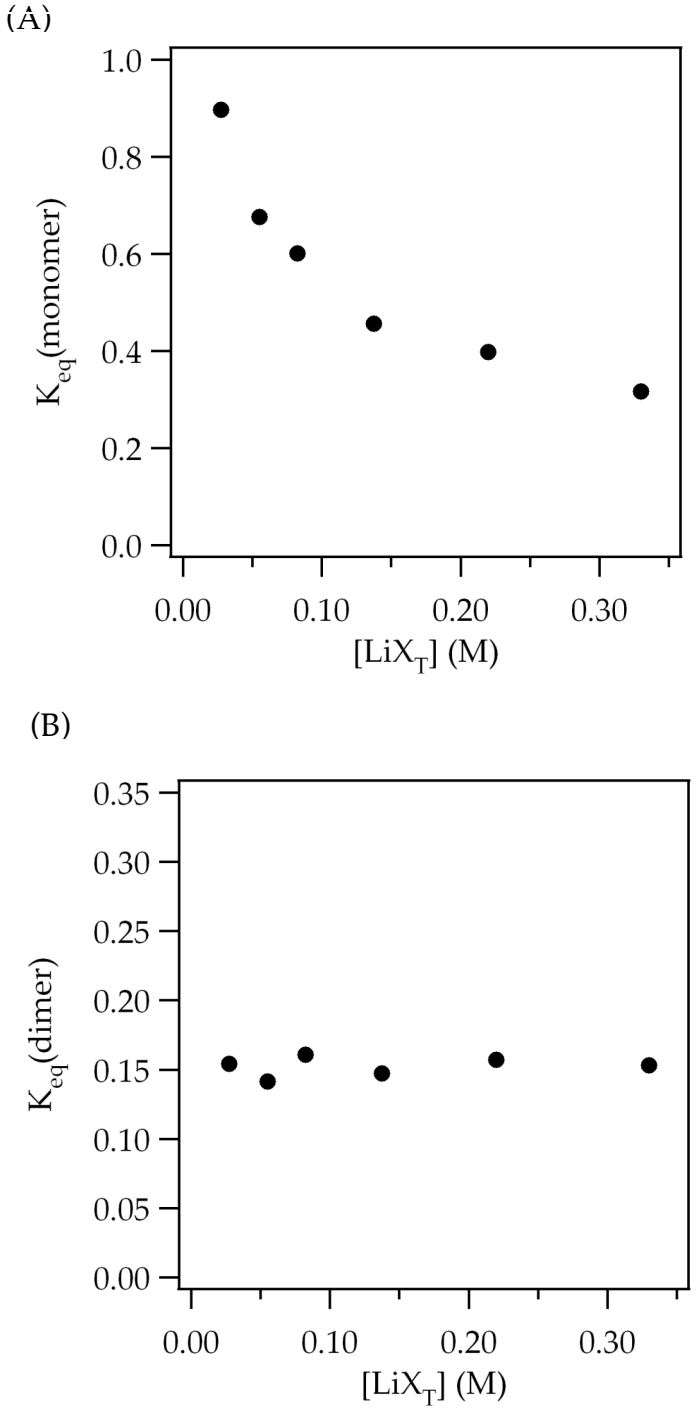



**Figure 35**. Plot of the equilibrium constant ($K_{eq}$) versus total concentration of lithium titer $LiX_T$ (=LDA+LiCl) assuming (A) monomeric lithium chloride and (B) dimeric lithium chloride. Amounts of LDA-LiCl mixed dimer AX and mixed trimer $A_2X$ and lithium chloride $X_n$ are measured by $^6$Li NMR for solutions of 2:1 ratios of LiCl to LDA in 12.2 M THF at -78 °C.

**Figure 35 (continued).**

$$K_{equ}(\text{monomer}) = [AX]^2/([X][A_2X])$$

$$K_{equ}(\text{dimer}) = [AX]^2/([X_2]^{0.5}[A_2X])$$

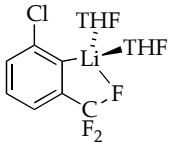
where values of AX, $X_n$ and $A_2X$ are expressed in units of molarity.

| $[LiX_T]$ (M)* | $K_{equ}$ (monomer) | $K_{equ}$(dimer) |
|---|---|---|
| 0.023 | 0.90 | 0.15 |
| 0.055 | 0.68 | 0.14 |
| 0.083 | 0.60 | 0.16 |
| 0.14 | 0.46 | 0.16 |
| 0.22 | 0.40 | 0.16 |
| 0.33 | 0.32 | 0.15 |

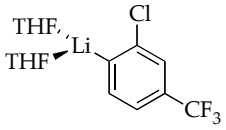
*The concentration of $LiX_T$, although expressed in units of molarity, refers to concentration of monomer unit (normality).

## Part 4: Computational Studies

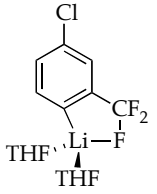
**A**



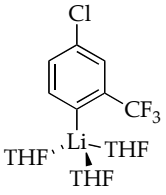
**B**



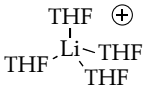
**C**



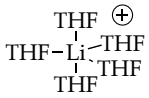
**D**



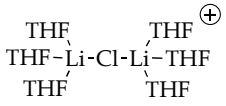
**E**



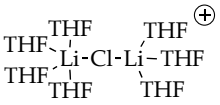
**F**



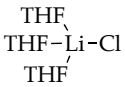
**G**



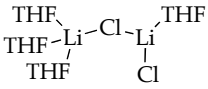
**H**



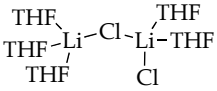
**I**



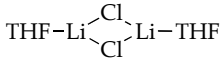
**J**



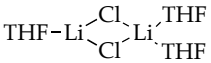
**K**



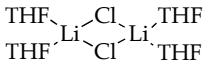
**L**



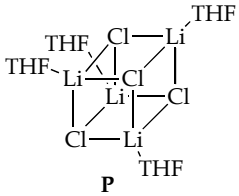
**M**



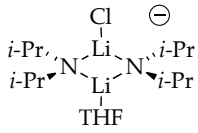
**N**



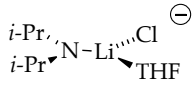
**O**



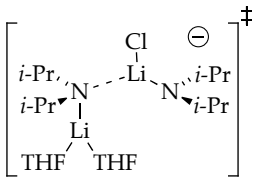
**P**



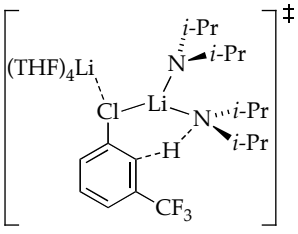
**Q**



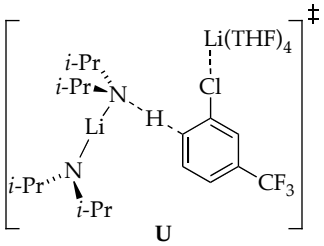
**R**



**S**



**T**



**U**

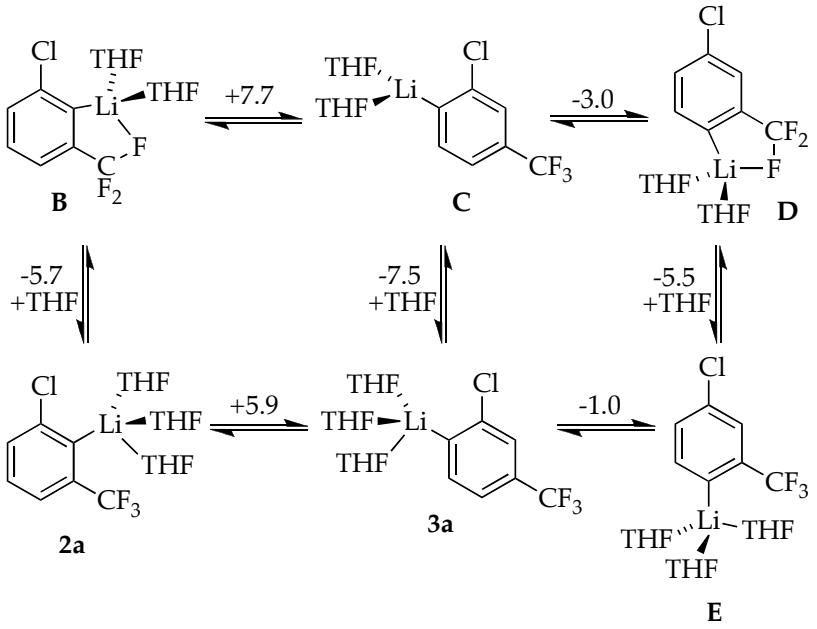



**Figure 36.** Relative free energies for the solvation (Δ*G*, kcal/mol) of of **2**, **3**, and 4-lithio-1-chloro-3-(trifluoromethyl)benzene at -78 °C calculated at the MP2 level of theory with the 6-31G(d) basis set. Relative free energies are given in kcal/mol.

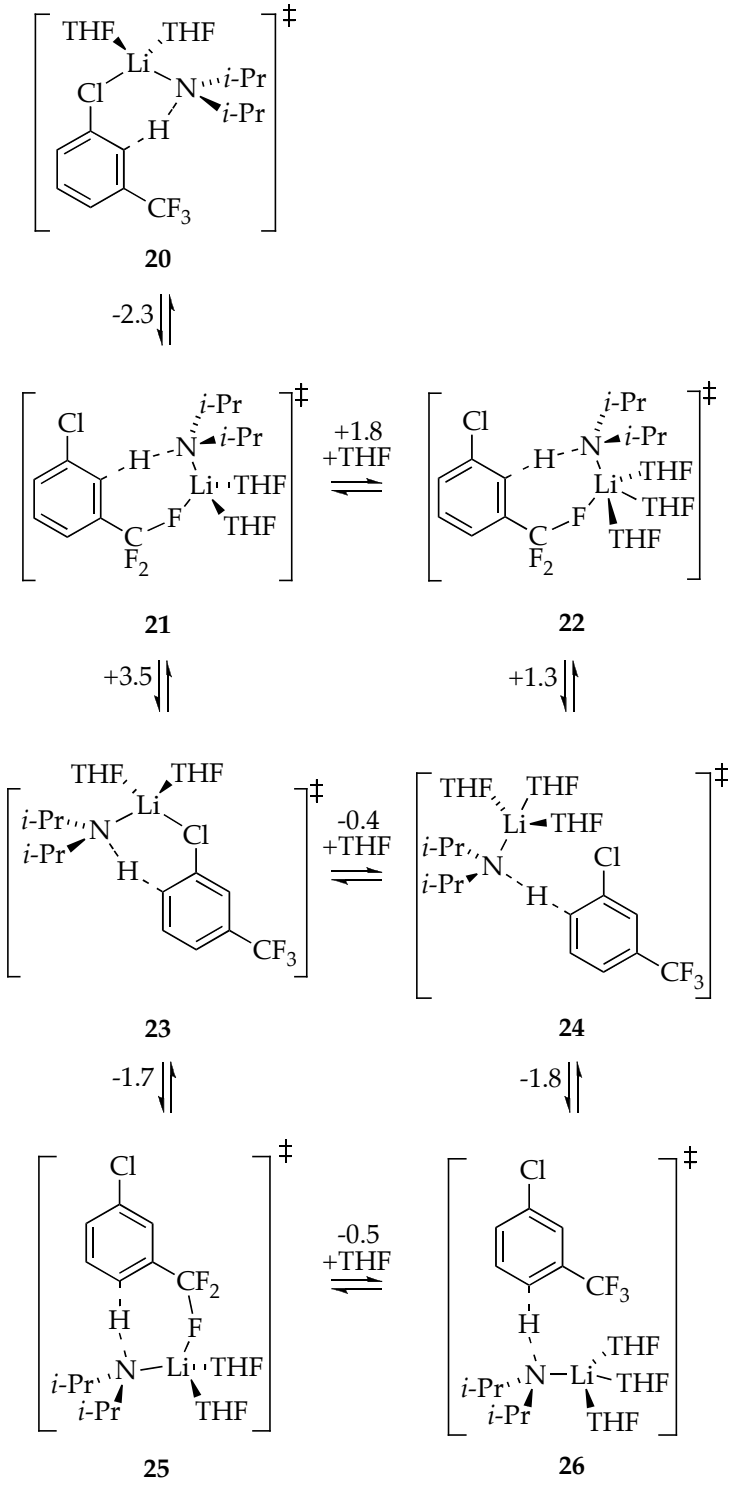



**Figure 37.** DFT computations [MP2/6–31G(d)//B3LYP/6–31G(d)] of monomer-based transition structures for the metalation of **1**. The free energy of activation for the formation of **18** ($\Delta G^{\ddagger}$) is 14.5 kcal/mol calculated at –78 °C. The numbers affiliated with the arrows represent the relative free energies ($\Delta G$).

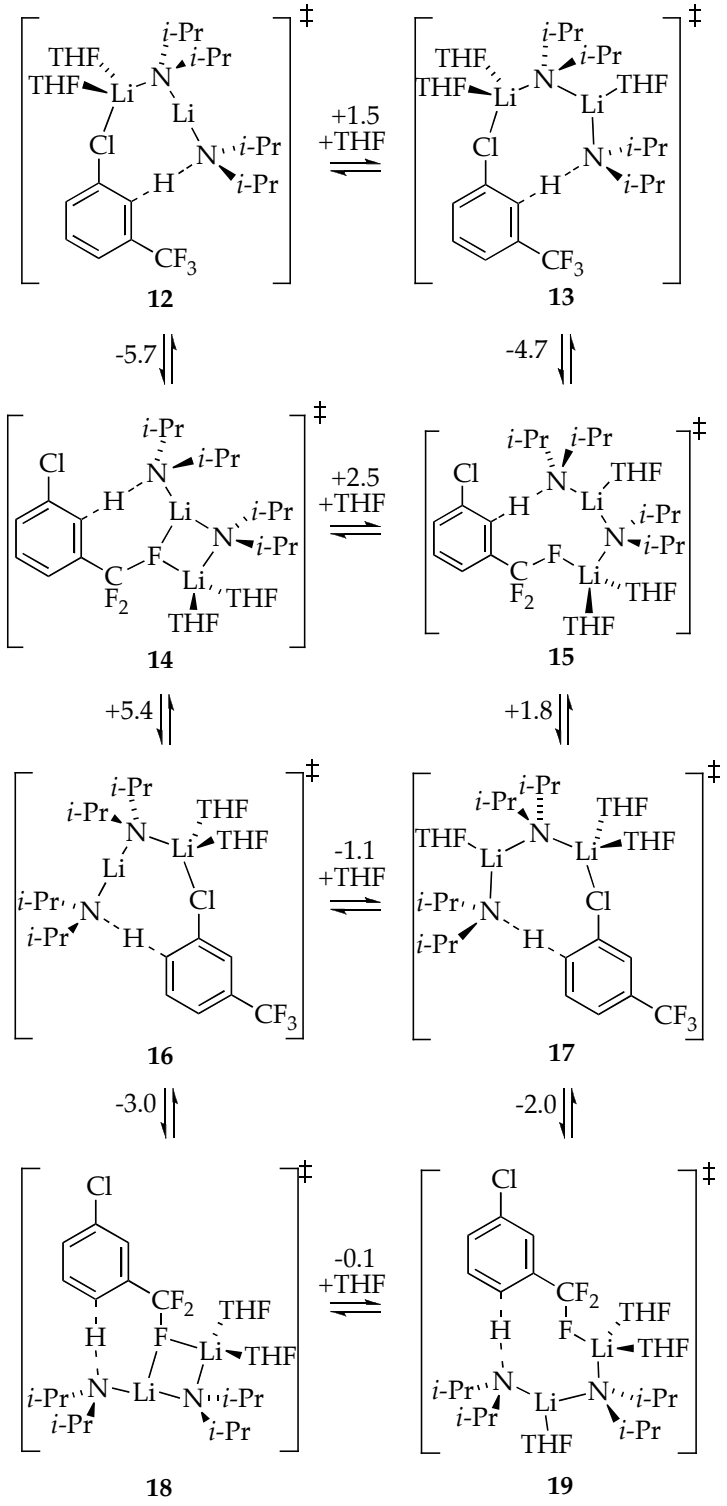
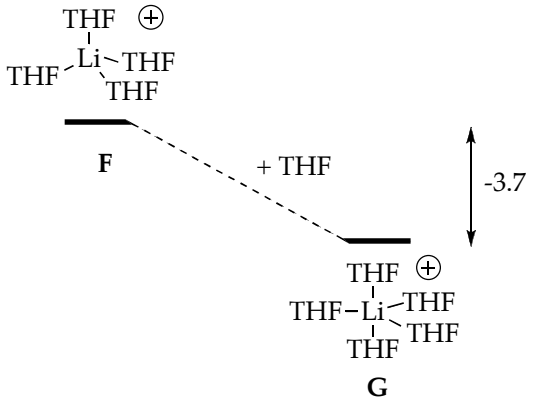
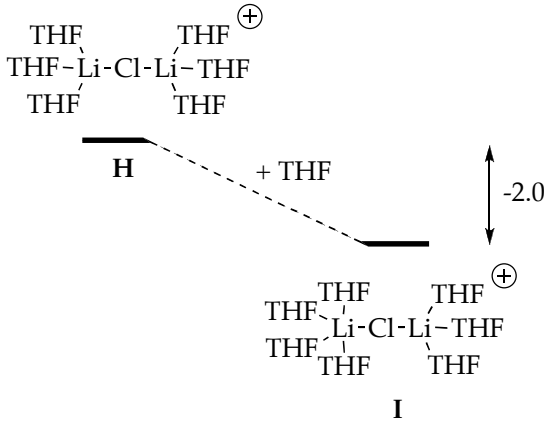



**Figure 38.** DFT computations [MP2/6–31G(d)//B3LYP/6–31G(d)] of dimer-based transition structures for the metalation of **1**. The free energy of activation for the formation of **12** ($\Delta G^{\ddagger}$) is 19.3 kcal/mol calculated at –78 °C. The numbers affiliated with the arrows represent the relative free energies ($\Delta G$).

(A)




(B)




(C)

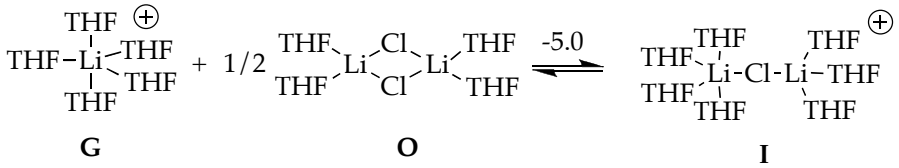
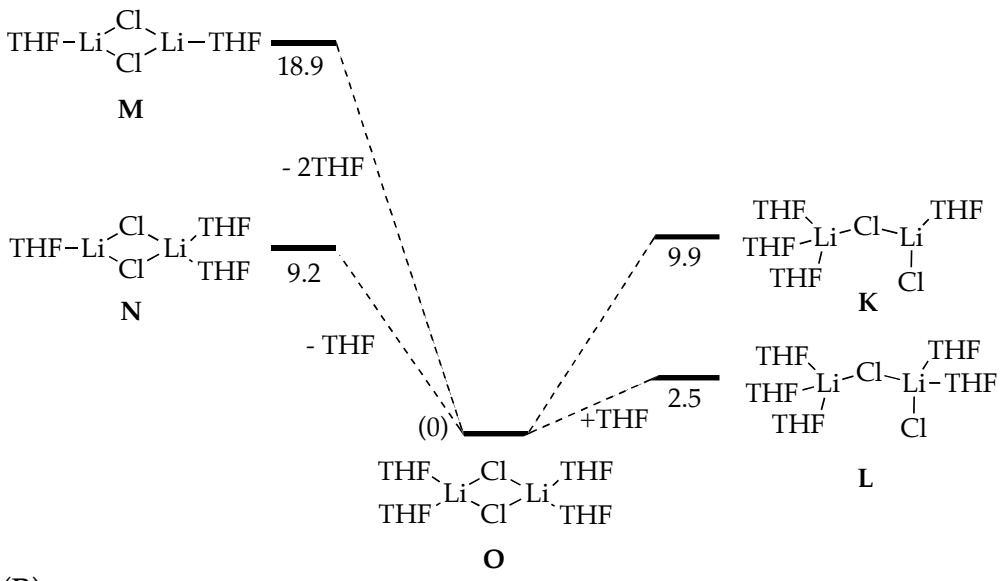



**Figure 39.** Relative free energies (ΔG, kcal/mol) at -78 °C for the solvation of (A) THF-tetrasolvated lithium ion and (B) THF-hexasolvated LiCl triple ion. (C) Relative free energy (ΔG, kcal/mol) at -78 °C showing the relative propensity of the lithium ion to exist in the triple-ion form rather than the simple ion pair.

(A)




(B)

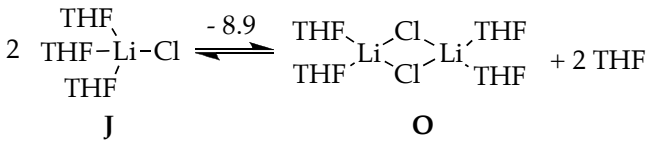



**Figure 40.** Relative free energies (ΔG, kcal/mol) at -78 °C of (A) dimeric LiCl and relative free energy of monomeric and dimeric LiCl at -78 °C. Tetrasolvated monomeric LiCl failed to minimize.

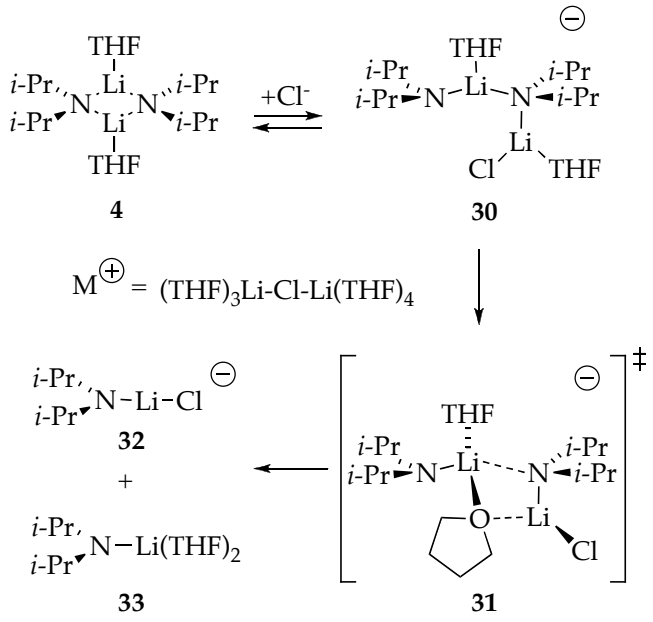
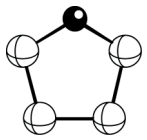



**Figure 41.** Reaction scheme showing lithium chloride deaggregating THF-disolvated closed dimer. The free energy of **31** is + 5.0 kcal/mol at -78 °C relative to chloride-solvated opendimer **30**. The left side of the equation could, in principle, be balanced by the inclusion of LDA-LiCl mixed aggregates. Because a comparison in free energies of neutral and ionic/charge-separated species results in large errors in DFT, the equation was not balanced. The negatively charged triple ions all have the counterion $(THF)_3Li\text{-}Cl\text{-}Li(THF)_3$.

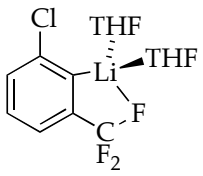
**Table 5.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of **2**, **3**, and 4-lithio-1-chloro-3-(trifluoromethyl)benzene at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

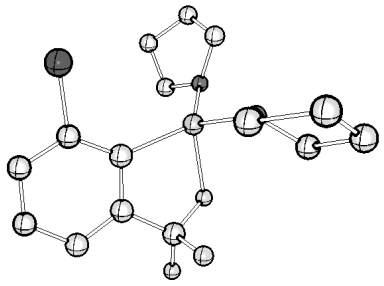



**A**
$G$ = -232.349385
$G_{MP2}$ = -231.669937

| Atom | X | Y | Z |
|---|---|---|---|
| C | -0.77676 | 0.78926 | -0.12614 |
| C | -1.13241 | -0.69941 | 0.08086 |
| O | -0.00028 | -1.43271 | -0.37154 |
| C | 1.13192 | -0.69999 | 0.08156 |
| C | 0.77743 | 0.78860 | -0.12707 |
| H | -1.99954 | -1.03544 | -0.49441 |
| H | -1.32099 | -0.90818 | 1.14790 |
| H | 1.99943 | -1.03711 | -0.49250 |
| H | 1.31917 | -0.90803 | 1.14900 |
| H | 1.16400 | 1.14893 | -1.08517 |
| H | 1.20108 | 1.42138 | 0.65905 |
| H | -1.16426 | 1.15158 | -1.08311 |
| H | -1.19880 | 1.42112 | 0.66158 |

**Table 5 (Continued).**

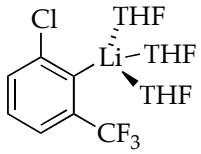


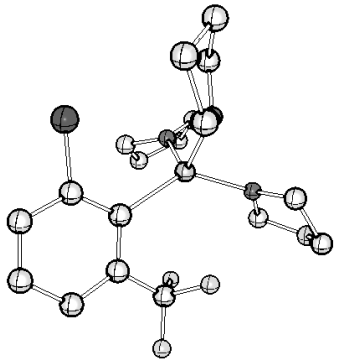



**B**
$G$ = -1500.483215
$G_{MP2}$ = -1496.753504

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 0.171979 | -0.561478 | 0.062389 | H | 5.498146 | -3.424722 | -1.329519 |
| C | 0.115382 | -0.096682 | 1.487325 | H | 3.920372 | -4.197710 | -1.491305 |
| C | 1.349549 | 0.202902 | 2.104120 | H | 2.756084 | -2.150808 | -1.356020 |
| C | 1.200229 | 0.563148 | 3.436685 | H | 4.317262 | -1.364466 | -1.710260 |
| C | -0.002228 | 0.636029 | 4.139933 | O | 3.958476 | 1.725702 | 0.304060 |
| C | -1.185051 | 0.324860 | 3.462701 | C | 5.375893 | 1.748285 | 0.611941 |
| C | -1.134155 | -0.046403 | 2.121014 | C | 5.683633 | 3.171821 | 1.090353 |
| H | -2.047243 | -0.284615 | 1.582034 | C | 4.329084 | 3.632441 | 1.652367 |
| H | -2.137281 | 0.377840 | 3.983600 | C | 3.349609 | 2.992331 | 0.673148 |
| H | -0.024323 | 0.929828 | 5.185307 | H | 3.222735 | 3.595648 | -0.235417 |
| Cl | 2.685533 | 0.995259 | 4.385639 | H | 2.370730 | 2.769833 | 1.104270 |
| Li | 2.892118 | 0.159067 | 0.718571 | H | 4.227816 | 4.721024 | 1.693493 |
| O | 3.847390 | -1.497348 | 0.282465 | H | 4.167290 | 3.228522 | 2.657484 |
| C | 3.803669 | -2.061661 | -1.044191 | H | 5.983391 | 3.804271 | 0.246470 |
| C | 4.480416 | -3.444418 | -0.929722 | H | 6.488348 | 3.191965 | 1.831025 |
| C | 4.488085 | -3.736530 | 0.596515 | H | 5.567031 | 1.005192 | 1.395041 |
| C | 3.638868 | -2.604887 | 1.186698 | H | 5.929358 | 1.461708 | -0.287793 |
| H | 3.940943 | -2.275017 | 2.182116 | F | 1.221839 | 0.027145 | -0.631663 |
| H | 2.571142 | -2.856052 | 1.202110 | F | 0.404427 | -1.900989 | -0.058579 |
| H | 5.507792 | -3.692138 | 0.990997 | F | -0.937557 | -0.302515 | -0.654913 |
| H | 4.077820 | -4.720544 | 0.840800 | | | | |

**Table 5 (Continued).**

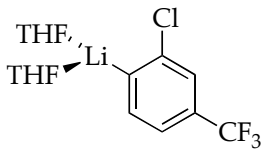


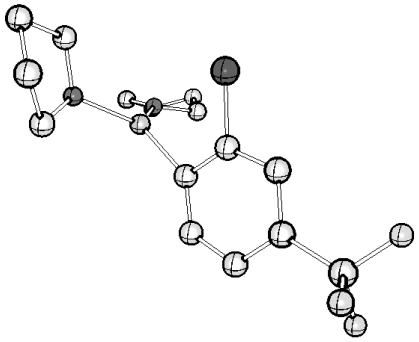



**2a**
$G$ = -1732.830143
$G_{MP2}$ = -1728.332611

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 0.017822 | 2.843992 | -0.388654 | C | 1.021688 | -0.478445 | 3.941691 |
| C | -1.339085 | 2.265150 | -0.112398 | C | -0.071618 | -0.931617 | 2.966786 |
| C | -1.397940 | 0.868650 | 0.120209 | H | -0.773197 | -0.154462 | 2.664612 |
| C | -2.694989 | 0.456009 | 0.397622 | H | -0.631199 | -1.794293 | 3.355846 |
| C | -3.840393 | 1.253842 | 0.451419 | H | 1.249998 | 0.579629 | 3.780988 |
| C | -3.699465 | 2.619132 | 0.206201 | H | 0.719272 | -0.601434 | 4.985878 |
| C | -2.435315 | 3.135009 | -0.077081 | H | 3.137326 | -0.755203 | 3.413316 |
| H | -2.309189 | 4.196535 | -0.266188 | H | 2.469974 | -2.104778 | 4.331560 |
| H | -4.568006 | 3.271566 | 0.238257 | H | 1.519471 | -3.100741 | 2.427504 |
| H | -4.812554 | 0.826152 | 0.678373 | H | 2.542349 | -2.019728 | 1.446948 |
| Cl | -3.003377 | -1.311472 | 0.745665 | O | -0.078641 | -1.957407 | -1.352658 |
| Li | 0.294935 | -0.475574 | 0.001013 | C | -0.179857 | -3.331650 | -0.920970 |
| O | 2.278988 | -0.225409 | -0.588333 | C | -0.943451 | -4.054940 | -2.031449 |
| C | 2.539633 | -0.262144 | -2.011693 | C | -1.896257 | -2.954620 | -2.524227 |
| C | 3.553526 | 0.850425 | -2.277492 | C | -1.027127 | -1.698915 | -2.418904 |
| C | 4.359282 | 0.863739 | -0.970271 | H | -1.586584 | -0.797235 | -2.158990 |
| C | 3.268432 | 0.603024 | 0.071072 | H | -0.459627 | -1.518768 | -3.342173 |
| H | 2.785441 | 1.529006 | 0.390784 | H | -2.757408 | -2.869420 | -1.854493 |
| H | 3.632086 | 0.065460 | 0.952954 | H | -2.261923 | -3.122807 | -3.541809 |
| H | 4.883574 | 1.807524 | -0.792949 | H | -1.463148 | -4.946458 | -1.667350 |
| H | 5.101158 | 0.055935 | -0.967418 | H | -0.258691 | -4.360681 | -2.831823 |
| H | 3.033423 | 1.804155 | -2.411581 | H | 0.834566 | -3.712121 | -0.764133 |
| H | 4.164434 | 0.657529 | -3.164648 | H | -0.724981 | -3.362613 | 0.029905 |
| H | 2.941893 | -1.250880 | -2.269129 | F | 0.865438 | 2.702856 | 0.677114 |
| H | 1.592795 | -0.122323 | -2.536255 | F | 0.650378 | 2.227029 | -1.432185 |
| O | 0.650776 | -1.330273 | 1.787958 | F | 0.007908 | 4.163940 | -0.684460 |
| C | 1.800123 | -2.052723 | 2.246807 | | | | |
| C | 2.239799 | -1.363506 | 3.560118 | | | | |

**Table 5 (Continued).**

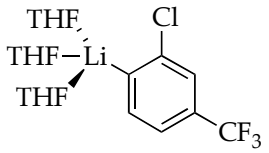


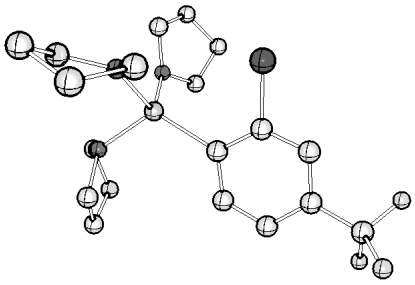



**C**
$G$ = -1500.472097
$G_{MP2}$ = -1496.741357

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 4.228498 | -1.630255 | -0.619511 | C | 1.726562 | 2.794350 | -1.282569 |
| O | 2.877050 | -1.419008 | -0.152078 | H | 2.273506 | 3.163010 | -2.160724 |
| Li | 1.656774 | 0.036753 | -0.472780 | H | 0.794132 | 2.322429 | -1.600537 |
| C | -0.387058 | -0.159538 | -0.721856 | H | 1.332794 | 4.859306 | -0.663125 |
| C | -1.331327 | -0.362525 | -1.756929 | H | 0.738244 | 3.613785 | 0.455994 |
| C | -2.709566 | -0.442054 | -1.545263 | H | 3.662707 | 4.390870 | -0.063380 |
| C | -3.220465 | -0.320538 | -0.248363 | H | 2.867534 | 4.244894 | 1.513379 |
| C | -2.346981 | -0.119577 | 0.824270 | H | 2.862492 | 1.837671 | 1.405926 |
| C | -0.990575 | -0.050571 | 0.523365 | H | 4.299277 | 2.122366 | 0.387380 |
| Cl | 0.112580 | 0.211146 | 1.974581 | C | 2.318401 | -2.659529 | 0.362600 |
| H | -2.720957 | -0.029876 | 1.838178 | C | 3.513197 | -3.597898 | 0.523913 |
| C | -4.701189 | -0.338895 | -0.013961 | C | 4.432626 | -3.147281 | -0.622400 |
| F | -5.260594 | 0.889051 | -0.171340 | H | 5.480238 | -3.425803 | -0.475640 |
| F | -5.019486 | -0.745436 | 1.238368 | H | 4.095696 | -3.576706 | -1.572904 |
| F | -5.344397 | -1.161715 | -0.877106 | H | 4.000738 | -3.437602 | 1.492707 |
| H | -3.391136 | -0.605959 | -2.375710 | H | 3.225457 | -4.651031 | 0.457744 |
| H | -0.977859 | -0.468811 | -2.783991 | H | 1.796768 | -2.427836 | 1.293819 |
| O | 2.525862 | 1.767909 | -0.635611 | H | 1.591270 | -3.037927 | -0.364923 |
| C | 3.231104 | 2.333916 | 0.501043 | H | 4.328027 | -1.171807 | -1.608279 |
| C | 2.906349 | 3.833029 | 0.500916 | H | 4.919705 | -1.130360 | 0.071226 |
| C | 1.552788 | 3.880923 | -0.226001 | | | | |

**Table 5 (Continued).**

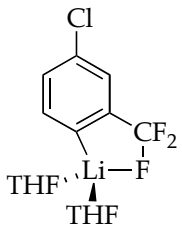


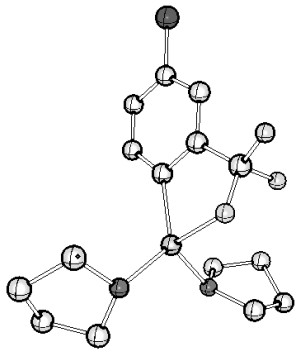



**3a**
$G$ = -1732.822222
$G_{MP2}$ = -1728.323065

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 1.414884 | 0.079137 | -0.074857 | O | 2.344193 | -0.242844 | 1.673865 |
| C | -0.709391 | 0.224189 | -0.043682 | C | 3.692392 | 0.178926 | 1.980854 |
| C | -1.493806 | 1.330662 | -0.459511 | C | 3.711550 | 0.529382 | 3.480924 |
| C | -2.889252 | 1.368287 | -0.432017 | C | 2.221032 | 0.718350 | 3.812610 |
| C | -3.597033 | 0.254816 | 0.030979 | C | 1.564848 | -0.304181 | 2.889933 |
| C | -2.896048 | -0.877654 | 0.451294 | H | 0.530871 | -0.087316 | 2.618419 |
| C | -1.504453 | -0.834355 | 0.387809 | H | 1.618589 | -1.318988 | 3.306587 |
| Cl | -0.689662 | -2.378199 | 0.934688 | H | 1.888821 | 1.730167 | 3.551711 |
| H | -3.424713 | -1.755922 | 0.804637 | H | 1.990859 | 0.544727 | 4.868053 |
| C | -5.091590 | 0.299065 | 0.130641 | H | 4.316411 | 1.416610 | 3.690630 |
| F | -5.513104 | 0.911761 | 1.267810 | H | 4.125264 | -0.301156 | 4.063899 |
| F | -5.650470 | 0.986124 | -0.896275 | H | 4.386823 | -0.632869 | 1.733197 |
| F | -5.646735 | -0.936050 | 0.133017 | H | 3.915908 | 1.037010 | 1.340102 |
| H | -3.430971 | 2.247137 | -0.772589 | O | 2.131888 | -1.265583 | -1.401593 |
| H | -0.990801 | 2.223434 | -0.838908 | C | 2.851694 | -2.422939 | -0.909231 |
| O | 2.421217 | 1.782679 | -0.660842 | C | 2.574105 | -3.546315 | -1.910744 |
| C | 2.988107 | 1.915474 | -1.974400 | C | 1.166981 | -3.187725 | -2.413561 |
| C | 2.024005 | 2.847823 | -2.704661 | C | 1.224704 | -1.661353 | -2.465205 |
| C | 1.637106 | 3.852043 | -1.597125 | H | 0.264836 | -1.174952 | -2.276726 |
| C | 1.864475 | 3.062714 | -0.284414 | H | 1.635955 | -1.303294 | -3.419225 |
| H | 0.943138 | 2.857213 | 0.264747 | H | 0.409504 | -3.508812 | -1.691711 |
| H | 2.569229 | 3.578240 | 0.380806 | H | 0.930859 | -3.628130 | -3.387003 |
| H | 0.603402 | 4.194373 | -1.694800 | H | 2.627633 | -4.535689 | -1.446701 |
| H | 2.282726 | 4.735886 | -1.630316 | H | 3.297606 | -3.516848 | -2.734490 |
| H | 1.146265 | 2.284418 | -3.038205 | H | 3.911276 | -2.157321 | -0.832934 |
| H | 2.475993 | 3.329335 | -3.577137 | H | 2.471644 | -2.665045 | 0.089263 |
| H | 3.994653 | 2.356166 | -1.901175 | | | | |
| H | 3.065675 | 0.909809 | -2.390627 | | | | |

**Table 5 (Continued).**

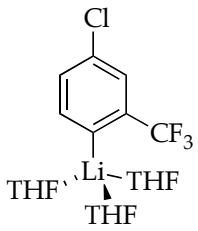


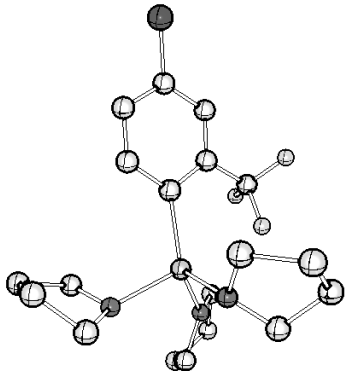



**D**
$G$ = -1500.475537
$G_{MP2}$ = -1496.746032

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 0.928658 | -1.012816 | 1.482744 | O | -2.299268 | -1.328246 | -0.680100 |
| C | 1.584391 | -0.172928 | 0.426750 | C | -1.748621 | -1.930597 | -1.881721 |
| C | 2.986545 | -0.101788 | 0.456051 | C | -1.412668 | -3.363833 | -1.483259 |
| C | 3.615938 | 0.617026 | -0.550917 | C | -2.559332 | -3.697790 | -0.515193 |
| C | 2.873361 | 1.242314 | -1.552503 | C | -2.772809 | -2.368023 | 0.219323 |
| C | 1.478800 | 1.138183 | -1.527622 | H | -2.179853 | -2.309365 | 1.137511 |
| C | 0.752596 | 0.430434 | -0.543355 | H | -3.822383 | -2.168200 | 0.458139 |
| Li | -1.228053 | 0.161675 | 0.028393 | H | -2.318014 | -4.512283 | 0.173744 |
| O | -2.414558 | 1.597610 | 0.591841 | H | -3.460506 | -3.980430 | -1.071828 |
| C | -3.685001 | 1.862119 | -0.032705 | H | -0.450699 | -3.388534 | -0.961525 |
| C | -3.498856 | 3.212694 | -0.718366 | H | -1.363035 | -4.038487 | -2.343076 |
| C | -2.636748 | 3.968272 | 0.309662 | H | -2.509025 | -1.894967 | -2.673993 |
| C | -1.771916 | 2.857531 | 0.935483 | H | -0.883206 | -1.330569 | -2.172890 |
| H | -1.711113 | 2.932259 | 2.026135 | H | 0.939113 | 1.647314 | -2.329082 |
| H | -0.759119 | 2.816629 | 0.524806 | H | 3.384723 | 1.801577 | -2.331573 |
| H | -3.274602 | 4.434364 | 1.068871 | Cl | 5.380289 | 0.744753 | -0.557808 |
| H | -2.028154 | 4.755727 | -0.143374 | H | 3.570370 | -0.582161 | 1.234878 |
| H | -4.447118 | 3.713763 | -0.934719 | F | 0.748409 | -2.312037 | 1.110809 |
| H | -2.954283 | 3.082178 | -1.660493 | F | 1.581797 | -1.044088 | 2.659751 |
| H | -3.894406 | 1.028414 | -0.707441 | F | -0.357376 | -0.565965 | 1.776938 |
| H | -4.470327 | 1.906035 | 0.735823 | | | | |

**Table 5 (Continued).**

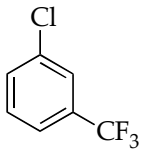


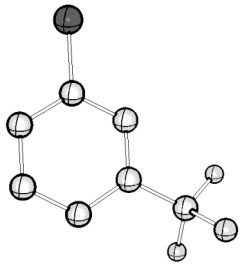



**E**
$G$ = -1732.822473
$G_{MP2}$ = -1728.324732

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.362083 | -2.061318 | -0.542082 | H | -5.302976 | -0.890849 | -2.460373 |
| C | 1.977997 | -0.694734 | -0.435157 | H | -3.931275 | 0.076652 | -3.036293 |
| C | 3.378274 | -0.638230 | -0.530033 | H | -3.904220 | -2.900539 | -2.296116 |
| C | 3.986268 | 0.609180 | -0.493216 | H | -3.287784 | -2.175582 | -3.789894 |
| C | 3.222304 | 1.766658 | -0.363672 | H | -1.365095 | -1.231360 | -2.655703 |
| C | 1.831116 | 1.646140 | -0.273308 | H | -1.598911 | -2.650666 | -1.622697 |
| C | 1.120742 | 0.422996 | -0.307311 | O | -1.928390 | 2.047014 | -0.115734 |
| Li | -0.960239 | 0.210810 | 0.114260 | C | -1.524996 | 2.835676 | -1.262682 |
| O | -1.354895 | -0.144046 | 2.097916 | C | -1.350574 | 4.285558 | -0.762185 |
| C | -2.088741 | -1.329699 | 2.470324 | C | -1.355003 | 4.140185 | 0.771972 |
| C | -1.105062 | -2.175068 | 3.275626 | C | -2.263027 | 2.929105 | 0.968110 |
| C | -0.315992 | -1.095270 | 4.033898 | H | -3.325098 | 3.213216 | 0.902376 |
| C | -0.239095 | 0.048075 | 3.011722 | H | -2.101834 | 2.373935 | 1.894106 |
| H | 0.676666 | 0.023419 | 2.415019 | H | -1.721366 | 5.034631 | 1.285153 |
| H | -0.334565 | 1.037540 | 3.472793 | H | -0.349388 | 3.915794 | 1.143642 |
| H | 0.676477 | -1.430380 | 4.348593 | H | -2.190166 | 4.909926 | -1.087546 |
| H | -0.864984 | -0.780107 | 4.929205 | H | -0.431570 | 4.741953 | -1.140217 |
| H | -0.446829 | -2.726833 | 2.597989 | H | -0.597561 | 2.394446 | -1.636408 |
| H | -1.605641 | -2.888677 | 3.937337 | H | -2.296382 | 2.757478 | -2.038772 |
| H | -2.959992 | -1.040867 | 3.076924 | H | 1.277616 | 2.582621 | -0.165647 |
| H | -2.435120 | -1.800202 | 1.547502 | H | 3.711285 | 2.737032 | -0.330954 |
| O | -2.388145 | -0.878552 | -0.888548 | Cl | 5.749590 | 0.726110 | -0.602319 |
| C | -2.079722 | -1.751213 | -2.009238 | H | 3.980293 | -1.536152 | -0.623468 |
| C | -3.413297 | -2.014102 | -2.715206 | F | 1.016705 | -2.388769 | -1.820074 |
| C | -4.220763 | -0.751240 | -2.378001 | F | 2.170004 | -3.059502 | -0.108244 |
| C | -3.771254 | -0.471722 | -0.944651 | F | 0.201784 | -2.178032 | 0.180739 |
| H | -4.351139 | -1.067219 | -0.224349 | | | | |
| H | -3.815293 | 0.580027 | -0.655885 | | | | |

**Table 6.** Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the ortholithiation of **1** at -78 °C with free energies (Hartrees), and cartesian coordinates (X,Y,Z). (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures)

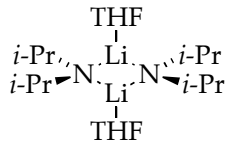


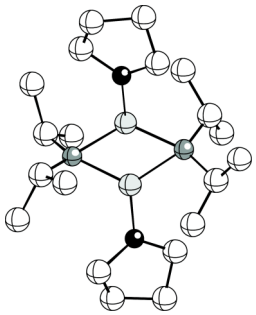



**1**
$G$ = -1028.806251
$G_{MP2}$ = -1026.746114

| Atom | X | Y | Y |
|---|---|---|---|
| C | -2.022802 | -0.354078 | -0.001457 |
| C | -0.643328 | 0.251689 | -0.033108 |
| C | -0.495501 | 1.640876 | -0.019701 |
| C | 0.783061 | 2.195416 | 0.003163 |
| C | 1.912125 | 1.375235 | 0.012535 |
| C | 1.743556 | -0.009039 | -0.002061 |
| C | 0.475114 | -0.584206 | -0.024773 |
| H | 0.360420 | -1.661422 | -0.043478 |
| Cl | 3.156784 | -1.051435 | 0.002466 |
| H | 2.910210 | 1.799814 | 0.027779 |
| H | 0.905815 | 3.274380 | 0.009824 |
| H | -1.372674 | 2.278709 | -0.035400 |
| F | -2.913870 | 0.401844 | -0.679607 |
| F | -2.486544 | -0.467172 | 1.264392 |
| F | -2.042081 | -1.591612 | -0.541256 |

**Table 6 (Continued).**

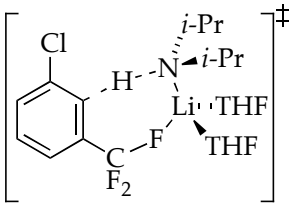


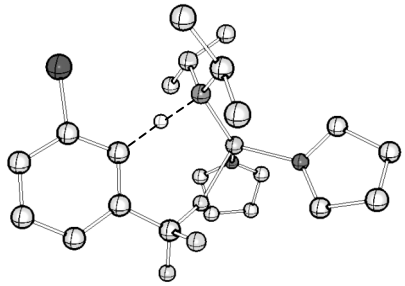



**4**
$G$ = -1063.135499
$G_{MP2}$ = -1059.937725

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.19464 | -0.00774 | 0.01421 | H | 1.83816 | -3.21720 | 1.36630 |
| O | -3.18299 | 0.01572 | -0.13583 | H | -2.15959 | -1.60468 | 1.84082 |
| C | -3.98409 | -1.09503 | -0.60154 | H | -1.26327 | -2.26497 | 3.22164 |
| C | -5.41144 | -0.77445 | -0.16155 | H | -0.80287 | -0.70251 | 2.54173 |
| C | -5.43839 | 0.75767 | -0.27769 | H | -0.65863 | -3.39245 | 1.09537 |
| C | -4.03238 | 1.14387 | 0.19102 | H | -1.65573 | -2.60864 | -2.05785 |
| N | -0.01403 | -1.64369 | 0.06875 | H | -0.68498 | -4.07367 | -2.32132 |
| C | -0.19692 | -2.41025 | 1.31036 | H | -1.50052 | -3.82045 | -0.77116 |
| C | -1.16039 | -1.70758 | 2.28179 | H | 1.87669 | -1.33857 | -1.92728 |
| C | 1.13099 | -2.71953 | 2.04026 | H | 1.14764 | -2.49745 | -3.05209 |
| Li | 1.19465 | 0.00783 | 0.01436 | H | 0.26500 | -1.03245 | -2.60504 |
| N | 0.01400 | 1.64376 | 0.06872 | H | 1.00263 | -3.33501 | -0.73003 |
| C | 0.19652 | 2.41040 | 1.31033 | H | 3.90323 | 1.15737 | -1.69393 |
| C | 1.15952 | 1.70771 | 2.28220 | H | 3.57283 | 2.00952 | -0.16815 |
| C | -1.13164 | 2.71990 | 2.03968 | H | 6.16235 | 1.26993 | -0.78433 |
| C | -0.27768 | 2.55391 | -1.04433 | H | 5.57076 | 1.08298 | 0.87817 |
| C | -0.93195 | 1.81412 | -2.22127 | H | 5.59112 | -1.05745 | -1.32156 |
| C | 0.96199 | 3.31164 | -1.57823 | H | 6.21990 | -1.22706 | 0.32667 |
| O | 3.18302 | -0.01557 | -0.13517 | H | 3.99129 | -1.30081 | 1.27554 |
| C | 4.03229 | -1.14374 | 0.19184 | H | 3.63030 | -2.03115 | -0.30431 |
| C | 5.43806 | -0.75816 | -0.27799 | H | -1.87605 | 1.33861 | -1.92791 |
| C | 5.41178 | 0.77396 | -0.16178 | H | -1.14658 | 2.49738 | -3.05257 |
| C | 3.98424 | 1.09517 | -0.60075 | H | -0.26417 | 1.03236 | -2.60515 |
| C | 0.27810 | -2.55390 | -1.04412 | H | 1.65649 | 2.60840 | -2.05742 |
| C | 0.93270 | -1.81416 | -2.22091 | H | 0.68595 | 4.07349 | -2.32131 |
| C | -0.96133 | -3.31179 | -1.57838 | H | 1.50097 | 3.82031 | -0.77087 |
| H | 2.15887 | 1.60463 | 1.84163 | H | -1.00225 | 3.33509 | -0.73054 |
| H | 1.26211 | 2.26520 | 3.22203 | H | -3.99064 | 1.30159 | 1.27458 |
| H | 0.80177 | 0.70272 | 2.54212 | H | -3.63100 | 2.03110 | -0.30596 |
| H | -1.59922 | 1.79146 | 2.39591 | H | -6.21992 | 1.22625 | 0.32760 |
| H | -0.98370 | 3.37716 | 2.90874 | H | -5.59242 | 1.05690 | -1.32113 |
| H | -1.83853 | 3.21752 | 1.36538 | H | -5.56953 | -1.08360 | 0.87850 |
| H | 0.65842 | 3.39254 | 1.09542 | H | -6.16225 | -1.27067 | -0.78359 |
| H | 1.59838 | -1.79101 | 2.39653 | H | -3.90377 | -1.15665 | -1.69482 |
| H | 0.98277 | -3.37667 | 2.90936 | H | -3.57208 | -2.00943 | -0.16966 |

**Table 6 (Continued).**

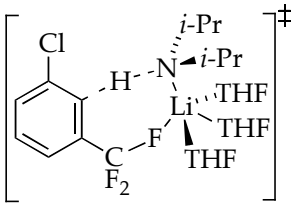


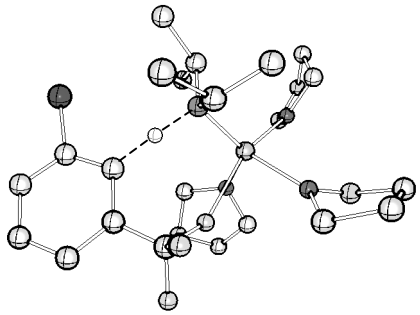



**21**
$G$ = -1792.691253
$G_{MP2}$ = -1787.893790
$\Delta G^{‡}$ = 20.2 kcal/mol
$\Delta G_{MP2}^{‡}$ = 12.2 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 0.547744 | -1.751918 | -1.431940 | H | -1.619713 | -4.202638 | 2.584304 |
| C | 1.964405 | -1.475261 | -1.021925 | H | -1.437177 | -3.604604 | 0.927775 |
| C | 2.923706 | -2.416344 | -1.426851 | H | -0.017417 | -1.998246 | 2.042620 |
| C | 4.262518 | -2.197764 | -1.117503 | H | -1.015858 | -2.037437 | 3.519128 |
| C | 4.623060 | -1.053991 | -0.405722 | C | 0.742327 | 2.131285 | 1.792377 |
| C | 3.624101 | -0.155589 | -0.028813 | H | 1.718436 | 2.642057 | 1.764642 |
| C | 2.266898 | -0.295004 | -0.308794 | C | -0.276591 | 3.144338 | 2.350397 |
| H | 1.326341 | 0.696764 | 0.079079 | H | -0.353782 | 4.042927 | 1.728836 |
| N | 0.390341 | 1.615552 | 0.453824 | H | -1.277707 | 2.692910 | 2.413298 |
| Li | -1.103124 | 0.283914 | 0.467077 | H | 0.009120 | 3.467961 | 3.359714 |
| O | -2.847194 | 0.610487 | -0.496225 | C | 0.897395 | 0.969109 | 2.783267 |
| C | -3.488886 | 1.911085 | -0.441893 | H | 1.590898 | 0.213976 | 2.400179 |
| C | -4.600047 | 1.865473 | -1.491818 | H | 1.291875 | 1.331159 | 3.740465 |
| C | -4.007071 | 0.916670 | -2.545317 | H | -0.069056 | 0.490221 | 2.983151 |
| C | -3.277833 | -0.111185 | -1.679342 | C | 0.332044 | 2.678199 | -0.573894 |
| H | -2.393687 | -0.542051 | -2.154087 | H | -0.511294 | 3.362000 | -0.355683 |
| H | -3.945853 | -0.923962 | -1.364703 | C | 1.589631 | 3.568433 | -0.678707 |
| H | -3.293175 | 1.451098 | -3.181716 | H | 1.467784 | 4.301860 | -1.486362 |
| H | -4.762027 | 0.456601 | -3.189432 | H | 1.782435 | 4.128377 | 0.241805 |
| H | -4.836742 | 2.857264 | -1.887555 | H | 2.478764 | 2.966028 | -0.892299 |
| H | -5.517050 | 1.441355 | -1.065739 | C | 0.050600 | 2.063432 | -1.952503 |
| H | -3.852805 | 2.066679 | 0.578156 | H | 0.875388 | 1.420638 | -2.274281 |
| H | -2.739515 | 2.676798 | -0.670628 | H | -0.861358 | 1.457514 | -1.941615 |
| O | -1.804050 | -0.993815 | 1.904336 | H | -0.076582 | 2.850272 | -2.706549 |
| C | -1.034761 | -2.096153 | 2.421358 | Cl | 4.191448 | 1.272307 | 0.900050 |
| C | -1.782143 | -3.340208 | 1.931366 | H | 5.660658 | -0.865356 | -0.146496 |
| C | -3.264505 | -2.879528 | 1.898408 | H | 5.021564 | -2.913280 | -1.421135 |
| C | -3.183580 | -1.347925 | 2.101138 | H | 2.629517 | -3.308398 | -1.971130 |
| H | -3.482056 | -1.066075 | 3.120584 | F | 0.292116 | -3.061369 | -1.649381 |
| H | -3.765474 | -0.766819 | 1.384753 | F | 0.153045 | -1.097745 | -2.551959 |
| H | -3.857771 | -3.345953 | 2.690659 | F | -0.373417 | -1.373305 | -0.462774 |
| H | -3.734112 | -3.134009 | 0.943808 | | | | |

**Table 6 (Continued).**



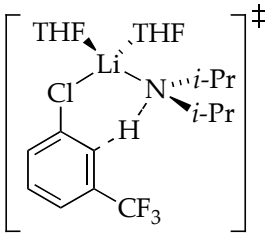



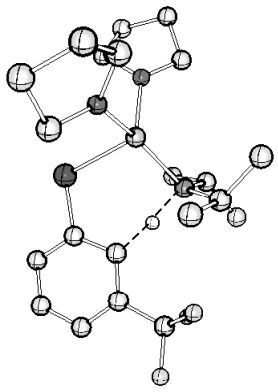
**22**
$G$ = -2025.024264
$G_{MP2}$ = -2019.460718
$\Delta G^{‡}$ = 30.4 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 14.0 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.894567 | -2.056084 | -0.592524 | H | 1.526579 | -2.207951 | 2.576220 |
| C | 2.970506 | -1.087248 | -0.191325 | H | 1.128542 | 0.113056 | 2.024400 |
| C | 4.241742 | -1.635777 | 0.032121 | H | 0.230658 | 0.392432 | 3.542001 |
| C | 5.297999 | -0.796993 | 0.372383 | O | -3.039261 | 0.926147 | 0.722114 |
| C | 5.067082 | 0.571809 | 0.490684 | C | -3.387435 | 1.211770 | 2.098918 |
| C | 3.780958 | 1.060984 | 0.254389 | C | -4.507042 | 2.263921 | 2.057430 |
| C | 2.672201 | 0.292301 | -0.099803 | C | -4.316279 | 2.906956 | 0.674542 |
| Cl | 3.618310 | 2.838758 | 0.452326 | C | -3.872641 | 1.707562 | -0.157534 |
| H | 5.870767 | 1.249749 | 0.762072 | H | -3.278140 | 1.965389 | -1.035224 |
| H | 6.290448 | -1.201862 | 0.549969 | H | -4.736913 | 1.104709 | -0.477696 |
| H | 4.401597 | -2.705974 | -0.053431 | H | -3.518792 | 3.657685 | 0.701734 |
| F | 2.123392 | -3.316399 | -0.139251 | H | -5.224101 | 3.379304 | 0.287384 |
| F | 1.737821 | -2.165915 | -1.938693 | H | -4.431127 | 2.979635 | 2.881212 |
| F | 0.664066 | -1.715135 | -0.103897 | H | -5.491290 | 1.784811 | 2.119385 |
| Li | -1.103446 | -0.018679 | 0.127261 | H | -3.698532 | 0.281455 | 2.586927 |
| O | -2.172304 | -1.633827 | -0.749242 | H | -2.489259 | 1.580910 | 2.601529 |
| C | -3.516352 | -2.027136 | -0.436960 | N | 0.170999 | 1.237104 | -0.919056 |
| C | -4.171417 | -2.342441 | -1.793923 | C | -0.216503 | 2.629055 | -0.621107 |
| C | -2.963814 | -2.692178 | -2.708130 | H | -1.287487 | 2.773661 | -0.868298 |
| C | -1.746701 | -2.545084 | -1.779040 | C | -0.091250 | 2.862394 | 0.894121 |
| H | -0.860088 | -2.128007 | -2.252077 | H | -0.649041 | 2.108346 | 1.459372 |
| H | -1.479780 | -3.506357 | -1.315774 | H | 0.954844 | 2.820127 | 1.210527 |
| H | -2.895017 | -1.990418 | -3.543957 | H | -0.486467 | 3.848422 | 1.170835 |
| H | -3.029592 | -3.701287 | -3.125579 | C | 0.523187 | 3.765405 | -1.366015 |
| H | -4.707189 | -1.469190 | -2.177863 | H | 0.257137 | 3.799566 | -2.426614 |
| H | -4.891093 | -3.162534 | -1.711411 | H | 0.247308 | 4.737720 | -0.935200 |
| H | -3.489558 | -2.922726 | 0.203452 | H | 1.607667 | 3.654620 | -1.287473 |
| H | -3.973012 | -1.206492 | 0.115016 | C | 0.157464 | 0.835950 | -2.343790 |
| O | -0.791772 | -0.658660 | 2.067490 | H | 0.254144 | -0.257341 | -2.319368 |
| C | 0.449891 | -0.336804 | 2.750683 | C | -1.166305 | 1.127239 | -3.077552 |
| C | 0.952657 | -1.657858 | 3.329322 | H | -1.149504 | 0.700233 | -4.089029 |
| C | -0.361622 | -2.387390 | 3.646568 | H | -2.019087 | 0.690114 | -2.543001 |
| C | -1.250710 | -1.968535 | 2.472242 | H | -1.349309 | 2.202962 | -3.185743 |
| H | -2.311795 | -1.897236 | 2.735137 | C | 1.354255 | 1.297692 | -3.215186 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.144990 | -2.649350 | 1.620721 | H | 1.382920 | 0.713329 | -4.145369 |
| H | -0.779998 | -2.028100 | 4.594453 | H | 1.299741 | 2.353039 | -3.495115 |
| H | -0.251091 | -3.473827 | 3.714990 | H | 2.299350 | 1.135743 | -2.689473 |
| H | 1.589725 | -1.511824 | 4.206616 | H | 1.415445 | 0.841583 | -0.453604 |



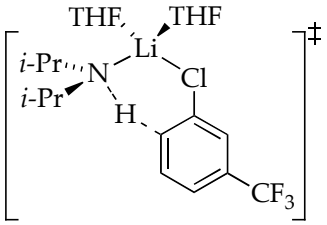



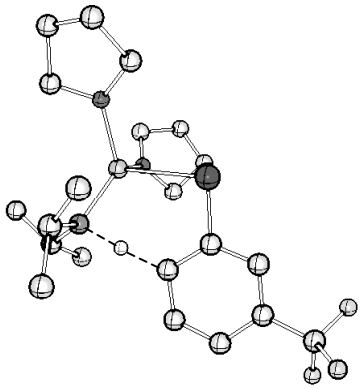
**20**
$G$ = -1792.687140
$G_{MP2}$ = -1787.890107
$\Delta G^{‡}$ = 22.7 kcal/mol
$\Delta G_{MP2}^{‡}$ = 14.5 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 3.479230 | -2.218775 | -0.393569 | H | 4.518384 | 3.116270 | 2.579946 |
| O | 2.999478 | -0.885316 | -0.689354 | H | 2.511843 | 4.762001 | 1.718754 |
| Li | 1.313725 | -0.041099 | 0.004941 | H | 3.598642 | 4.064870 | 0.501901 |
| N | -0.196507 | -1.149082 | 0.696694 | H | 1.462015 | 3.216000 | -0.314552 |
| C | -0.389619 | -1.078667 | 2.156223 | H | 0.835341 | 3.028322 | 1.341132 |
| H | -1.341898 | -1.549451 | 2.449065 | C | 3.742283 | -0.322021 | -1.798089 |
| C | 0.719332 | -1.789126 | 2.958159 | C | 4.642055 | -1.448157 | -2.317347 |
| H | 0.784215 | -2.856056 | 2.718321 | C | 4.850587 | -2.307602 | -1.060690 |
| H | 1.701353 | -1.339496 | 2.746681 | H | 5.139965 | -3.338414 | -1.284713 |
| H | 0.538463 | -1.705300 | 4.037802 | H | 5.621335 | -1.868108 | -0.416339 |
| C | -0.484696 | 0.387823 | 2.601039 | H | 4.124289 | -2.026252 | -3.091045 |
| H | -1.285296 | 0.907689 | 2.068472 | H | 5.574860 | -1.069565 | -2.745301 |
| H | -0.694654 | 0.453183 | 3.675925 | H | 3.029203 | 0.043079 | -2.542922 |
| H | 0.457596 | 0.917094 | 2.410346 | H | 4.325616 | 0.528242 | -1.423565 |
| C | -0.224505 | -2.528131 | 0.162652 | H | 3.499349 | -2.334134 | 0.693125 |
| H | 0.669329 | -3.081709 | 0.510790 | H | 2.777248 | -2.949682 | -0.811623 |
| C | -1.442651 | -3.378489 | 0.582772 | C | -3.437435 | 0.546428 | -0.495085 |
| H | -1.398682 | -4.363669 | 0.100759 | C | -4.223218 | 1.399041 | -1.279664 |
| H | -1.475392 | -3.549593 | 1.663904 | C | -3.628127 | 2.162034 | -2.283358 |
| H | -2.381062 | -2.897772 | 0.291714 | C | -2.253761 | 2.065449 | -2.494916 |
| C | -0.147037 | -2.491040 | -1.372708 | C | -1.538478 | 1.194877 | -1.675907 |
| H | -1.027939 | -1.999135 | -1.798232 | C | -2.042811 | 0.403810 | -0.663191 |
| H | 0.737054 | -1.944365 | -1.720108 | Cl | 0.263812 | 1.141837 | -2.037840 |
| H | -0.097957 | -3.508098 | -1.781297 | H | -1.762036 | 2.646681 | -3.269254 |
| O | 2.234445 | 1.615295 | 0.729682 | H | -4.227459 | 2.828791 | -2.897022 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.734404 | 2.975449 | 0.714586 | H | -5.291907 | 1.470665 | -1.106013 |
| C | 2.869272 | 3.823845 | 1.284377 | C | -4.144560 | -0.297623 | 0.535928 |
| C | 3.484261 | 2.870514 | 2.321018 | F | -3.450122 | -0.410314 | 1.690587 |
| C | 3.367008 | 1.510400 | 1.624488 | F | -4.362677 | -1.564912 | 0.091579 |
| H | 3.186662 | 0.684131 | 2.319223 | F | -5.364027 | 0.198725 | 0.864650 |
| H | 4.256478 | 1.277642 | 1.026511 | H | -1.176942 | -0.419911 | 0.071609 |
| H | 2.892392 | 2.880135 | 3.243337 | | | | |



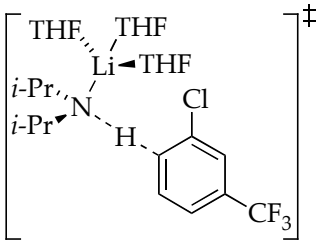



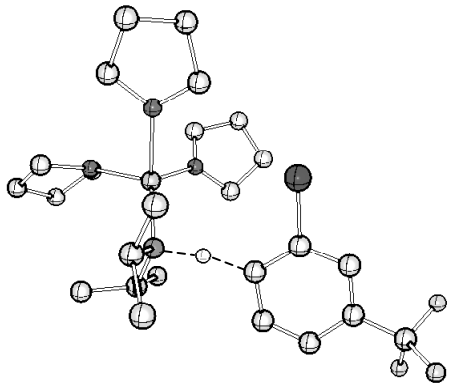
**23**
$G$ = -1792.686523
$G_{MP2}$ = -1787.888105
$\Delta G^{‡}$ = 23.1 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 15.7 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 4.548756 | -0.324498 | -0.770219 | H | 2.327883 | 4.614006 | 0.576521 |
| O | 3.332471 | 0.449856 | -0.936476 | H | -0.106306 | 4.363551 | 1.990944 |
| Li | 1.703537 | 0.047088 | 0.181556 | H | 0.138061 | 3.709961 | 0.360225 |
| N | 1.149821 | -1.810359 | 0.725085 | H | -0.377417 | 1.655127 | 1.551745 |
| C | 1.473961 | -2.202789 | 2.110056 | H | 0.499070 | 2.207716 | 3.005120 |
| H | 1.102926 | -3.220765 | 2.320304 | C | 3.307758 | 1.066048 | -2.249334 |
| C | 2.993125 | -2.225986 | 2.374908 | C | 4.425592 | 0.389082 | -3.042702 |
| H | 3.520664 | -2.869606 | 1.661689 | C | 5.449517 | 0.064330 | -1.943960 |
| H | 3.410789 | -1.212726 | 2.290904 | H | 6.139694 | -0.738275 | -2.219155 |
| H | 3.217744 | -2.598086 | 3.383586 | H | 6.042294 | 0.953129 | -1.697503 |
| C | 0.792147 | -1.274964 | 3.125859 | H | 4.058036 | -0.532337 | -3.508204 |
| H | -0.294336 | -1.267263 | 2.996584 | H | 4.824713 | 1.033662 | -3.831187 |
| H | 1.013346 | -1.599465 | 4.150094 | H | 2.312311 | 0.917692 | -2.675316 |
| H | 1.154855 | -0.246187 | 3.017237 | H | 3.487507 | 2.142744 | -2.132455 |
| C | 1.320427 | -2.933974 | -0.221680 | H | 4.972734 | -0.085053 | 0.209141 |
| H | 2.305222 | -3.406313 | -0.055485 | H | 4.285613 | -1.387874 | -0.788786 |
| C | 0.259357 | -4.049220 | -0.073989 | C | -2.561586 | -1.482525 | 0.968015 |
| H | 0.477466 | -4.884750 | -0.751719 | C | -3.864004 | -1.071913 | 0.683547 |
| H | 0.226800 | -4.455087 | 0.942563 | C | -4.078229 | -0.039595 | -0.237665 |
| H | -0.738307 | -3.666431 | -0.315661 | C | -2.989213 | 0.570463 | -0.865250 |
| C | 1.306960 | -2.426267 | -1.670597 | C | -1.722994 | 0.103341 | -0.526681 |
| H | 0.350117 | -1.949788 | -1.909737 | C | -1.424574 | -0.903484 | 0.368523 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.100926 | -1.690383 | -1.841922 | Cl | -0.331664 | 0.960654 | -1.375104 |
| H | 1.454356 | -3.253822 | -2.375538 | H | -3.136445 | 1.375044 | -1.577256 |
| O | 1.668402 | 1.657810 | 1.372684 | C | -5.476277 | 0.371613 | -0.596472 |
| C | 0.465850 | 2.248209 | 1.906611 | F | -6.311780 | 0.306098 | 0.467187 |
| C | 0.505941 | 3.684437 | 1.390487 | F | -5.531856 | 1.638364 | -1.072852 |
| C | 2.014399 | 4.027844 | 1.445039 | F | -6.013106 | -0.424858 | -1.554153 |
| C | 2.711497 | 2.645016 | 1.492700 | H | -4.714385 | -1.538655 | 1.172955 |
| H | 3.237897 | 2.494358 | 2.444672 | H | -2.423388 | -2.290982 | 1.687356 |
| H | 3.408731 | 2.467708 | 0.672002 | H | -0.104959 | -1.399607 | 0.609165 |
| H | 2.257958 | 4.610130 | 2.339152 | | | | |



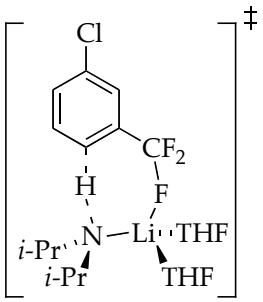



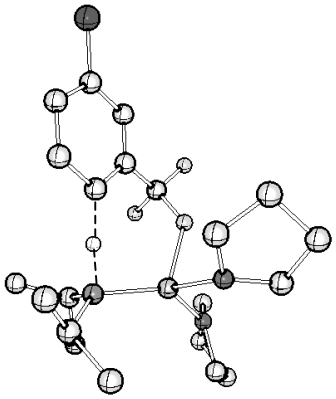
**24**
$G$ = -2025.025028
$G_{MP2}$ = -2019.458608
$\Delta G^{‡}$ = 30.0 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 15.3 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 1.859866 | -0.091191 | 0.010361 | C | 4.873500 | -2.289455 | 2.016501 |
| N | 0.605071 | -1.545310 | -0.771106 | C | 4.259025 | -0.890996 | 1.943776 |
| C | 0.598268 | -2.821929 | -0.021326 | H | 5.004113 | -0.111003 | 2.166087 |
| H | -0.297909 | -3.413326 | -0.282334 | H | 3.388997 | -0.744583 | 2.585906 |
| C | 1.804971 | -3.738063 | -0.296356 | H | 5.603040 | -2.383992 | 2.826239 |
| H | 1.866938 | -4.044064 | -1.345619 | H | 4.085508 | -3.030822 | 2.178639 |
| H | 2.739433 | -3.229342 | -0.035360 | H | 6.585565 | -2.298318 | 0.638404 |
| H | 1.736163 | -4.652875 | 0.306677 | H | 5.333745 | -3.470074 | 0.220756 |
| C | 0.500611 | -2.544274 | 1.484777 | H | 4.287339 | -1.787122 | -1.121852 |
| H | -0.386134 | -1.949409 | 1.718088 | H | 5.524138 | -0.622957 | -0.586044 |
| H | 0.435982 | -3.483179 | 2.049032 | O | 1.345027 | 0.951877 | 1.698270 |
| H | 1.383134 | -1.998222 | 1.843482 | C | 2.138571 | 1.967932 | 2.330260 |
| C | 0.685346 | -1.751244 | -2.237075 | C | 1.151192 | 3.060156 | 2.796754 |
| H | 1.654917 | -2.217645 | -2.491796 | C | -0.239133 | 2.375658 | 2.708530 |
| C | -0.410986 | -2.664552 | -2.831254 | C | 0.091117 | 0.908653 | 2.411495 |
| H | -0.292445 | -2.739964 | -3.919600 | H | -0.633708 | 0.408698 | 1.768598 |
| H | -0.369418 | -3.682935 | -2.430203 | H | 0.225390 | 0.326940 | 3.335583 |
| H | -1.408550 | -2.262821 | -2.624072 | H | -0.825918 | 2.794359 | 1.887351 |
| C | 0.649104 | -0.396229 | -2.955342 | H | -0.820636 | 2.482231 | 3.628835 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.293307 | 0.126406 | -2.761327 | H | 1.196789 | 3.941830 | 2.150438 |
| H | 1.466992 | 0.249737 | -2.618973 | H | 1.388123 | 3.389426 | 3.813116 |
| H | 4.032885 | 0.850155 | -2.256263 | H | 2.672501 | 1.531401 | 3.187258 |
| C | 3.887886 | 1.738878 | -1.633315 | H | 2.870467 | 2.306750 | 1.594616 |
| O | 2.613618 | 1.634694 | -0.958800 | C | -2.862419 | -1.721783 | 0.104666 |
| C | 1.799790 | 2.791220 | -1.270366 | C | -4.233111 | -1.549406 | 0.299276 |
| C | 2.792777 | 3.868998 | -1.695537 | C | -4.798815 | -0.283956 | 0.116151 |
| C | 3.841922 | 3.037762 | -2.450351 | C | -3.985175 | 0.786375 | -0.261031 |
| H | 3.498553 | 2.835809 | -3.471082 | C | -2.624738 | 0.540711 | -0.437416 |
| H | 4.820434 | 3.522915 | -2.513512 | C | -1.984638 | -0.680738 | -0.273342 |
| H | 2.330709 | 4.644201 | -2.313675 | Cl | -1.654363 | 2.001911 | -0.911055 |
| H | 3.239164 | 4.351645 | -0.817435 | H | -4.404221 | 1.776677 | -0.402223 |
| H | 1.106112 | 2.535636 | -2.079368 | C | -6.277231 | -0.083330 | 0.267067 |
| H | 1.215572 | 3.029564 | -0.380152 | F | -6.807474 | -0.900342 | 1.209156 |
| H | 4.674039 | 1.761548 | -0.869330 | F | -6.589227 | 1.187471 | 0.619184 |
| H | 0.747064 | -0.530611 | -4.039907 | F | -6.952238 | -0.338490 | -0.882574 |
| O | 3.812203 | -0.763333 | 0.585602 | H | -4.862218 | -2.383074 | 0.598821 |
| C | 4.807943 | -1.384646 | -0.250110 | H | -2.455592 | -2.721354 | 0.256602 |
| C | 5.504103 | -2.464533 | 0.614154 | H | -0.600274 | -1.040914 | -0.535784 |



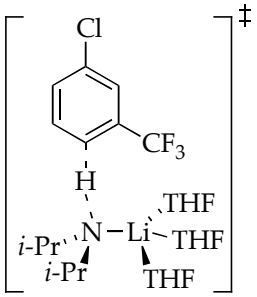



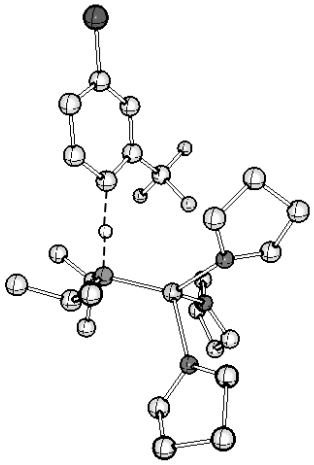
**25**
$G$ = -1792.689753
$G_{MP2}$ = -1787.890791
$\Delta G^{‡}$ = 21.1 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 14.0 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.009448 | -0.601446 | -1.699157 | H | 1.208483 | -3.581788 | 2.830537 |
| C | 2.113782 | -0.072290 | -0.835471 | H | 0.967471 | -3.275082 | 1.098909 |
| C | 3.421763 | -0.460759 | -1.165118 | H | 0.768205 | -1.009541 | 1.967823 |
| C | 4.465995 | 0.033170 | -0.393768 | H | -0.076997 | -1.583686 | 3.434476 |
| C | 4.217682 | 0.890961 | 0.675835 | C | -1.109307 | 2.306452 | 2.036829 |
| C | 2.897032 | 1.250185 | 0.960978 | H | -1.359123 | 3.373586 | 1.939071 |
| C | 1.785976 | 0.793410 | 0.228839 | C | -2.353440 | 1.631257 | 2.649442 |
| H | 0.463742 | 1.302074 | 0.559530 | H | -3.216296 | 1.731787 | 1.980029 |
| N | -0.769510 | 1.744743 | 0.712389 | H | -2.174466 | 0.560960 | 2.816220 |
| Li | -1.366694 | -0.128080 | 0.336673 | H | -2.623424 | 2.079015 | 3.615762 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -2.966953 | -0.663162 | -0.744886 | C | 0.066640 | 2.232386 | 3.027349 |
| C | -4.333537 | -0.554919 | -0.275256 | H | 0.912551 | 2.828121 | 2.670249 |
| C | -5.221999 | -0.732287 | -1.511923 | H | -0.222805 | 2.612507 | 4.015617 |
| C | -4.306974 | -0.246743 | -2.647408 | H | 0.414225 | 1.200064 | 3.154876 |
| C | -2.943073 | -0.758047 | -2.191220 | C | -0.932617 | 2.697220 | -0.406132 |
| H | -2.096743 | -0.171392 | -2.551922 | H | -0.595762 | 2.150460 | -1.297449 |
| H | -2.791279 | -1.808449 | -2.473662 | C | -2.394439 | 3.108454 | -0.662220 |
| H | -4.304348 | 0.847803 | -2.699203 | H | -2.477807 | 3.744765 | -1.553363 |
| H | -4.592265 | -0.636416 | -3.628938 | H | -3.023371 | 2.223159 | -0.813704 |
| H | -6.154694 | -0.166238 | -1.434883 | H | -2.809596 | 3.673579 | 0.181744 |
| H | -5.477977 | -1.788663 | -1.654239 | C | -0.030887 | 3.948464 | -0.313974 |
| H | -4.498618 | -1.319395 | 0.490607 | H | -0.115977 | 4.557729 | -1.223122 |
| H | -4.458896 | 0.432965 | 0.181996 | H | -0.301382 | 4.590568 | 0.533212 |
| O | -1.183312 | -1.606045 | 1.669418 | H | 1.017443 | 3.655284 | -0.198787 |
| C | 0.081129 | -1.761478 | 2.362114 | H | 2.737127 | 1.922865 | 1.803531 |
| C | 0.501112 | -3.201824 | 2.087718 | H | 5.045775 | 1.267610 | 1.269918 |
| C | -0.851462 | -3.932164 | 2.110142 | Cl | 6.124604 | -0.440781 | -0.773771 |
| C | -1.803254 | -2.901758 | 1.483730 | H | 3.625812 | -1.130277 | -1.993239 |
| H | -2.789785 | -2.890275 | 1.960285 | F | 1.368605 | -1.629247 | -2.493087 |
| H | -1.936385 | -3.058458 | 0.408035 | F | 0.442099 | 0.329993 | -2.507842 |
| H | -1.147284 | -4.150240 | 3.142702 | F | -0.052833 | -1.089716 | -0.938652 |
| H | -0.843300 | -4.875741 | 1.556751 | | | | |



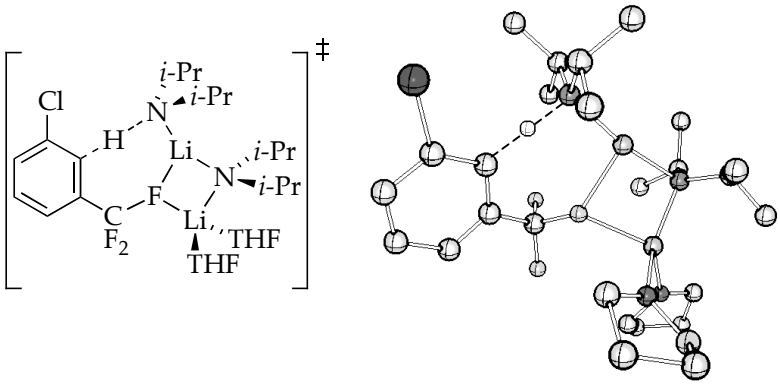
**26**
$G$ = -2025.02701
$G_{MP2}$ = -2019.461570
$\Delta G^{‡}$ = 28.7 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 13.5 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 2.099262 | -1.624323 | -0.721682 | H | 1.728408 | -1.635521 | 2.639896 |
| C | 2.891387 | -0.407130 | -0.340558 | H | 0.931180 | 0.500589 | 1.876597 |
| C | 4.250683 | -0.583469 | -0.043147 | H | -0.013717 | 0.767339 | 3.371211 |

**Table 6 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.997620 | 0.536319 | 0.302979 | O | -3.336708 | 0.752425 | 0.863634 |
| C | 4.410773 | 1.798412 | 0.348970 | C | -3.649895 | 0.807927 | 2.276546 |
| C | 3.052332 | 1.920404 | 0.037999 | C | -4.943238 | 1.620522 | 2.395066 |
| C | 2.227421 | 0.837168 | -0.316901 | C | -4.864250 | 2.538287 | 1.165905 |
| H | 2.626619 | 2.924127 | 0.079406 | C | -4.238956 | 1.609291 | 0.127020 |
| H | 5.008667 | 2.663988 | 0.621231 | H | -3.660107 | 2.125822 | -0.640170 |
| Cl | 6.712246 | 0.349289 | 0.693571 | H | -5.002565 | 0.987743 | -0.363178 |
| H | 4.717189 | -1.561609 | -0.076280 | H | -4.200686 | 3.388156 | 1.361791 |
| F | 2.763043 | -2.790248 | -0.537732 | H | -5.836562 | 2.927797 | 0.850114 |
| F | 1.697469 | -1.616813 | -2.022139 | H | -5.004878 | 2.165527 | 3.341648 |
| F | 0.942830 | -1.734096 | 0.009690 | H | -5.819724 | 0.965199 | 2.325066 |
| Li | -1.419150 | 0.008313 | 0.143985 | H | -3.746023 | -0.215273 | 2.652190 |
| O | -2.204758 | -1.785105 | -0.607560 | H | -2.814120 | 1.289450 | 2.795368 |
| C | -3.561247 | -2.215728 | -0.420267 | N | -0.404284 | 1.334372 | -1.073042 |
| C | -4.023051 | -2.724452 | -1.799195 | C | -0.732472 | 2.752432 | -0.842172 |
| C | -2.692621 | -3.067307 | -2.526597 | H | -1.785416 | 2.942256 | -1.123002 |
| C | -1.614383 | -2.774363 | -1.471536 | C | -0.623908 | 3.046192 | 0.664366 |
| H | -0.686024 | -2.367798 | -1.866484 | H | -1.270943 | 2.379339 | 1.244319 |
| H | -1.383490 | -3.671163 | -0.877174 | H | 0.404555 | 2.909717 | 1.016126 |
| H | -2.554730 | -2.423415 | -3.399701 | H | -0.918920 | 4.079824 | 0.884455 |
| H | -2.651662 | -4.105984 | -2.867416 | C | 0.096426 | 3.806203 | -1.615832 |
| H | -4.570040 | -1.945794 | -2.338717 | H | -0.126307 | 3.799240 | -2.686191 |
| H | -4.686197 | -3.589474 | -1.703332 | H | -0.130368 | 4.815084 | -1.245618 |
| H | -3.580048 | -3.026828 | 0.324323 | H | 1.171381 | 3.633948 | -1.496570 |
| H | -4.119268 | -1.364251 | -0.032044 | C | -0.545449 | 0.834256 | -2.462252 |
| O | -0.833885 | -0.572395 | 2.010383 | H | -0.501673 | -0.258986 | -2.363539 |
| C | 0.332406 | 0.015233 | 2.649334 | C | -1.905601 | 1.147890 | -3.111824 |
| C | 1.049314 | -1.142090 | 3.342118 | H | -1.997488 | 0.632809 | -4.076751 |
| C | -0.116992 | -2.072549 | 3.707426 | H | -2.736686 | 0.820647 | -2.474594 |
| C | -1.036157 | -1.919802 | 2.493561 | H | -2.031565 | 2.219727 | -3.306811 |
| H | -2.097625 | -2.044297 | 2.733689 | C | 0.600082 | 1.177656 | -3.446961 |
| H | -0.771695 | -2.620659 | 1.695055 | H | 0.527176 | 0.538301 | -4.337302 |
| H | -0.618276 | -1.721483 | 4.617617 | H | 0.568805 | 2.216004 | -3.789440 |
| H | 0.188500 | -3.110990 | 3.867403 | H | 1.573966 | 0.999982 | -2.984742 |
| H | 1.629976 | -0.812777 | 4.208739 | H | 0.835446 | 1.089365 | -0.702770 |

**Table 7.** Optimized geometries of reactants and dimer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the ortholithiation of **1** at -78 °C with free energies (Hartrees), and cartesian coordinates (X,Y,Z). (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

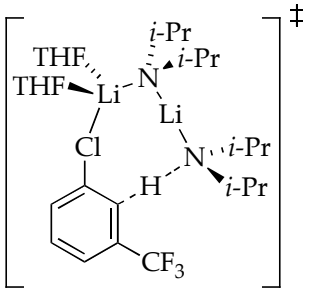


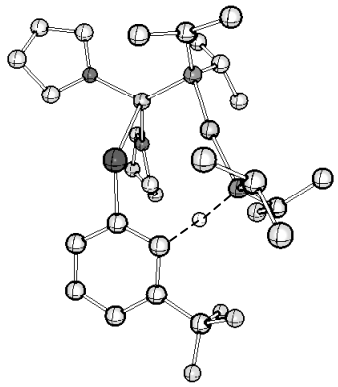

**14**
$G$ = -2091.909073
$G_{MP2}$ = -2085.993661
$\Delta G^{‡}$ = 20.5 kcal/mol
$\Delta G_{MP2}^{‡}$ = 13.5 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -0.494484 | -1.372784 | -1.460317 | O | 1.927643 | -1.290283 | 1.636969 |
| F | 0.489120 | -2.297221 | -1.620070 | C | 3.033433 | -1.608191 | 2.510313 |
| F | 0.029259 | -0.476610 | -0.521918 | C | 2.393771 | -2.028433 | 3.831237 |
| Li | 2.126407 | 0.098417 | 0.192018 | C | 1.126970 | -2.750103 | 3.347737 |
| N | 1.606287 | 2.037170 | 0.167737 | C | 0.708676 | -1.916085 | 2.131731 |
| Li | -0.380619 | 1.652531 | 0.033998 | H | 0.006426 | -1.120169 | 2.397139 |
| N | -2.375370 | 1.599570 | 0.003300 | H | 0.273559 | -2.513373 | 1.327355 |
| C | -2.970577 | 1.868175 | 1.327903 | H | 0.339126 | -2.794696 | 4.104729 |
| H | -4.057690 | 1.687000 | 1.307707 | H | 1.365036 | -3.777197 | 3.047637 |
| C | -2.402239 | 0.883271 | 2.360986 | H | 2.132108 | -1.143940 | 4.423212 |
| H | -2.871924 | 1.035144 | 3.340532 | H | 3.051996 | -2.662026 | 4.433080 |
| H | -2.582193 | -0.152017 | 2.057262 | H | 3.620109 | -2.425235 | 2.068148 |
| H | -1.320543 | 1.020262 | 2.493280 | H | 3.668335 | -0.721700 | 2.587517 |
| C | -2.772410 | 3.316095 | 1.817351 | O | 3.799721 | -0.641004 | -0.629558 |
| H | -3.257759 | 4.043129 | 1.157598 | C | 3.878567 | -1.938047 | -1.268409 |
| H | -3.195486 | 3.450394 | 2.821483 | C | 4.939968 | -1.782738 | -2.354522 |
| H | -1.705165 | 3.574144 | 1.863307 | C | 5.930789 | -0.816860 | -1.686677 |
| C | -2.959430 | 2.429743 | -1.075846 | C | 5.005236 | 0.122657 | -0.905178 |
| H | -2.697099 | 3.491957 | -0.912913 | H | 4.718776 | 1.002948 | -1.489758 |
| C | -2.345013 | 2.031310 | -2.424913 | H | 5.428065 | 0.457995 | 0.045476 |
| H | -2.591653 | 0.996123 | -2.682063 | H | 6.557204 | -0.276444 | -2.402034 |
| H | -2.719697 | 2.678784 | -3.226904 | H | 6.592314 | -1.362870 | -1.004030 |
| H | -1.252626 | 2.124411 | -2.417305 | H | 4.502085 | -1.328818 | -3.250913 |
| C | -4.497161 | 2.376493 | -1.196356 | H | 5.390893 | -2.737859 | -2.639268 |
| H | -4.843263 | 1.353309 | -1.376492 | H | 2.183997 | 2.414203 | -3.201461 |
| H | -4.998162 | 2.741833 | -0.294269 | C | 1.210468 | 4.069403 | -1.296293 |
| H | -4.831103 | 3.004996 | -2.031869 | H | 1.242491 | 4.734589 | -0.426874 |
| F | -0.551499 | -0.672911 | -2.609251 | H | 1.609099 | 4.628699 | -2.153599 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.098689 | 2.725271 | 1.374759 | H | 0.155064 | 3.848672 | -1.506865 |
| H | 1.940544 | 3.817070 | 1.300177 | H | 4.174471 | -2.687808 | -0.521796 |
| C | 3.614125 | 2.537193 | 1.629098 | H | 2.884783 | -2.185258 | -1.644262 |
| H | 4.210351 | 2.818882 | 0.754210 | C | -1.801784 | -1.962503 | -1.027212 |
| H | 3.961060 | 3.147619 | 2.473769 | C | -2.788439 | -1.109918 | -0.489550 |
| H | 3.839315 | 1.486485 | 1.865946 | C | -3.971448 | -1.771176 | -0.168160 |
| C | 1.326439 | 2.266274 | 2.617311 | C | -4.207100 | -3.134302 | -0.356701 |
| H | 0.272283 | 2.555649 | 2.557003 | C | -3.195237 | -3.923966 | -0.901341 |
| H | 1.371619 | 1.173112 | 2.721417 | C | -1.978763 | -3.338675 | -1.239321 |
| H | 1.738207 | 2.706916 | 3.534028 | H | -1.183038 | -3.943041 | -1.663115 |
| C | 2.009733 | 2.767011 | -1.050284 | H | -3.356840 | -4.986802 | -1.057780 |
| H | 3.073509 | 3.072627 | -0.990521 | H | -5.162989 | -3.570158 | -0.081580 |
| C | 1.895048 | 1.870642 | -2.293543 | Cl | -5.328434 | -0.855247 | 0.560090 |
| H | 2.539768 | 0.987223 | -2.212319 | H | -2.602969 | 0.262955 | -0.270294 |
| H | 0.869402 | 1.513885 | -2.441531 | | | | |



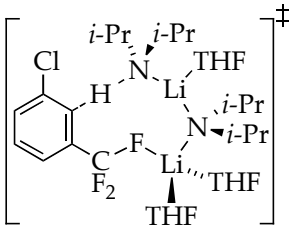
**12**
$G$ = -2091.897802
$G_{MP2}$ = -2085.98452
$\Delta G^{‡}$ = 27.6 kcal/mol
$\Delta G_{MP2}^{‡}$ = 19.3 kcal/mol

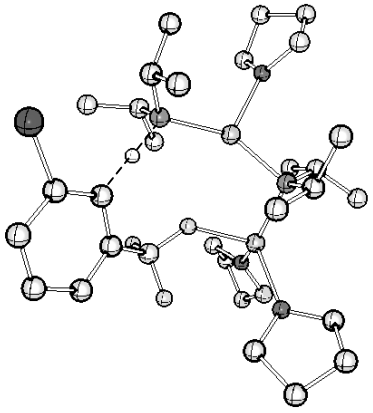
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| N | 1.999882 | 1.967933 | 0.292844 | H | -2.006141 | 1.319855 | -2.783326 |
| Li | 2.393813 | 0.005958 | 0.226267 | H | -1.996502 | 3.031866 | -3.249239 |
| O | 1.876794 | -1.403614 | 1.532529 | H | -0.633496 | 2.351113 | -2.358615 |
| C | 2.838468 | -1.990841 | 2.440064 | C | -3.949484 | 2.755344 | -1.400180 |
| C | 2.130009 | -3.190306 | 3.068961 | H | -4.335502 | 1.779798 | -1.708974 |
| C | 0.672916 | -2.705600 | 3.116011 | H | -4.511130 | 3.069885 | -0.514833 |
| C | 0.545806 | -1.928840 | 1.805210 | H | -4.164302 | 3.478610 | -2.197201 |
| H | -0.151513 | -1.090605 | 1.858422 | C | 2.476053 | 2.474924 | 1.595181 |
| H | 0.254959 | -2.574510 | 0.970386 | H | 2.489231 | 3.579876 | 1.600571 |
| H | 0.519308 | -2.040661 | 3.973686 | C | 3.922290 | 2.036056 | 1.936826 |
| H | -0.053537 | -3.520186 | 3.184149 | H | 4.616452 | 2.277394 | 1.123969 |
| H | 2.536068 | -3.444096 | 4.052544 | H | 4.293716 | 2.530006 | 2.845030 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.221296 | -4.072032 | 2.423538 | H | 3.970149 | 0.950491 | 2.112450 |
| H | 3.731126 | -2.249836 | 1.864128 | C | 1.543668 | 2.053933 | 2.736502 |
| H | 3.110967 | -1.243741 | 3.197000 | H | 0.554182 | 2.510022 | 2.626990 |
| O | 3.962426 | -0.906608 | -0.604941 | H | 1.414930 | 0.963067 | 2.752464 |
| C | 3.817780 | -2.113446 | -1.394704 | H | 1.941816 | 2.356820 | 3.713275 |
| C | 4.964724 | -2.074696 | -2.402336 | C | 2.558299 | 2.795555 | -0.796605 |
| C | 6.074936 | -1.388981 | -1.591077 | H | 3.621620 | 3.030485 | -0.593064 |
| C | 5.293783 | -0.352739 | -0.777696 | C | 2.539401 | 2.057055 | -2.143505 |
| H | 5.199640 | 0.600654 | -1.308889 | H | 3.095569 | 1.113306 | -2.092886 |
| H | 5.718072 | -0.162368 | 0.211804 | H | 1.516714 | 1.818925 | -2.458437 |
| H | 6.845736 | -0.927912 | -2.215095 | H | 2.987364 | 2.670976 | -2.934790 |
| H | 6.564014 | -2.111589 | -0.927285 | C | 1.845742 | 4.158745 | -0.963195 |
| H | 4.688650 | -1.464517 | -3.269917 | H | 1.817461 | 4.716189 | -0.020715 |
| H | 5.240878 | -3.071229 | -2.759031 | H | 2.350415 | 4.791211 | -1.706288 |
| H | 3.894618 | -2.983632 | -0.728887 | H | 0.808538 | 4.018558 | -1.297582 |
| H | 2.823581 | -2.100484 | -1.847310 | C | -3.520024 | -1.705945 | -0.620448 |
| Li | 0.006074 | 1.758639 | 0.020637 | C | -2.383980 | -0.877317 | -0.758275 |
| N | -1.989861 | 1.783907 | -0.058426 | C | -1.324124 | -1.511712 | -1.377664 |
| C | -2.680302 | 2.027993 | 1.224028 | C | -1.300482 | -2.817097 | -1.866318 |
| H | -3.766758 | 1.876248 | 1.113219 | C | -2.455638 | -3.582046 | -1.715566 |
| C | -2.214764 | 1.001378 | 2.267370 | C | -3.567798 | -3.025831 | -1.084699 |
| H | -2.751790 | 1.140894 | 3.213782 | H | -4.469128 | -3.616138 | -0.957575 |
| H | -2.401251 | -0.020346 | 1.928727 | H | -2.486507 | -4.602128 | -2.088123 |
| H | -1.143634 | 1.109169 | 2.479346 | H | -0.418379 | -3.221791 | -2.354123 |
| C | -2.485373 | 3.453202 | 1.777495 | Cl | 0.236863 | -0.584345 | -1.614589 |
| H | -2.894620 | 4.216432 | 1.107294 | C | -4.725974 | -1.191432 | 0.128081 |
| H | -2.986271 | 3.565384 | 2.747761 | F | -5.042404 | 0.081621 | -0.189604 |
| H | -1.418635 | 3.675801 | 1.920685 | F | -4.526437 | -1.215071 | 1.473900 |
| C | -2.428956 | 2.696583 | -1.140883 | F | -5.835914 | -1.937207 | -0.100601 |
| H | -2.118190 | 3.730613 | -0.899390 | H | -2.256870 | 0.457281 | -0.405062 |
| C | -1.725368 | 2.326357 | -2.454603 | | | | |

**Table 7 (Continued).**



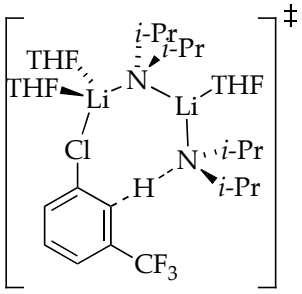
**15**
$G$ = -2324.240665
$G_{MP2}$ = -2317.559550
$\Delta G^{‡}$ = 31.7 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 16.0 kcal/mol

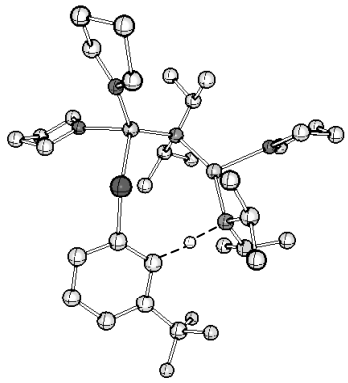
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 1.994601 | -0.544030 | -0.065503 | H | -3.484859 | -3.537886 | -1.771787 |
| F | 0.644657 | 0.935800 | 0.488421 | H | -1.888819 | -4.320632 | -1.689205 |
| C | 0.859981 | 2.199555 | 0.991710 | C | 0.765266 | -1.566299 | -2.432405 |
| F | 2.191240 | 2.427839 | 0.816594 | H | 1.756674 | -1.861889 | -2.837219 |
| F | 0.687042 | 2.093326 | 2.334931 | C | -0.256440 | -2.360746 | -3.278874 |
| C | -0.013184 | 3.242832 | 0.367087 | H | -0.129041 | -2.146174 | -4.347973 |
| C | -1.362772 | 2.939181 | 0.074619 | H | -0.142550 | -3.442540 | -3.148690 |
| C | -2.068977 | 4.054919 | -0.383251 | H | -1.286821 | -2.095926 | -3.007036 |
| C | -1.536888 | 5.333201 | -0.569032 | C | 0.619885 | -0.069986 | -2.751894 |
| C | -0.194972 | 5.559456 | -0.274555 | H | -0.339265 | 0.326068 | -2.403127 |
| C | 0.574600 | 4.507102 | 0.206987 | H | 1.413356 | 0.517803 | -2.278283 |
| H | 1.618224 | 4.666417 | 0.459000 | H | 0.679130 | 0.106872 | -3.833395 |
| H | 0.238812 | 6.545808 | -0.413229 | C | 0.897956 | -3.197151 | -0.609384 |
| H | -2.166429 | 6.138380 | -0.935536 | H | 0.098729 | -3.845001 | -1.017738 |
| Cl | -3.815363 | 3.939417 | -0.775100 | C | 2.224149 | -3.829618 | -1.094811 |
| N | 0.689488 | -1.787428 | -0.977426 | H | 2.299101 | -4.875781 | -0.769555 |
| Li | -1.220812 | -1.168606 | -0.283536 | C | 0.830802 | -3.356328 | 0.916150 |
| N | -2.529984 | 0.373599 | 0.287851 | H | -0.088926 | -2.921575 | 1.321434 |
| C | -3.677405 | 0.480357 | -0.647531 | H | 0.856065 | -4.414648 | 1.206395 |
| H | -4.253842 | 1.393717 | -0.442848 | H | 1.681173 | -2.856185 | 1.394406 |
| C | -4.692276 | -0.678932 | -0.591396 | O | 2.916818 | -0.715793 | 1.742340 |
| H | -5.242133 | -0.710414 | 0.355798 | C | 4.324221 | -1.031646 | 1.847398 |
| H | -5.437160 | -0.563087 | -1.389377 | C | 4.675386 | -0.881779 | 3.328550 |
| H | -4.190295 | -1.643067 | -0.723125 | C | 3.352752 | -1.265203 | 4.009267 |
| C | -3.148748 | 0.618600 | -2.079893 | C | 2.321028 | -0.648679 | 3.065381 |
| H | -2.415792 | 1.427529 | -2.153005 | H | 2.122978 | 0.400193 | 3.302952 |
| H | -2.668254 | -0.310359 | -2.418654 | H | 1.371296 | -1.187939 | 3.034923 |
| H | -3.964399 | 0.839361 | -2.779246 | H | 3.262545 | -0.881432 | 5.029669 |
| C | -2.981412 | 0.223088 | 1.688775 | H | 3.241902 | -2.355464 | 4.042837 |
| H | -3.690646 | -0.619602 | 1.759864 | H | 4.934430 | 0.158744 | 3.557046 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.804344 | -0.138248 | 2.605559 | H | 5.517139 | -1.515490 | 3.623329 |
| H | -1.283460 | -1.040401 | 2.255265 | H | 2.315848 | -3.823647 | -2.186286 |
| H | -1.075144 | 0.672409 | 2.656318 | H | 3.087962 | -3.289864 | -0.679950 |
| H | -2.155003 | -0.338150 | 3.626483 | H | 4.476615 | -2.062932 | 1.501193 |
| C | -3.719955 | 1.450392 | 2.271560 | H | 4.873797 | -0.355126 | 1.189213 |
| H | -4.600079 | 1.715832 | 1.677451 | O | 3.686692 | 0.133556 | -1.110013 |
| H | -4.060458 | 1.246782 | 3.295670 | C | 4.056213 | 1.514624 | -1.370505 |
| H | -3.064235 | 2.327256 | 2.298503 | C | 5.127709 | 1.474583 | -2.468249 |
| O | -2.385961 | -3.153647 | -0.054410 | C | 4.853650 | 0.130770 | -3.161131 |
| C | -2.778307 | -4.058303 | -1.112214 | C | 4.437969 | -0.741726 | -1.981113 |
| C | -3.435067 | -5.258280 | -0.424518 | H | 5.315322 | -1.124852 | -1.439278 |
| C | -4.027355 | -4.617807 | 0.839285 | H | 3.791551 | -1.578738 | -2.247414 |
| C | -2.953389 | -3.591186 | 1.199977 | H | 5.722462 | -0.267308 | -3.693679 |
| H | -2.158912 | -4.042927 | 1.809825 | H | 4.024122 | 0.221858 | -3.871239 |
| H | -3.343420 | -2.714031 | 1.721018 | H | 6.131875 | 1.476370 | -2.028229 |
| H | -4.209759 | -5.334067 | 1.646271 | H | 5.056264 | 2.332037 | -3.143519 |
| H | -4.973018 | -4.114651 | 0.607257 | H | 3.155706 | 2.047429 | -1.691120 |
| H | -2.680282 | -6.006665 | -0.155221 | H | 4.411339 | 1.964575 | -0.439484 |
| H | -4.183087 | -5.743257 | -1.058891 | H | -1.922346 | 1.634804 | 0.199905 |

**Table 7 (Continued).**



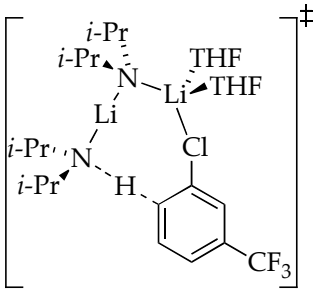
**13**
$G$ = -2324.230678
$G_{MP2}$ = -2317.552005
$\Delta G^{‡}$ = 37.9 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 20.8 kcal/mol

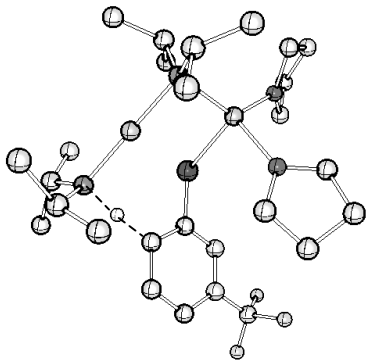
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 3.382045 | 1.015891 | -0.332080 | H | -2.824007 | 3.851274 | 0.707015 |
| N | 2.203611 | 0.714380 | 0.519915 | H | -2.979647 | 2.124380 | 1.081464 |
| Li | 0.466508 | 1.561708 | -0.285372 | O | 0.762616 | 3.802775 | -0.250152 |
| N | -1.467645 | 1.287755 | -1.107929 | C | 0.909357 | 4.662765 | -1.404321 |
| Li | -2.300505 | -0.239856 | -0.118292 | C | 1.043327 | 6.089375 | -0.860769 |
| O | -3.362212 | -0.245306 | 1.649267 | C | 1.668112 | 5.852625 | 0.522379 |
| C | -4.808641 | -0.261167 | 1.648793 | C | 0.974175 | 4.563144 | 0.958891 |
| C | -5.224051 | -0.355642 | 3.117705 | H | 0.001053 | 4.773516 | 1.423908 |
| C | -4.083964 | 0.398676 | 3.818722 | H | 1.568107 | 3.951605 | 1.642021 |
| C | -2.867045 | -0.026970 | 2.996743 | H | 1.499326 | 6.676832 | 1.222208 |
| H | -2.434472 | -0.965087 | 3.362064 | H | 2.748716 | 5.693058 | 0.434254 |
| H | -2.078319 | 0.727470 | 2.950170 | H | 0.056278 | 6.555766 | -0.758598 |
| H | -3.979937 | 0.142099 | 4.876989 | H | 1.652637 | 6.725287 | -1.509948 |
| H | -4.239462 | 1.481250 | 3.743809 | H | 1.808610 | 4.354006 | -1.951999 |
| H | -5.248020 | -1.402108 | 3.444099 | H | 0.039869 | 4.525147 | -2.051455 |
| H | -6.210810 | 0.080385 | 3.299810 | C | 2.424610 | 1.096429 | 1.930643 |
| H | -5.168500 | 0.669126 | 1.189416 | H | 2.690656 | 2.167437 | 1.984048 |
| H | -5.138542 | -1.104106 | 1.037062 | C | 1.133342 | 0.944261 | 2.746173 |
| O | -3.480779 | -1.670937 | -0.990813 | H | 0.302690 | 1.501902 | 2.290771 |
| C | -3.374890 | -3.073395 | -0.637457 | H | 0.828863 | -0.103216 | 2.816850 |
| C | -4.399248 | -3.797184 | -1.511847 | H | 1.271693 | 1.329124 | 3.764953 |
| C | -4.400443 | -2.931468 | -2.780956 | C | 3.565079 | 0.340891 | 2.649418 |
| C | -4.258453 | -1.522321 | -2.204670 | H | 4.526140 | 0.478600 | 2.145146 |
| H | -5.234512 | -1.093509 | -1.941698 | H | 3.675968 | 0.703938 | 3.680055 |
| H | -3.733044 | -0.826667 | -2.862162 | H | 3.364127 | -0.734557 | 2.684921 |
| H | -5.305232 | -3.045685 | -3.385119 | H | 4.213176 | 0.337549 | -0.092412 |
| H | -3.536424 | -3.175483 | -3.409464 | F | 4.581298 | -1.794996 | -1.393960 |
| H | -5.388935 | -3.785889 | -1.039343 | C | 4.493295 | -2.519192 | -0.249989 |
| H | -4.123450 | -4.839348 | -1.697486 | C | 3.089793 | -3.012270 | 0.016731 |
| H | -2.352703 | -3.409100 | -0.845831 | C | 2.066169 | -2.093321 | 0.365132 |
| H | -3.559688 | -3.167187 | 0.436019 | C | 0.855957 | -2.723445 | 0.601520 |

**Table 7 (Continued).**

| | | | |
|---|---|---|---|
| C | -1.350071 | 0.893230 | -2.522863 |
| H | -2.350715 | 0.741381 | -2.979435 |
| C | -0.652996 | 1.921690 | -3.442865 |
| H | -0.614449 | 1.557672 | -4.477950 |
| H | -1.180926 | 2.881738 | -3.454464 |
| H | 0.378172 | 2.107971 | -3.117040 |
| C | -0.626343 | -0.457457 | -2.635639 |
| H | 0.382998 | -0.407330 | -2.214374 |
| H | -1.165192 | -1.247464 | -2.099931 |
| H | -0.534730 | -0.768905 | -3.683952 |
| C | -2.246084 | 2.525410 | -0.933232 |
| H | -1.741190 | 3.392634 | -1.401998 |
| C | -3.670943 | 2.501740 | -1.537875 |
| H | -3.660654 | 2.374077 | -2.625417 |
| H | -4.260998 | 1.676637 | -1.111525 |
| H | -4.202933 | 3.438562 | -1.325401 |
| C | -2.363433 | 2.865819 | 0.559729 |
| H | -1.380127 | 2.881815 | 1.040951 |
| C | 0.585221 | -4.089242 | 0.511509 |
| C | 1.625161 | -4.935918 | 0.142877 |
| C | 2.884607 | -4.392601 | -0.099257 |
| H | 3.708888 | -5.042845 | -0.369363 |
| H | 1.459276 | -6.006471 | 0.060248 |
| H | -0.402745 | -4.479821 | 0.737154 |
| Cl | -0.579216 | -1.746297 | 1.159745 |
| F | 4.964073 | -1.734696 | 0.747833 |
| F | 5.385926 | -3.534073 | -0.383462 |
| C | 3.953573 | 2.441885 | -0.203936 |
| H | 4.395615 | 2.633292 | 0.779744 |
| H | 4.747186 | 2.592799 | -0.946984 |
| H | 3.171998 | 3.189021 | -0.378421 |
| C | 3.017802 | 0.757772 | -1.799140 |
| H | 2.590950 | -0.239401 | -1.931586 |
| H | 2.288241 | 1.496354 | -2.160452 |
| H | 3.902779 | 0.829497 | -2.443124 |
| H | 2.144451 | -0.690918 | 0.462667 |

**Table 7 (Continued).**



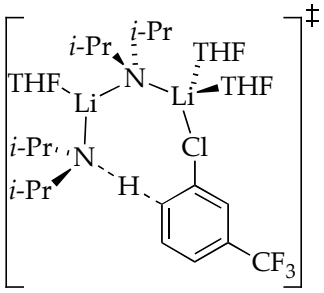



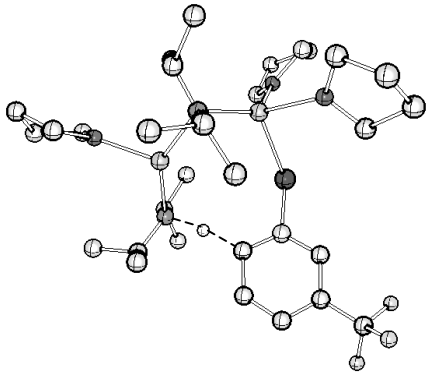
**16**
$G$ = -2091.89831
$G_{MP2}$ = -2085.985027
$\Delta G^{‡}$ = 27.3 kcal/mol
$\Delta G_{MP2}^{‡}$ = 18.9 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| N | 2.930733 | 0.326087 | 0.398201 | H | -1.558793 | 3.972213 | -2.169631 |
| Li | 1.560061 | -1.178484 | 0.276513 | H | -1.367006 | 5.337343 | -1.059285 |
| O | 0.129324 | -1.712758 | 1.596862 | H | -0.750023 | 5.456579 | -2.711446 |
| C | -0.205904 | -3.100920 | 1.844125 | C | 3.565880 | 0.266455 | 1.730843 |
| C | -1.227502 | -3.092615 | 2.982977 | H | 4.520511 | 0.820851 | 1.729356 |
| C | -1.934002 | -1.744388 | 2.774811 | C | 3.917654 | -1.171843 | 2.180741 |
| C | -0.775189 | -0.849021 | 2.341747 | H | 4.524985 | -1.685116 | 1.426702 |
| H | -0.235773 | -0.448656 | 3.208665 | C | 2.694202 | 0.931408 | 2.800643 |
| H | -1.070069 | -0.025208 | 1.689868 | H | 2.578849 | 2.003303 | 2.606245 |
| H | -2.422448 | -1.372207 | 3.680169 | H | 1.693835 | 0.481707 | 2.823638 |
| H | -2.690745 | -1.814435 | 1.986384 | H | 3.128835 | 0.820808 | 3.802197 |
| H | -0.720002 | -3.113990 | 3.954621 | C | 3.969294 | 0.282391 | -0.652070 |
| H | -1.905322 | -3.949987 | 2.935052 | H | 4.717909 | -0.503877 | -0.423229 |
| H | -0.634230 | -3.523239 | 0.927451 | C | 3.373425 | -0.076079 | -2.021716 |
| H | 0.714343 | -3.641601 | 2.083750 | H | 2.871536 | -1.049967 | -2.001233 |
| O | 1.918988 | -2.982739 | -0.593910 | H | 2.637033 | 0.670394 | -2.343631 |
| C | 1.089818 | -3.632234 | -1.589161 | H | 4.154310 | -0.113732 | -2.791341 |
| C | 2.062350 | -4.389520 | -2.489395 | C | 4.768955 | 1.599889 | -0.796824 |
| C | 3.137369 | -4.831133 | -1.484575 | H | 5.199803 | 1.923393 | 0.156382 |
| C | 3.219496 | -3.628997 | -0.537844 | H | 5.595029 | 1.492350 | -1.512847 |
| H | 3.970382 | -2.900526 | -0.861281 | H | 4.119646 | 2.409476 | -1.158797 |
| H | 3.424102 | -3.906255 | 0.499988 | C | -3.076702 | 2.075887 | 0.074746 |
| H | 4.101082 | -5.054667 | -1.950895 | C | -1.797884 | 1.732307 | -0.408240 |
| H | 2.807597 | -5.726004 | -0.944029 | C | -1.733266 | 0.460588 | -0.945175 |
| H | 2.488569 | -3.715944 | -3.241549 | C | -2.770603 | -0.462237 | -1.022647 |
| H | 1.585618 | -5.225700 | -3.009126 | C | -4.008739 | -0.076256 | -0.500779 |
| H | 0.397592 | -4.319358 | -1.083698 | C | -4.165549 | 1.202308 | 0.044937 |
| H | 0.511767 | -2.858358 | -2.097725 | H | -5.132094 | 1.503323 | 0.438570 |
| H | 4.487155 | -1.176444 | 3.120201 | C | -5.121387 | -1.078504 | -0.445809 |
| H | 3.004454 | -1.762241 | 2.348069 | F | -6.340362 | -0.500079 | -0.410802 |
| Li | 1.667132 | 1.835339 | 0.003959 | H | 1.145995 | 5.064040 | -1.229988 |
| N | 0.405417 | 3.383759 | -0.174600 | C | 1.110411 | 3.400049 | -2.557750 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.282812 | 4.241352 | 1.023235 | H | 0.525680 | 2.499725 | -2.778071 |
| H | -0.413202 | 5.076385 | 0.825685 | H | 1.158140 | 3.999135 | -3.475665 |
| C | -0.304165 | 3.458578 | 2.206704 | H | 2.136254 | 3.093302 | -2.315198 |
| H | -0.348247 | 4.090461 | 3.102083 | C | -0.878472 | 4.773529 | -1.861881 |
| H | -1.314769 | 3.100297 | 1.993468 | F | -5.103041 | -1.926379 | -1.500826 |
| H | 0.315303 | 2.586706 | 2.451583 | F | -5.033753 | -1.861129 | 0.669047 |
| C | 1.624980 | 4.878498 | 1.436542 | H | -2.636839 | -1.442629 | -1.467851 |
| H | 2.076758 | 5.443643 | 0.614211 | Cl | -0.132556 | -0.110390 | -1.621528 |
| H | 1.493781 | 5.569194 | 2.280172 | H | -3.229755 | 3.069028 | 0.498586 |
| H | 2.343943 | 4.107012 | 1.743107 | H | -0.682222 | 2.606036 | -0.292946 |
| C | 0.483967 | 4.200981 | -1.409481 | | | | |



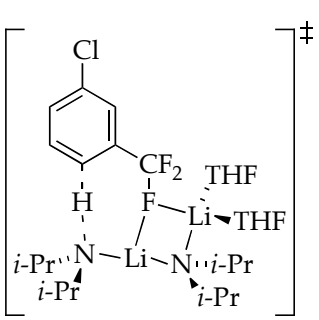
**17**
$G$ = -2324.23695
$G_{MP2}$ = -2317.556712
$\Delta G^{‡}$ = 34.0 kcal/mol
$\Delta G_{MP2}^{‡}$ = 17.8 kcal/mol

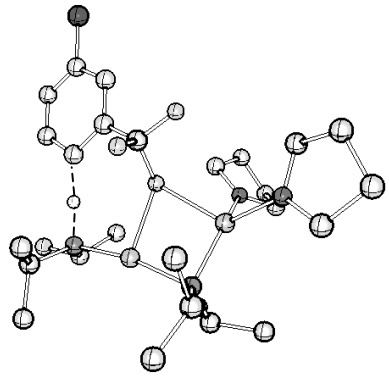
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| N | 1.718676 | 1.115895 | -1.084696 | H | -0.555634 | -3.224665 | 2.672606 |
| Li | 0.233451 | 1.974734 | -0.017449 | O | 4.184641 | -1.235028 | -0.394244 |
| O | 0.384983 | 3.018609 | 1.752338 | C | 4.995955 | -1.435919 | -1.575260 |
| C | 0.113239 | 4.436696 | 1.831944 | C | 6.429202 | -1.635428 | -1.074709 |
| C | -0.080454 | 4.735645 | 3.318099 | C | 6.203164 | -2.263451 | 0.308698 |
| C | 0.878482 | 3.726987 | 3.968301 | C | 4.960642 | -1.516404 | 0.792523 |
| C | 0.714169 | 2.500498 | 3.068461 | H | 5.227409 | -0.565963 | 1.274209 |
| H | -0.107632 | 1.856609 | 3.398378 | H | 4.335880 | -2.097177 | 1.474934 |
| H | 1.619892 | 1.895944 | 2.979818 | H | 7.054050 | -2.141639 | 0.985766 |
| H | 0.636777 | 3.509046 | 5.012614 | H | 4.626168 | -2.324537 | -2.102693 |
| H | 1.908673 | 4.100128 | 3.927894 | H | 4.878471 | -0.566276 | -2.225867 |
| H | -1.114452 | 4.529580 | 3.618657 | C | 1.241288 | 0.970393 | -2.471708 |
| H | 0.147476 | 5.776186 | 3.567973 | H | 1.089238 | 1.959488 | -2.952449 |
| H | 0.973508 | 4.984588 | 1.423014 | C | 2.195084 | 0.212454 | -3.423994 |
| H | -0.762531 | 4.644328 | 1.214051 | H | 1.771669 | 0.151907 | -4.435005 |
| O | -1.154623 | 3.238722 | -0.915194 | H | 3.169481 | 0.706473 | -3.508044 |
| C | -2.598566 | 3.072184 | -0.858175 | H | 2.366571 | -0.814509 | -3.075094 |
| C | -3.178680 | 4.056785 | -1.878860 | C | -0.131857 | 0.282754 | -2.484098 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.033968 | 4.193044 | -2.893790 | H | -0.093396 | -0.702163 | -2.007314 |
| C | -0.808940 | 4.150428 | -1.983953 | H | -0.879504 | 0.873845 | -1.944403 |
| H | -0.596154 | 5.140096 | -1.554686 | H | -0.496862 | 0.146291 | -3.510029 |
| H | 0.093465 | 3.772996 | -2.467418 | C | 2.989937 | 1.855370 | -1.001442 |
| H | -2.084697 | 5.111698 | -3.485856 | H | 3.808524 | 1.310987 | -1.513865 |
| H | -2.024934 | 3.340078 | -3.581812 | C | 2.982465 | 3.269729 | -1.629063 |
| H | -3.387126 | 5.025110 | -1.408396 | H | 2.762678 | 3.249259 | -2.701812 |
| H | -4.109238 | 3.689313 | -2.320794 | H | 2.229149 | 3.906449 | -1.142877 |
| H | -2.830490 | 2.032605 | -1.110702 | H | 3.959217 | 3.756527 | -1.507384 |
| H | -2.929163 | 3.259770 | 0.167178 | C | 3.426764 | 1.988624 | 0.464440 |
| Li | 2.077962 | -0.810087 | -0.314074 | H | 3.444205 | 1.014052 | 0.964258 |
| N | 1.154304 | -2.455745 | 0.545580 | H | 4.432357 | 2.422038 | 0.540325 |
| C | 1.271972 | -3.723131 | -0.210526 | H | 2.736571 | 2.637040 | 1.016542 |
| H | 0.496509 | -4.439930 | 0.119647 | C | -2.373948 | -0.963684 | 0.631578 |
| C | 2.621263 | -4.450756 | -0.056546 | H | 0.755753 | -3.660827 | 3.789424 |
| H | 2.800434 | -4.796120 | 0.967037 | C | -1.571984 | -2.040002 | 0.298949 |
| H | 2.652427 | -5.334953 | -0.705982 | C | -2.305231 | -3.143465 | -0.192692 |
| H | 3.445370 | -3.786618 | -0.342152 | C | -3.692713 | -3.147119 | -0.336559 |
| C | 1.014593 | -3.460153 | -1.700035 | C | -4.426740 | -2.011615 | 0.020937 |
| H | 0.060905 | -2.949418 | -1.857038 | C | -3.760081 | -0.890382 | 0.519034 |
| H | 1.809979 | -2.837213 | -2.131793 | H | -4.312358 | -0.006471 | 0.818959 |
| H | 0.992723 | -4.400895 | -2.264467 | C | -5.911403 | -1.972529 | -0.183989 |
| C | 1.437818 | -2.626922 | 1.985696 | F | -6.243930 | -1.619530 | -1.453101 |
| H | 2.451828 | -3.044336 | 2.119025 | F | -6.520272 | -1.078175 | 0.632005 |
| C | 1.439373 | -1.259720 | 2.681094 | F | -6.488218 | -3.176509 | 0.039037 |
| H | 2.180381 | -0.584881 | 2.230815 | H | -4.209498 | -4.025238 | -0.714058 |
| H | 0.459117 | -0.780406 | 2.604695 | H | -1.767733 | -4.048166 | -0.473714 |
| H | 1.689598 | -1.360824 | 3.744933 | Cl | -1.606619 | 0.548624 | 1.320147 |
| C | 0.477534 | -3.582693 | 2.730429 | H | -0.150161 | -2.166926 | 0.444391 |
| H | 0.503420 | -4.594135 | 2.310769 | | | | |

**Table 7 (Continued).**



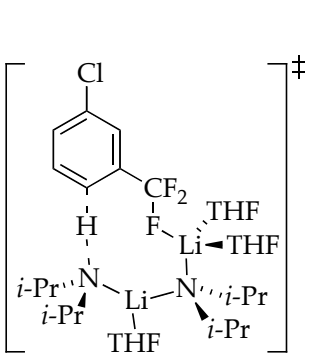



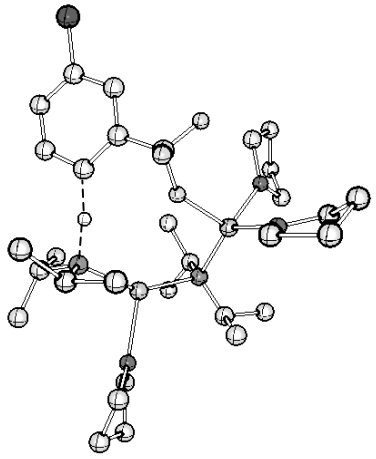
**18**
$G$ = -2091.906847
$G_{MP2}$ = -2085.989806
$\Delta G^{‡}$ = 21.9 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 15.9 kcal/mol

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -1.016912 | -1.025891 | -1.186328 | C | 2.651738 | -1.665946 | 2.780365 |
| F | -0.440688 | -2.259098 | -1.190432 | C | 1.891826 | -2.055811 | 4.046670 |
| F | -0.181076 | -0.261089 | -0.360827 | C | 0.634859 | -2.720392 | 3.465214 |
| Li | 2.050968 | -0.260269 | 0.151503 | C | 0.344196 | -1.854693 | 2.237722 |
| N | 2.181464 | 1.725892 | -0.166606 | H | -0.302917 | -1.005350 | 2.476976 |
| Li | 0.193359 | 1.958297 | -0.113946 | H | -0.094896 | -2.408446 | 1.405567 |
| N | -1.678389 | 2.564426 | 0.185278 | H | -0.207022 | -2.740360 | 4.162856 |
| C | -1.971104 | 2.934364 | 1.587532 | H | 0.852203 | -3.752933 | 3.167297 |
| H | -1.322845 | 3.775691 | 1.894393 | H | 1.623327 | -1.160419 | 4.618857 |
| C | -3.420897 | 3.382675 | 1.871380 | H | 2.473146 | -2.716468 | 4.696469 |
| H | -3.541093 | 3.619955 | 2.935973 | H | 3.253497 | -2.501641 | 2.397547 |
| H | -3.699815 | 4.276967 | 1.305335 | H | 3.299547 | -0.794232 | 2.904745 |
| H | -4.134946 | 2.589254 | 1.622308 | O | 3.252352 | -1.582775 | -0.724780 |
| C | -1.632751 | 1.748474 | 2.505776 | C | 2.916185 | -2.983080 | -0.896148 |
| H | -0.598477 | 1.414261 | 2.364208 | C | 3.910773 | -3.522001 | -1.924979 |
| H | -1.747062 | 2.027403 | 3.560283 | C | 5.151630 | -2.657064 | -1.655289 |
| H | -2.294243 | 0.899695 | 2.301417 | C | 4.528808 | -1.294388 | -1.352498 |
| C | -2.129575 | 3.558299 | -0.807609 | H | 4.344465 | -0.719183 | -2.266945 |
| H | -3.224967 | 3.693354 | -0.750192 | H | 5.112794 | -0.680105 | -0.663133 |
| C | -1.495074 | 4.948693 | -0.624743 | H | 5.844646 | -2.617696 | -2.500583 |
| H | -0.400164 | 4.884884 | -0.689491 | H | 5.699228 | -3.033579 | -0.783085 |
| H | -1.839407 | 5.639421 | -1.405157 | H | 3.539177 | -3.351372 | -2.941902 |
| H | -1.745103 | 5.395047 | 0.343668 | H | 4.093227 | -4.593844 | -1.805011 |
| C | -1.835252 | 3.031491 | -2.219859 | H | 3.022832 | -3.487263 | 0.072779 |
| H | -0.753220 | 2.971113 | -2.404677 | H | 1.873664 | -3.045329 | -1.213793 |
| H | -2.262207 | 2.035126 | -2.367372 | C | -2.441153 | -1.024142 | -0.728364 |
| H | -2.254824 | 3.701254 | -2.980379 | C | -3.018788 | 0.194628 | -0.325377 |
| F | -0.833325 | -0.513835 | -2.419423 | C | -4.387799 | 0.104182 | -0.012451 |
| C | 2.930290 | 2.404520 | 0.905031 | C | -5.125554 | -1.080425 | -0.082714 |
| H | 3.074396 | 3.475501 | 0.675093 | C | -4.481990 | -2.251860 | -0.480418 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.348897 | 1.834382 | 1.145714 | C | -3.134424 | -2.243569 | -0.813672 |
| H | 4.953021 | 1.852813 | 0.231862 | H | 2.477726 | 1.362541 | -3.563755 |
| H | 4.890587 | 2.410671 | 1.907565 | C | 2.626946 | 3.517317 | -1.921571 |
| H | 4.297415 | 0.790997 | 1.491488 | H | 3.149972 | 4.184010 | -1.228707 |
| C | 2.139843 | 2.364423 | 2.219509 | H | 3.063643 | 3.675042 | -2.916531 |
| H | 1.197439 | 2.918409 | 2.133054 | H | 1.576666 | 3.835900 | -1.960512 |
| H | 1.897297 | 1.330903 | 2.502876 | O | 1.634657 | -1.333325 | 1.807861 |
| H | 2.709190 | 2.812542 | 3.043342 | H | -2.647337 | -3.158633 | -1.132628 |
| C | 2.731592 | 2.032963 | -1.501182 | Cl | -5.385820 | -3.767997 | -0.563470 |
| H | 3.811241 | 1.782193 | -1.554863 | H | -6.182816 | -1.103718 | 0.167009 |
| C | 2.041894 | 1.176758 | -2.574369 | H | -4.920166 | 1.002230 | 0.303591 |
| H | 2.135024 | 0.104715 | -2.364904 | H | -2.308937 | 1.443608 | -0.085067 |
| H | 0.972041 | 1.406265 | -2.644811 | | | | |



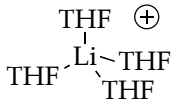
**19**
$G$ = -2324.242208
$G_{MP2}$ = -2317.55991
$\Delta G^{‡}$ = 30.7 kcal/mol
$\Delta G_{MP2}^{‡}$ = 15.8 kcal/mol

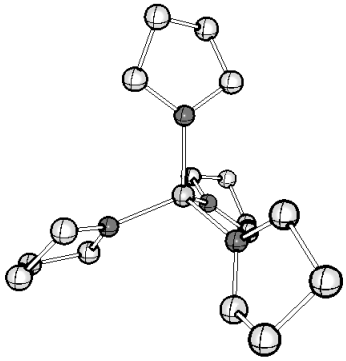
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -0.272486 | 1.933725 | -0.045018 | H | 6.705227 | 0.601706 | -0.476194 |
| F | -1.066358 | 0.176203 | 0.617594 | H | 7.252240 | -0.838950 | -1.354867 |
| C | -2.210185 | -0.412128 | 1.124240 | H | 4.979452 | -1.470722 | -1.924707 |
| F | -3.176513 | 0.539150 | 1.036513 | H | 4.802161 | 0.301060 | -1.938842 |
| F | -1.968428 | -0.564587 | 2.453434 | C | 1.103494 | 1.282301 | -2.458562 |
| C | -2.545381 | -1.690166 | 0.423256 | H | 0.840322 | 2.273557 | -2.883972 |
| C | -1.497930 | -2.560571 | 0.063241 | C | 2.250223 | 0.761981 | -3.356466 |
| C | -1.941231 | -3.761348 | -0.529386 | H | 1.938406 | 0.729697 | -4.408586 |
| C | -3.284543 | -4.075305 | -0.752849 | H | 3.138515 | 1.400940 | -3.300042 |
| C | -4.262924 | -3.159519 | -0.370157 | H | 2.547514 | -0.255093 | -3.067925 |
| C | -3.910732 | -1.956671 | 0.224928 | C | -0.134376 | 0.396818 | -2.669456 |
| H | -4.678396 | -1.250680 | 0.522986 | H | 0.016192 | -0.608991 | -2.263962 |
| Cl | -5.970584 | -3.525672 | -0.646504 | H | -1.015857 | 0.819219 | -2.176339 |
| H | -3.574640 | -5.014147 | -1.216642 | H | 3.482898 | 1.919477 | -1.211730 |

**Table 7 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.205990 | -4.501911 | -0.841668 | C | 2.379802 | 3.736995 | -1.269331 |
| N | 1.417860 | 1.380141 | -1.022053 | H | 2.251418 | 3.778989 | -2.356398 |
| Li | 1.950534 | -0.540460 | -0.320384 | H | 1.506997 | 4.220568 | -0.807015 |
| N | 1.269358 | -2.400283 | 0.344700 | H | 3.262775 | 4.341872 | -1.023984 |
| C | 1.638588 | -3.543957 | -0.521899 | C | 2.814269 | 2.352699 | 0.759648 |
| H | 1.017842 | -4.425980 | -0.276228 | H | 2.954753 | 1.351740 | 1.181369 |
| C | 3.102729 | -4.009700 | -0.406448 | H | 3.718177 | 2.936270 | 0.977291 |
| H | 3.335644 | -4.429816 | 0.577746 | H | 1.974285 | 2.824693 | 1.282829 |
| H | 3.310164 | -4.791755 | -1.147936 | O | -0.481151 | 2.889014 | 1.746045 |
| H | 3.785374 | -3.172114 | -0.589669 | C | -0.948764 | 4.249934 | 1.865862 |
| C | 1.338061 | -3.194278 | -1.984989 | C | -1.431921 | 4.388238 | 3.308443 |
| H | 0.305088 | -2.858328 | -2.109055 | C | -0.450877 | 3.471730 | 4.055185 |
| H | 2.002553 | -2.395967 | -2.343417 | C | -0.262457 | 2.318608 | 3.065115 |
| H | 1.492980 | -4.064877 | -2.634857 | H | -0.993882 | 1.520462 | 3.215013 |
| C | 1.581786 | -2.651007 | 1.768363 | H | 0.740877 | 1.884809 | 3.087856 |
| H | 2.651928 | -2.898580 | 1.873859 | H | -0.829461 | 3.127310 | 5.021877 |
| C | 1.355820 | -1.377971 | 2.595445 | H | 0.498589 | 3.991864 | 4.227904 |
| H | 1.941751 | -0.534994 | 2.204491 | H | -2.457357 | 4.012440 | 3.404861 |
| H | 0.303412 | -1.086874 | 2.596157 | H | -1.412036 | 5.424273 | 3.659753 |
| H | 1.661965 | -1.533261 | 3.638028 | H | -0.114002 | 4.933546 | 1.656256 |
| H | -0.368966 | 0.296472 | -3.736858 | H | -1.726563 | 4.400102 | 1.114708 |
| C | 2.544804 | 2.288272 | -0.750770 | O | -1.765508 | 3.020126 | -1.043126 |
| C | 0.802288 | -3.822090 | 2.409975 | C | -3.153287 | 2.619612 | -1.214364 |
| H | 0.989009 | -4.768623 | 1.891350 | C | -3.710642 | 3.473258 | -2.362431 |
| H | 1.103330 | -3.957795 | 3.456971 | C | -2.444148 | 3.877364 | -3.132665 |
| H | -0.276129 | -3.635881 | 2.384074 | C | -1.440821 | 4.055138 | -1.998011 |
| O | 4.151666 | -0.633512 | -0.213738 | H | -1.552106 | 5.038884 | -1.518209 |
| C | 5.076733 | -0.557356 | -1.322771 | H | -0.399660 | 3.918918 | -2.292555 |
| C | 6.469342 | -0.445536 | -0.699518 | H | -2.571326 | 4.785865 | -3.728880 |
| C | 6.299726 | -1.245704 | 0.599583 | H | -2.119439 | 3.069271 | -3.797421 |
| C | 4.875464 | -0.872254 | 1.015378 | H | -4.217348 | 4.363404 | -1.971641 |
| H | 4.863162 | 0.048316 | 1.614007 | H | -4.429664 | 2.919669 | -2.972870 |
| H | 4.359807 | -1.660711 | 1.567962 | H | -3.165839 | 1.551367 | -1.449150 |
| H | 7.037705 | -0.992967 | 1.366904 | H | -3.681644 | 2.771678 | -0.269241 |
| H | 6.370613 | -2.320977 | 0.398758 | H | -0.053390 | -2.377066 | 0.243261 |

**Table 8.** Optimized geometries at the B3LYP level of theory with 6-31G(d) basis set of lithium ions, lithium chloride aggregates, lithium chloride triple ions, lithium chloride-LDA mixed aggregates and lithium chloride-LDA triple ions at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z). Single point MP2 energies are included.

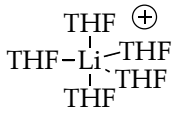


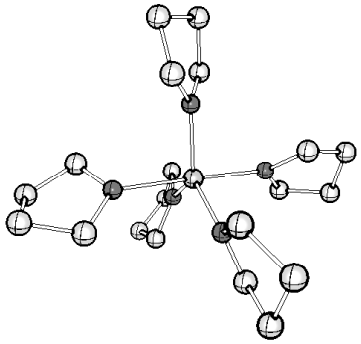



**F**
$G$ = -936.852895
$G_{MP2}$ = -933.704189

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -0.006449 | 0.001038 | -0.009157 | O | 1.191545 | 1.220605 | -0.970730 |
| O | -1.077777 | -1.026060 | -1.295317 | C | 2.297282 | 1.933630 | -0.357946 |
| C | -0.989910 | -2.462953 | -1.508784 | C | 3.270383 | 2.229150 | -1.496696 |
| C | -2.132747 | -2.816892 | -2.464896 | C | 2.314055 | 2.442198 | -2.680370 |
| C | -3.164470 | -1.715775 | -2.173973 | C | 1.225143 | 1.399943 | -2.415227 |
| C | -2.268061 | -0.502979 | -1.939270 | H | 1.461585 | 0.432429 | -2.872967 |
| H | -2.697261 | 0.253434 | -1.276585 | H | 0.230932 | 1.713191 | -2.746231 |
| H | -1.979832 | -0.025559 | -2.884933 | H | 2.793140 | 2.300813 | -3.652757 |
| H | -3.737433 | -1.950673 | -1.269413 | H | 1.893118 | 3.453407 | -2.654471 |
| H | -3.871172 | -1.560270 | -2.993477 | H | 3.923574 | 1.367847 | -1.678120 |
| H | -2.518079 | -3.825188 | -2.292093 | H | 3.901818 | 3.097306 | -1.290120 |
| H | -1.795718 | -2.758029 | -3.505587 | H | 1.915196 | 2.857533 | 0.095229 |
| H | 0.000191 | -2.692371 | -1.913886 | H | 2.708844 | 1.297860 | 0.430975 |
| H | -1.097298 | -2.956151 | -0.535998 | O | -1.236654 | 1.033713 | 1.121026 |
| O | 1.102928 | -1.230097 | 1.050946 | C | -2.269354 | 0.461832 | 1.968338 |
| C | 2.270584 | -1.905345 | 0.513630 | C | -3.249489 | 1.600110 | 2.249196 |
| C | 3.181542 | -2.153074 | 1.713094 | C | -2.324461 | 2.827204 | 2.240319 |
| C | 2.162391 | -2.403646 | 2.835346 | C | -1.344388 | 2.484692 | 1.118917 |
| C | 1.044761 | -1.414890 | 2.493348 | H | -0.344441 | 2.901385 | 1.265602 |
| H | 1.200174 | -0.438633 | 2.967237 | H | -1.719882 | 2.801928 | 0.138394 |
| H | 0.047388 | -1.780647 | 2.754423 | H | -1.797773 | 2.917682 | 3.196897 |
| H | 2.571312 | -2.234846 | 3.834979 | H | -2.854323 | 3.765320 | 2.055151 |
| H | 1.791464 | -3.433513 | 2.791200 | H | -3.780163 | 1.466271 | 3.195494 |
| H | 3.784018 | -1.263155 | 1.929201 | H | -3.995082 | 1.673546 | 1.449237 |
| H | 3.861908 | -2.993687 | 1.553117 | H | -2.712408 | -0.385399 | 1.436410 |
| H | 1.951993 | -2.846493 | 0.047474 | H | -1.800550 | 0.096006 | 2.889973 |
| H | 2.704206 | -1.258975 | -0.254455 | | | | |

**Table 8 (Continued).**

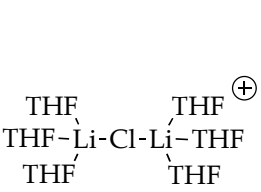


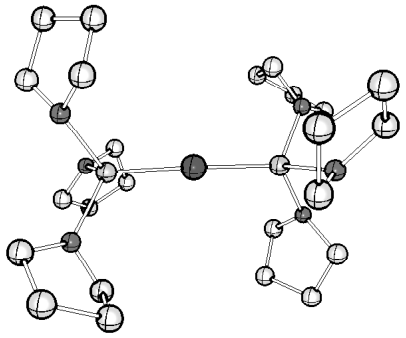



**G**
$G$ = -1169.19433
$G_{MP2}$ = -1165.279988

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -0.014627 | -0.019310 | 0.032833 | H | 2.105502 | -0.957041 | -2.234215 |
| O | 2.092823 | 0.695684 | 0.132841 | H | 0.663926 | -3.478052 | -3.212980 |
| C | 2.753883 | 1.717327 | -0.651421 | H | 2.365339 | -3.046867 | -3.454857 |
| C | 4.237583 | 1.343169 | -0.673616 | H | 1.749754 | -4.765441 | -1.422854 |
| C | 4.405092 | 0.626669 | 0.674675 | H | 2.876275 | -3.441408 | -1.085768 |
| C | 3.081276 | -0.129150 | 0.790943 | H | 1.191834 | -2.915250 | 0.565714 |
| H | 2.752971 | -0.297026 | 1.820427 | H | -0.114956 | -3.561982 | -0.454225 |
| H | 3.127996 | -1.099454 | 0.278859 | O | -2.115883 | -0.713223 | -0.140070 |
| H | 4.505837 | 1.355452 | 1.487182 | C | -3.179621 | 0.074960 | 0.441072 |
| H | 5.272077 | -0.038927 | 0.707813 | C | -4.441255 | -0.278173 | -0.346681 |
| H | 4.886478 | 2.216016 | -0.786043 | C | -4.185718 | -1.750183 | -0.702432 |
| H | 4.450674 | 0.655895 | -1.500977 | C | -2.677566 | -1.761326 | -0.966708 |
| H | 2.292211 | 1.745489 | -1.642609 | H | -2.447815 | -1.539982 | -2.017034 |
| H | 2.596879 | 2.690064 | -0.167155 | H | -2.200587 | -2.708729 | -0.701558 |
| O | -0.548295 | 1.758109 | -0.848809 | H | -4.762716 | -2.095358 | -1.564723 |
| C | -1.097509 | 1.827082 | -2.189010 | H | -4.431662 | -2.396007 | 0.148270 |
| C | -1.699024 | 3.227667 | -2.326913 | H | -4.511216 | 0.331022 | -1.255740 |
| C | -0.819185 | 4.054007 | -1.375803 | H | -5.355116 | -0.124672 | 0.233821 |
| C | -0.581281 | 3.068705 | -0.232604 | H | -3.283391 | -0.190291 | 1.502072 |
| H | -1.401543 | 3.096851 | 0.497594 | H | -2.893467 | 1.127458 | 0.371156 |
| H | 0.363099 | 3.217591 | 0.296537 | O | -0.091440 | -0.129446 | 2.047041 |
| H | -1.297287 | 4.977527 | -1.038237 | C | 0.201893 | 0.968188 | 2.949462 |
| H | 0.128387 | 4.318498 | -1.858858 | C | 0.128708 | 0.379635 | 4.359114 |
| H | -2.740856 | 3.234994 | -1.986586 | C | -0.916305 | -0.734379 | 4.188719 |
| H | -1.679043 | 3.588960 | -3.358567 | C | -0.582145 | -1.269212 | 2.796904 |
| H | -0.281315 | 1.665354 | -2.904968 | H | -1.435814 | -1.680961 | 2.253769 |
| H | -1.827311 | 1.020153 | -2.297534 | H | 0.210474 | -2.028087 | 2.841133 |
| O | 0.605380 | -1.690607 | -1.000315 | H | -1.929559 | -0.316465 | 4.207965 |
| C | 0.837295 | -3.017614 | -0.464154 | H | -0.853785 | -1.507708 | 4.959104 |
| C | 1.852666 | -3.677268 | -1.399304 | H | -0.151947 | 1.125820 | 5.107325 |
| C | 1.535138 | -3.006661 | -2.744517 | H | 1.096342 | -0.044823 | 4.650576 |
| C | 1.204232 | -1.577657 | -2.314267 | H | 1.182132 | 1.371763 | 2.683251 |
| H | 0.488597 | -1.076111 | -2.972997 | H | -0.553139 | 1.750803 | 2.801162 |

**Table 8 (Continued).**



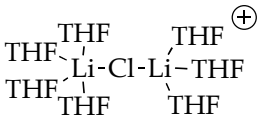



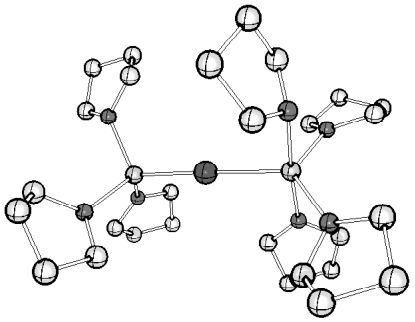
**H**
$G$ = -1869.437502
$G_{MP2}$ = -1864.094163

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -2.309220 | -0.063071 | 0.051572 | H | 3.036500 | 1.015043 | 3.617927 |
| Cl | 0.012786 | -0.023900 | -0.007906 | C | 2.262868 | -1.029499 | 3.735624 |
| Li | 2.335520 | 0.048590 | -0.000622 | H | 2.072138 | -0.908774 | 4.807453 |
| O | 3.149071 | 1.702927 | -0.861548 | H | 1.412497 | -1.558142 | 3.285558 |
| C | 2.366301 | 2.446946 | -1.821620 | C | 3.586950 | -1.767082 | 3.437391 |
| H | 1.483590 | 1.841057 | -2.054531 | H | 3.422549 | -2.831862 | 3.236283 |
| H | 2.963246 | 2.602161 | -2.733440 | H | 4.283140 | -1.689678 | 4.279391 |
| C | 2.054281 | 3.761185 | -1.114723 | C | 4.152774 | -1.035445 | 2.195016 |
| H | 1.794890 | 4.563710 | -1.814073 | H | 5.106958 | -0.538178 | 2.416750 |
| H | 1.209975 | 3.606363 | -0.430090 | H | 4.275863 | -1.682953 | 1.322802 |
| C | 3.353220 | 4.039094 | -0.335377 | O | -3.085002 | -1.736989 | 0.880236 |
| H | 3.170429 | 4.572586 | 0.604578 | C | -2.265737 | -2.607969 | 1.685614 |
| H | 4.040095 | 4.645874 | -0.936147 | H | -2.790685 | -2.833373 | 2.627471 |
| C | 3.945651 | 2.634694 | -0.090420 | H | -1.336514 | -2.066652 | 1.895995 |
| H | 4.991066 | 2.564337 | -0.419304 | C | -2.089919 | -3.854046 | 0.822363 |
| H | 3.880854 | 2.309829 | 0.951728 | H | -1.823587 | -4.739340 | 1.409954 |
| O | 3.216265 | -1.472276 | -0.995455 | H | -1.293480 | -3.667156 | 0.091131 |
| C | 2.464359 | -2.672411 | -1.272767 | C | -3.459873 | -3.984079 | 0.122383 |
| H | 1.511609 | -2.580290 | -0.740264 | H | -4.100361 | -4.705349 | 0.641629 |
| H | 3.020046 | -3.546215 | -0.898137 | H | -3.358514 | -4.315835 | -0.917188 |
| C | 2.341280 | -2.688856 | -2.792904 | C | -4.063773 | -2.561261 | 0.210162 |
| H | 2.119705 | -3.685522 | -3.190081 | H | -4.244062 | -2.097682 | -0.762927 |
| H | 1.535741 | -2.005521 | -3.091009 | H | -4.995709 | -2.553080 | 0.791901 |
| C | 3.713717 | -2.152687 | -3.245024 | O | -3.212861 | 0.011927 | -1.763012 |
| H | 3.649752 | -1.569698 | -4.170498 | C | -4.264640 | 0.946391 | -2.090622 |
| H | 4.412308 | -2.978693 | -3.418018 | H | -4.422767 | 1.557544 | -1.198333 |
| C | 4.185048 | -1.288071 | -2.053636 | H | -5.183112 | 0.384755 | -2.309705 |
| H | 5.175021 | -1.594994 | -1.689712 | C | -3.777216 | 1.747250 | -3.322812 |
| H | 4.205060 | -0.215596 | -2.268545 | H | -3.690540 | 2.816719 | -3.099139 |
| O | 3.178629 | -0.035980 | 1.826804 | H | -4.479596 | 1.635727 | -4.155856 |
| C | 2.443873 | 0.305665 | 3.018969 | H | -5.012534 | 1.357490 | 2.102851 |
| C | -2.406847 | 1.119842 | -3.658811 | C | -3.394006 | 2.211976 | 3.334972 |
| H | -1.592483 | 1.699062 | -3.204040 | | | | |

**Table 8 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -2.223242 | 1.042881 | -4.735956 | H | -4.159776 | 2.950827 | 3.596139 |
| C | -2.476172 | -0.243451 | -2.975481 | H | -3.084148 | 1.708900 | 4.258502 |
| H | -3.023966 | -0.980068 | -3.584072 | C | -2.210576 | 2.884884 | 2.613229 |
| H | -1.502555 | -0.651274 | -2.681317 | H | -1.276888 | 2.337404 | 2.798228 |
| O | -3.209282 | 1.432874 | 1.068675 | H | -2.069610 | 3.931404 | 2.905781 |
| C | -3.941940 | 1.208371 | 2.296495 | C | -2.586296 | 2.732023 | 1.143437 |
| H | -3.774697 | 0.162620 | 2.569849 | H | -3.306341 | 3.501084 | 0.822175 |
| H | 1.509872 | 0.779916 | 2.696561 | H | -1.728533 | 2.717724 | 0.458942 |



**I**
$G$ = -2101.774411
$G_{MP2}$ = -2095.667218

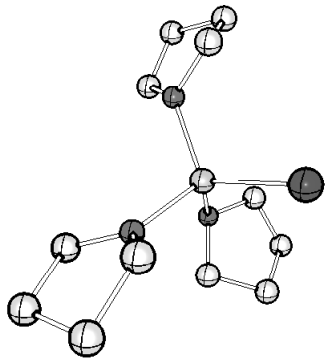
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 2.092644 | -0.204286 | 0.158816 | C | -2.657925 | 4.258283 | -0.147982 |
| Cl | -0.389978 | -0.130696 | -0.001816 | C | -2.534004 | 2.970481 | 0.664104 |
| Li | -2.704165 | 0.088780 | -0.123903 | H | -2.977136 | 3.081723 | 1.662926 |
| O | -3.635244 | -0.787110 | 1.398964 | H | -1.513522 | 2.593050 | 0.764508 |
| C | -4.856790 | -0.239895 | 1.965413 | H | -2.532860 | 5.154421 | 0.466367 |
| C | -4.876390 | -0.667542 | 3.440073 | H | -1.905056 | 4.281760 | -0.944769 |
| C | -3.390760 | -0.927738 | 3.739468 | H | -4.823775 | 4.409719 | -0.003605 |
| C | -2.905703 | -1.514472 | 2.417461 | H | -4.221913 | 4.736302 | -1.636818 |
| H | -3.151723 | -2.582650 | 2.339627 | H | -3.775104 | 2.388965 | -2.048381 |
| H | -1.842735 | -1.370802 | 2.212122 | H | -5.160524 | 2.214269 | -0.946338 |
| H | -3.236004 | -1.605563 | 4.583846 | O | -3.481095 | -0.694049 | -1.761838 |
| H | -2.866939 | 0.011524 | 3.952783 | C | -2.702904 | -0.744402 | -2.989600 |
| H | -5.454988 | -1.589265 | 3.565834 | C | -3.192056 | -1.981378 | -3.757181 |
| H | -5.319670 | 0.096058 | 4.085149 | C | -3.798180 | -2.856266 | -2.647440 |
| H | -4.815717 | 0.847003 | 1.842404 | C | -4.407162 | -1.805395 | -1.724363 |
| H | -5.709732 | -0.625636 | 1.397058 | H | -4.498934 | -2.113886 | -0.680864 |
| O | -3.294253 | 1.978277 | -0.071594 | H | -5.387492 | -1.470110 | -2.089787 |
| C | -4.151774 | 2.625407 | -1.046260 | H | -3.014809 | -3.414147 | -2.121445 |
| C | -4.068128 | 4.123784 | -0.744097 | H | -4.538586 | -3.570430 | -3.018770 |
| H | -2.382470 | -2.476106 | -4.301047 | H | 5.214521 | -1.050874 | -1.182708 |
| H | -3.963413 | -1.704348 | -4.484205 | H | 4.129033 | -2.445845 | -0.992925 |
| H | -2.861986 | 0.188439 | -3.541069 | O | 3.019001 | 0.289475 | 1.898603 |
| H | -1.649044 | -0.811571 | -2.701628 | C | 4.371926 | -0.005140 | 2.315054 |
| O | 2.043238 | -2.288081 | 0.724449 | C | 4.742508 | 1.081342 | 3.326973 |

**Table 8 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.655365 | -2.597688 | 2.080387 | C | 3.380727 | 1.406836 | 3.960021 |
| C | 1.103974 | -4.021412 | 2.035302 | C | 2.438090 | 1.298137 | 2.760715 |
| C | 0.425508 | -4.043545 | 0.657749 | H | 2.374600 | 2.236588 | 2.197757 |
| C | 1.377556 | -3.194108 | -0.190198 | H | 1.424837 | 0.977913 | 3.019022 |
| H | 0.854491 | -2.598012 | -0.942064 | H | 3.347170 | 2.394018 | 4.429540 |
| H | 2.143905 | -3.809956 | -0.678282 | H | 3.124835 | 0.660245 | 4.720637 |
| H | -0.556737 | -3.561242 | 0.711544 | H | 5.146087 | 1.962439 | 2.814405 |
| H | 0.293510 | -5.051769 | 0.254205 | H | 5.488195 | 0.740683 | 4.050641 |
| H | 0.418074 | -4.232916 | 2.861193 | H | 4.391868 | -1.004335 | 2.768853 |
| H | 1.920825 | -4.751356 | 2.076610 | H | 5.012154 | -0.014355 | 1.427663 |
| H | 2.535301 | -2.485672 | 2.719007 | O | 2.302456 | 1.948061 | -0.472769 |
| H | 0.888317 | -1.880301 | 2.400473 | C | 3.621237 | 2.498703 | -0.682438 |
| O | 3.194293 | -0.676031 | -1.497003 | C | 3.429912 | 3.835076 | -1.418757 |
| C | 4.338761 | -1.560070 | -1.599918 | C | 2.045548 | 3.666983 | -2.065274 |
| C | 4.497749 | -1.886988 | -3.092697 | C | 1.311603 | 2.847459 | -1.005877 |
| C | 3.087576 | -1.629910 | -3.649295 | H | 0.486423 | 2.237988 | -1.378222 |
| C | 2.634593 | -0.440566 | -2.806546 | H | 0.932113 | 3.495508 | -0.200764 |
| H | 1.551679 | -0.351469 | -2.689107 | H | 2.120321 | 3.101027 | -3.001534 |
| H | 3.026785 | 0.505202 | -3.206563 | H | 1.553413 | 4.619765 | -2.282553 |
| H | 2.436978 | -2.493385 | -3.468939 | H | 4.226810 | 4.029920 | -2.142073 |
| H | 3.081300 | -1.414467 | -4.721643 | H | 3.415006 | 4.668268 | -0.707048 |
| H | 4.846634 | -2.910052 | -3.257696 | H | 4.116452 | 2.620068 | 0.287857 |
| H | 5.218973 | -1.208177 | -3.561203 | H | 4.192154 | 1.773998 | -1.273130 |

**Table 8 (Continued).**

THF
THF–Li–Cl
THF

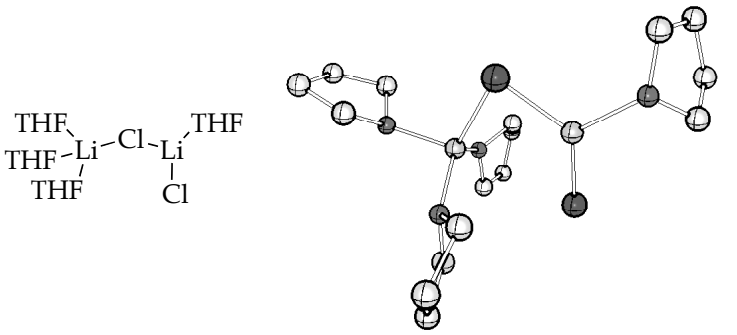


**J**
$G$ = -1164.913673
$G_{MP2}$ = -1161.942118

* Tetrasolvated lithium chloride monomer fails to minimize.

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -0.030161 | -0.109586 | 0.290648 | H | -1.942805 | -1.419516 | 1.805276 |
| Cl | -0.124011 | 0.560351 | 2.423159 | H | -4.470547 | -2.142028 | 0.967611 |
| O | -0.291182 | 1.484173 | -0.918817 | H | -3.901650 | -0.485490 | 0.682078 |
| C | -1.392889 | 2.318883 | -0.453211 | H | -3.860424 | -2.842244 | -1.276024 |
| C | -0.835540 | 3.743276 | -0.337165 | H | -4.380131 | -1.187066 | -1.613696 |
| C | 0.667081 | 3.495044 | -0.131166 | H | -2.104221 | -0.444894 | -1.880131 |
| C | 0.904132 | 2.290474 | -1.037109 | H | -1.750163 | -2.173243 | -2.097146 |
| H | 1.748831 | 1.665628 | -0.736625 | O | 1.758263 | -0.888047 | -0.121882 |
| H | 1.031328 | 2.589627 | -2.087939 | C | 2.582283 | -1.311417 | 0.985451 |
| H | 0.864680 | 3.217351 | 0.908989 | C | 4.001180 | -1.175372 | 0.442750 |
| H | 1.288981 | 4.354509 | -0.400889 | C | 3.841807 | -1.662279 | -1.013739 |
| H | -1.294269 | 4.292374 | 0.489891 | C | 2.359491 | -1.355775 | -1.343280 |
| H | -1.009692 | 4.308156 | -1.261123 | H | 1.826883 | -2.248225 | -1.695881 |
| H | -2.214187 | 2.234546 | -1.173382 | H | 2.237482 | -0.563376 | -2.088232 |
| H | -1.704012 | 1.929553 | 0.520848 | H | 4.032340 | -2.738446 | -1.082692 |
| O | -1.457624 | -1.409572 | -0.183798 | H | 4.529898 | -1.162106 | -1.701458 |
| C | -2.200144 | -1.434678 | -1.422696 | H | 4.731065 | -1.761580 | 1.008992 |
| C | -3.655910 | -1.788389 | -1.056036 | H | 4.310243 | -0.124508 | 0.471487 |
| C | -3.707652 | -1.541562 | 0.462941 | H | 2.323739 | -0.671722 | 1.830451 |
| C | -2.289801 | -1.905836 | 0.891116 | H | 2.347324 | -2.356082 | 1.238760 |
| H | -2.161906 | -2.995069 | 0.974030 | | | | |

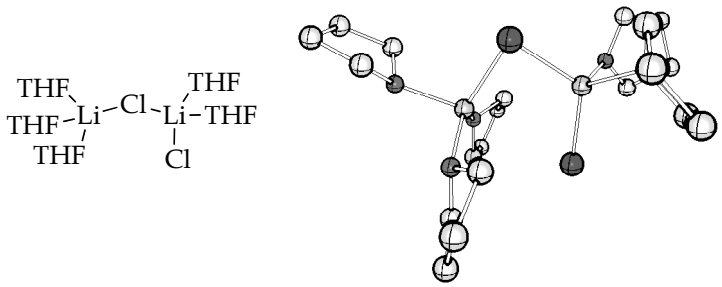
**Table 8 (Continued).**




**K**
$G$ = -1865.131896
$G_{MP2}$ = -1860.742824

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.157373 | -0.069142 | -0.069344 | H | -3.694448 | 1.053497 | -1.611361 |
| Cl | 0.402606 | -0.278979 | -1.812373 | H | -2.595701 | 0.176338 | -2.709544 |
| Li | 1.964071 | 0.577751 | -0.393609 | O | -1.567693 | 1.847739 | 0.296200 |
| Cl | 1.697598 | 1.043337 | 1.752870 | C | -1.878844 | 2.346929 | 1.614055 |
| O | 3.761042 | 0.629470 | -1.073347 | C | -2.085910 | 3.871714 | 1.451128 |
| C | 4.880917 | 0.703529 | -0.170100 | C | -1.556492 | 4.171604 | 0.024199 |
| C | 5.514841 | -0.685741 | -0.260085 | C | -0.803722 | 2.890919 | -0.344469 |
| C | 5.283833 | -1.088491 | -1.739917 | H | 0.213947 | 2.885326 | 0.066203 |
| C | 4.197943 | -0.102735 | -2.237356 | H | -0.770212 | 2.663377 | -1.411185 |
| H | 3.311700 | -0.578941 | -2.660997 | H | -0.910581 | 5.053869 | -0.011968 |
| H | 4.605100 | 0.608219 | -2.967955 | H | -2.388435 | 4.333671 | -0.669329 |
| H | 4.955415 | -2.128183 | -1.824869 | H | -1.523245 | 4.417124 | 2.214382 |
| H | 6.198461 | -0.983857 | -2.331880 | H | -3.138314 | 4.153273 | 1.551830 |
| H | 4.990238 | -1.371450 | 0.413184 | H | -2.769692 | 1.814289 | 1.957468 |
| H | 6.572662 | -0.681691 | 0.019314 | H | -1.034947 | 2.128122 | 2.278009 |
| H | 5.569898 | 1.488653 | -0.514837 | O | -0.916072 | -1.460161 | 1.336256 |
| H | 4.481177 | 0.967135 | 0.810840 | C | 0.221637 | -2.345658 | 1.259536 |
| O | -2.909575 | -0.674767 | -0.845469 | C | -0.019566 | -3.335278 | 2.398209 |
| C | -3.406119 | 0.066480 | -1.976913 | C | -0.624125 | -2.437791 | 3.504460 |
| C | -4.573595 | -0.771405 | -2.540769 | C | -1.129365 | -1.188660 | 2.740675 |
| C | -4.352828 | -2.183256 | -1.930095 | H | -0.556416 | -0.296799 | 3.013773 |
| C | -2.996933 | -2.060305 | -1.221655 | H | -2.199044 | -1.000009 | 2.868753 |
| H | -2.163481 | -2.302240 | -1.896294 | H | 0.136161 | -2.149602 | 4.236302 |
| H | -2.903659 | -2.649675 | -0.308178 | H | -1.429103 | -2.945340 | 4.044210 |
| H | -4.346607 | -2.975008 | -2.685105 | H | 0.898566 | -3.838852 | 2.715674 |
| H | -5.140744 | -2.417205 | -1.207371 | H | -0.737156 | -4.101897 | 2.085255 |
| H | -4.551619 | -0.786110 | -3.634484 | H | 0.227815 | -2.780907 | 0.258510 |
| H | -5.541177 | -0.361942 | -2.236263 | H | 1.138222 | -1.762471 | 1.413782 |

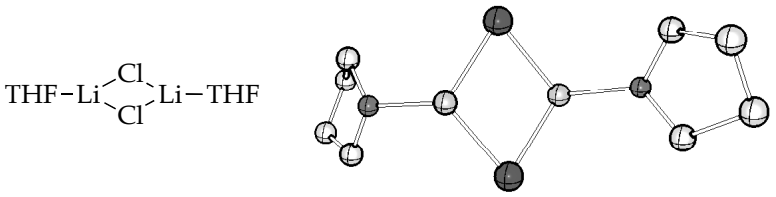
**Table 8 (Continued).**




**L**
$G$ = -2097.482363
$G_{MP2}$ = -2092.324568

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.645970 | -0.147008 | -0.040343 | H | -2.625812 | -1.494039 | -2.536674 |
| Cl | -0.091724 | 0.105549 | -1.764153 | H | -3.570044 | -2.349706 | -1.286694 |
| Li | 1.683314 | 0.007390 | -0.207878 | H | -4.648472 | -1.507463 | -3.786670 |
| Cl | 1.131884 | 0.172049 | 2.018032 | H | -5.649012 | -1.752078 | -2.352998 |
| O | 2.797808 | -1.647805 | -0.462347 | H | -5.081447 | 0.839031 | -3.586160 |
| C | 3.532934 | -1.814784 | -1.697075 | H | -5.954933 | 0.540331 | -2.079238 |
| C | 4.885199 | -2.443860 | -1.315640 | H | -4.027911 | 1.625590 | -1.101731 |
| C | 5.014032 | -2.099065 | 0.178284 | H | -2.975906 | 1.108417 | -2.449710 |
| C | 3.561482 | -2.183418 | 0.638831 | O | -1.623844 | -1.952134 | 0.820954 |
| H | 3.311028 | -1.589154 | 1.519984 | C | -1.890570 | -2.145614 | 2.223347 |
| H | 3.262481 | -3.227938 | 0.813949 | C | -1.700593 | -3.657417 | 2.474700 |
| H | 5.391446 | -1.078183 | 0.309177 | C | -0.878693 | -4.138677 | 1.247128 |
| H | 5.672762 | -2.782291 | 0.723377 | C | -0.522643 | -2.835871 | 0.519330 |
| H | 5.708272 | -2.054143 | -1.922238 | H | -0.456681 | -2.916681 | -0.566715 |
| H | 4.856532 | -3.531410 | -1.450647 | H | 0.400020 | -2.389038 | 0.905381 |
| H | 2.944887 | -2.439346 | -2.377254 | H | -1.488116 | -4.783888 | 0.605868 |
| H | 3.651113 | -0.823470 | -2.145946 | H | 0.015960 | -4.700668 | 1.532090 |
| O | 2.980903 | 1.487922 | -0.722441 | H | -2.661318 | -4.178068 | 2.531228 |
| C | 3.589086 | 2.272286 | 0.330466 | H | -1.174474 | -3.830615 | 3.418129 |
| C | 3.223537 | 3.749900 | 0.045643 | H | -1.173550 | -1.550427 | 2.801165 |
| C | 2.345541 | 3.681222 | -1.224372 | H | -2.906387 | -1.788991 | 2.412607 |
| C | 2.761823 | 2.351791 | -1.849809 | O | -2.066262 | 1.533927 | 0.966136 |
| H | 3.696076 | 2.452572 | -2.424655 | C | -1.243758 | 2.691534 | 0.713200 |
| H | 1.993736 | 1.884265 | -2.468171 | C | -1.905238 | 3.793620 | 1.543406 |
| H | 2.497591 | 4.532301 | -1.895678 | C | -2.405981 | 3.032352 | 2.797454 |
| H | 1.284379 | 3.637239 | -0.960090 | C | -2.332101 | 1.541848 | 2.385093 |
| H | 4.126248 | 4.343490 | -0.134208 | H | -3.267332 | 0.996516 | 2.538178 |
| H | 2.692543 | 4.204980 | 0.886565 | H | -1.511212 | 1.027591 | 2.896485 |
| H | 3.185013 | 1.891255 | 1.270708 | H | -3.422584 | 3.332867 | 3.068138 |
| H | 4.676016 | 2.116412 | 0.307812 | H | -1.764110 | 3.219263 | 3.663411 |
| O | -3.419588 | -0.326545 | -1.019539 | H | -2.747802 | 4.227577 | 0.994050 |
| C | -3.812606 | 0.815436 | -1.800408 | H | -1.209741 | 4.602331 | 1.788033 |
| C | -5.023540 | 0.335818 | -2.616295 | H | -0.222043 | 2.478893 | 1.050303 |
| C | -4.793529 | -1.195902 | -2.747904 | H | -1.246275 | 2.860674 | -0.365399 |
| C | -3.525685 | -1.454070 | -1.908567 | | | | |

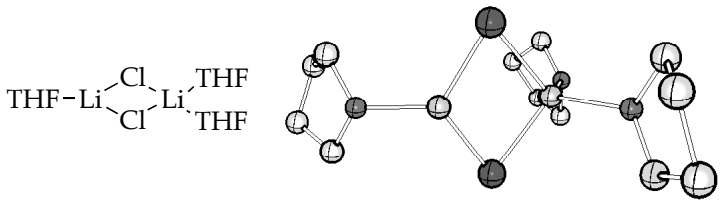
**Table 8 (Continued).**




**M**
$G$ = -1400.432963
$G_{MP2}$ = -1397.58876

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 1.224110 | 0.056448 | 0.583724 | H | -3.288569 | 1.815396 | 0.242365 |
| Cl | -0.000071 | 1.876521 | -0.000606 | H | -4.147110 | 1.720238 | -1.312896 |
| Li | -1.224402 | 0.056560 | -0.585074 | O | 3.114196 | 0.007075 | 0.737816 |
| Cl | -0.000216 | -1.771825 | -0.000681 | C | 3.828251 | -1.199145 | 0.369709 |
| O | -3.114591 | 0.006934 | -0.738054 | C | 4.735454 | -0.765170 | -0.776506 |
| C | -3.910617 | 1.177484 | -0.392669 | C | 5.160538 | 0.644126 | -0.327247 |
| C | -5.160087 | 0.644226 | 0.328488 | C | 3.910614 | 1.177530 | 0.393033 |
| C | -4.734737 | -0.765017 | 0.777665 | H | 3.289078 | 1.815532 | -0.242408 |
| C | -3.828352 | -1.199229 | -0.369104 | H | 4.146524 | 1.720236 | 1.313440 |
| H | -4.406690 | -1.551196 | -1.233802 | H | 5.459273 | 1.286858 | -1.160093 |
| H | -3.079620 | -1.949348 | -0.104241 | H | 6.005729 | 0.580776 | 0.367289 |
| H | -5.581491 | -1.441894 | 0.924423 | H | 4.164149 | -0.721081 | -1.710744 |
| H | -4.162781 | -0.720783 | 1.711499 | H | 5.582288 | -1.442100 | -0.922561 |
| H | -6.005723 | 0.580789 | -0.365500 | H | 4.405994 | -1.550881 | 1.234903 |
| H | -5.458268 | 1.287081 | 1.161437 | H | 3.079750 | -1.949374 | 0.104494 |

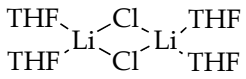
**Table 8 (Continued).**

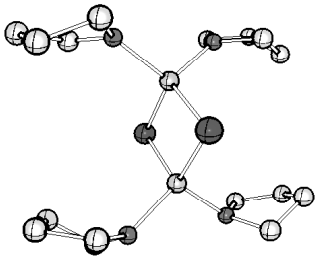



**N**
$G$ = -1632.79084
$G_{MP2}$ = -1629.174087

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.263759 | 0.257486 | -0.059976 | H | -2.520828 | -1.421331 | 1.882389 |
| Cl | 0.121472 | -0.564014 | -1.831186 | H | -4.220699 | -0.938594 | 1.639370 |
| Li | 1.211897 | -1.051697 | 0.075573 | H | -3.247450 | -3.650454 | 1.360859 |
| Cl | 0.083053 | -0.270455 | 1.851823 | H | -4.812599 | -3.050037 | 0.802190 |
| O | 3.064641 | -1.492822 | 0.088890 | H | -2.212313 | -3.253565 | -0.793013 |
| C | 3.880562 | -1.220161 | 1.262295 | H | -3.860028 | -3.622497 | -1.344036 |
| C | 5.194280 | -0.606732 | 0.738930 | H | -4.422917 | -1.219940 | -1.404551 |
| C | 4.855791 | -0.210999 | -0.710601 | H | -2.726570 | -1.207424 | -1.985669 |
| C | 3.853177 | -1.289784 | -1.106463 | O | -1.511893 | 2.204156 | -0.211716 |
| H | 4.353428 | -2.230753 | -1.373937 | C | -0.886485 | 2.948570 | -1.279686 |
| H | 3.160525 | -1.008265 | -1.902861 | C | 0.054274 | 3.916847 | -0.569347 |
| H | 5.733163 | -0.188094 | -1.363779 | C | -0.769698 | 4.302819 | 0.671314 |
| H | 4.376209 | 0.773901 | -0.744160 | C | -1.533308 | 3.007104 | 0.998699 |
| H | 5.996513 | -1.352778 | 0.749976 | H | -2.576251 | 3.190608 | 1.279062 |
| H | 5.521250 | 0.242244 | 1.345846 | H | -1.048099 | 2.418595 | 1.782791 |
| H | 3.306177 | -0.541019 | 1.898644 | H | -1.467420 | 5.111604 | 0.425230 |
| H | 4.039767 | -2.158363 | 1.803567 | H | -0.151812 | 4.637322 | 1.509696 |
| O | -2.957146 | -0.741652 | -0.002565 | H | 0.326175 | 4.776261 | -1.190075 |
| C | -3.383956 | -1.486822 | -1.160074 | H | 0.972849 | 3.395566 | -0.276736 |
| C | -3.260956 | -2.944672 | -0.728085 | H | -0.391052 | 2.224541 | -1.929840 |
| C | -3.730451 | -2.891080 | 0.739410 | H | -1.659779 | 3.484115 | -1.849317 |
| C | -3.365629 | -1.458504 | 1.190920 | | | | |

**Table 8 (Continued).**

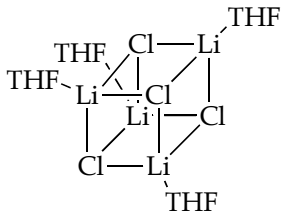


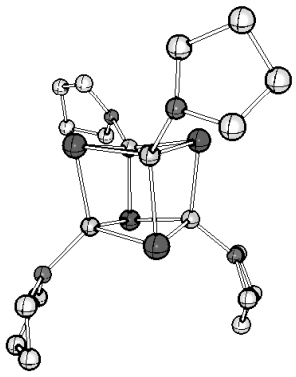



**O**
$G$ = -1865.144982
$G_{MP2}$ = -1860.758608

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 0.032551 | -1.524063 | 0.022267 | H | 2.632291 | 3.481070 | 1.528251 |
| Cl | 0.079285 | -0.094857 | 1.893780 | H | 2.302701 | 1.731682 | 1.694753 |
| Li | -0.041459 | 1.384887 | 0.065541 | O | -1.513441 | -2.762613 | 0.060842 |
| Cl | -0.100281 | -0.046379 | -1.805635 | C | -2.066179 | -3.166078 | -1.204530 |
| O | -1.659752 | 2.524905 | 0.169501 | C | -3.333512 | -2.325918 | -1.339722 |
| C | -2.376416 | 2.652219 | 1.413201 | C | -3.864923 | -2.283411 | 0.110839 |
| C | -3.765679 | 2.101625 | 1.105821 | C | -2.610703 | -2.552404 | 0.978849 |
| C | -4.003681 | 2.618518 | -0.324504 | H | -2.732094 | -3.451559 | 1.596123 |
| C | -2.588487 | 2.636821 | -0.938565 | H | -2.322910 | -1.717389 | 1.620997 |
| H | -2.383153 | 3.567264 | -1.480506 | H | -4.619770 | -3.059602 | 0.275947 |
| H | -2.392551 | 1.791142 | -1.603086 | H | -4.327693 | -1.320905 | 0.348419 |
| H | -4.424670 | 3.629912 | -0.296153 | H | -4.053071 | -2.753356 | -2.045043 |
| H | -4.691954 | 1.989197 | -0.896468 | H | -3.056496 | -1.325203 | -1.685044 |
| H | -4.525293 | 2.440538 | 1.817065 | H | -1.313754 | -2.962190 | -1.969036 |
| H | -3.738314 | 1.006362 | 1.125248 | H | -2.286305 | -4.244108 | -1.181877 |
| H | -1.821863 | 2.085588 | 2.164097 | O | 1.651191 | -2.660923 | -0.054328 |
| H | -2.419129 | 3.711881 | 1.705779 | C | 2.671173 | -2.457932 | -1.062610 |
| O | 1.527444 | 2.591616 | 0.002541 | C | 4.007685 | -2.278070 | -0.305880 |
| C | 2.574811 | 2.522423 | 0.992288 | C | 3.582414 | -2.178369 | 1.173112 |
| C | 3.846763 | 2.259184 | 0.190187 | C | 2.290921 | -2.990889 | 1.192357 |
| C | 3.602142 | 3.105054 | -1.070741 | H | 1.603337 | -2.713556 | 1.993774 |
| C | 2.083347 | 2.979900 | -1.280405 | H | 2.488310 | -4.072656 | 1.230171 |
| H | 1.816923 | 2.197699 | -1.997660 | H | 3.355183 | -1.143100 | 1.447866 |
| H | 1.620684 | 3.922653 | -1.592162 | H | 4.339516 | -2.563932 | 1.863002 |
| H | 4.167602 | 2.756690 | -1.940112 | H | 4.555139 | -1.393266 | -0.644712 |
| H | 3.882381 | 4.148390 | -0.884606 | H | 4.657643 | -3.146144 | -0.461540 |
| H | 3.914083 | 1.195248 | -0.065491 | H | 2.691494 | -3.330680 | -1.726498 |
| H | 4.755287 | 2.542671 | 0.730585 | H | 2.368509 | -1.581724 | -1.640600 |

**Table 8 (Continued).**

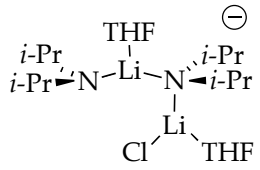


**P**
$G$ = -2800.897208
$G_{MP2}$ = -2795.229129

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | 0.485646 | -1.117847 | 1.156965 | H | -0.196529 | 5.228972 | 0.561741 |
| Cl | 0.679319 | -1.786881 | -1.135521 | H | -0.567354 | 6.169025 | 2.023413 |
| Li | -1.567669 | -0.957524 | -1.052778 | H | -1.265891 | 4.138158 | 3.223286 |
| Cl | -1.849460 | -0.735402 | 1.347813 | H | 0.116353 | 3.516848 | 2.272921 |
| Li | -1.090489 | 1.441055 | 0.757779 | O | -2.991248 | -2.074226 | -1.726702 |
| Cl | -1.269625 | 1.320005 | -1.639666 | C | -4.344334 | -1.621542 | -1.442615 |
| Li | 0.977393 | 0.617485 | -1.283952 | C | -5.123633 | -2.865044 | -0.990229 |
| Cl | 1.298108 | 1.159241 | 1.029019 | C | -4.009715 | -3.798675 | -0.487551 |
| O | 2.434591 | 1.073452 | -2.456532 | C | -2.885996 | -3.495776 | -1.473753 |
| C | 3.632758 | 1.742328 | -1.983476 | H | -3.017893 | -4.036094 | -2.421140 |
| C | 4.757499 | 1.317201 | -2.937334 | H | -1.880078 | -3.687199 | -1.092226 |
| C | 4.245887 | -0.024125 | -3.488524 | H | -4.298593 | -4.854236 | -0.488966 |
| C | 2.744957 | 0.232546 | -3.592756 | H | -3.701231 | -3.518105 | 0.525205 |
| H | 2.129559 | -0.666429 | -3.512577 | H | -5.649713 | -3.320839 | -1.837331 |
| H | 2.487169 | 0.770672 | -4.514664 | H | -5.863920 | -2.627077 | -0.221037 |
| H | 4.439325 | -0.834717 | -2.776539 | H | -4.279589 | -0.867601 | -0.651393 |
| H | 4.694145 | -0.294812 | -4.449222 | H | -4.749612 | -1.159153 | -2.347543 |
| H | 5.721559 | 1.235187 | -2.426708 | O | 1.493622 | -2.188849 | 2.400605 |
| H | 4.868132 | 2.043389 | -3.751053 | C | 1.919193 | -1.604663 | 3.661087 |
| H | 3.450504 | 2.821312 | -1.984784 | C | 3.217816 | -2.328010 | 4.044208 |
| H | 3.809717 | 1.418301 | -0.952784 | C | 3.744758 | -2.821407 | 2.686244 |
| O | -1.728986 | 3.122218 | 1.464646 | C | 2.449878 | -3.181011 | 1.962129 |
| C | -0.859803 | 4.002432 | 2.210897 | H | 2.089146 | -4.177176 | 2.252705 |
| C | -0.871817 | 5.307517 | 1.421220 | H | 2.503291 | -3.124811 | 0.872523 |
| C | -2.337082 | 5.381336 | 0.957817 | H | 4.428481 | -3.671499 | 2.771465 |
| C | -2.705147 | 3.905492 | 0.724565 | H | 4.262341 | -2.013168 | 2.156761 |
| H | -2.625896 | 3.608908 | -0.325190 | H | 3.006439 | -3.180105 | 4.700741 |
| H | -3.705203 | 3.654362 | 1.092923 | H | 3.918120 | -1.668011 | 4.564384 |
| H | -2.470544 | 5.984293 | 0.055064 | H | 2.072108 | -0.533747 | 3.491745 |
| H | -2.962401 | 5.815243 | 1.746510 | H | 1.116457 | -1.740164 | 4.392060 |

**Table 8 (Continued).**

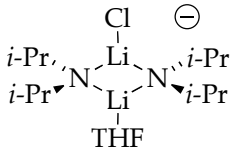


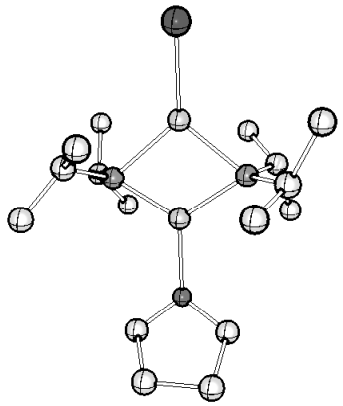

**30**
$G$ = -1523.430812
$G_{MP2}$ = -1519.042557

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.940275 | -0.992163 | -0.318219 | C | 5.174999 | -1.255140 | 0.360461 |
| N | 1.156792 | 2.004180 | -0.145390 | C | 5.219053 | 0.244615 | -0.049563 |
| C | 1.289829 | 2.886835 | 0.997919 | C | 3.962379 | 0.422358 | -0.919395 |
| C | 2.294392 | 2.314662 | 2.012573 | H | 4.195119 | 0.249910 | -1.983654 |
| H | 3.293617 | 2.240091 | 1.566968 | H | 3.419929 | 1.364548 | -0.799458 |
| H | 2.365379 | 2.936852 | 2.916131 | H | 6.132778 | 0.507410 | -0.593525 |
| H | 1.993946 | 1.306189 | 2.327266 | H | 5.161012 | 0.885795 | 0.835539 |
| C | -0.049175 | 3.187729 | 1.724494 | H | 6.036387 | -1.820516 | -0.011918 |
| H | -0.468398 | 2.265796 | 2.144919 | H | 5.157497 | -1.360883 | 1.449957 |
| H | 0.073592 | 3.919851 | 2.539079 | H | 3.288781 | -2.444035 | 0.374292 |
| H | -0.785022 | 3.598185 | 1.022445 | H | 4.041705 | -2.254569 | -1.229297 |
| H | 1.696742 | 3.882452 | 0.710269 | C | 0.628430 | 2.690489 | -1.309036 |
| Li | 1.052586 | 0.029062 | -0.011853 | C | 0.159704 | 1.676320 | -2.361837 |
| N | -0.125715 | -1.648400 | 0.324822 | H | -0.628301 | 1.025306 | -1.964818 |
| C | -0.224951 | -2.051587 | 1.733329 | H | -0.233244 | 2.168274 | -3.261772 |
| C | 1.029559 | -2.749189 | 2.316646 | H | 0.995368 | 1.033726 | -2.672994 |
| H | 1.902050 | -2.083975 | 2.246401 | C | 1.633547 | 3.663380 | -1.987775 |
| H | 0.879999 | -2.999083 | 3.376630 | H | 2.476701 | 3.100643 | -2.411466 |
| H | 1.271565 | -3.680462 | 1.792390 | H | 1.163412 | 4.237498 | -2.801422 |
| C | -0.539049 | -0.834165 | 2.615821 | H | 2.040993 | 4.384950 | -1.269797 |
| H | -1.404036 | -0.279657 | 2.241575 | H | -0.264891 | 3.314034 | -1.066650 |
| H | -0.739181 | -1.140680 | 3.652244 | O | -3.058000 | 0.398904 | 0.709225 |
| H | 0.309959 | -0.138645 | 2.633850 | C | -3.324410 | 1.572571 | -0.096280 |
| H | -1.057746 | -2.772197 | 1.896784 | C | -4.839922 | 1.603017 | -0.293694 |
| C | 0.244166 | -2.767818 | -0.558210 | C | -5.346399 | 0.962663 | 1.007899 |
| C | -0.731112 | -3.970489 | -0.532694 | C | -4.294309 | -0.123154 | 1.248939 |
| H | -1.730421 | -3.662561 | -0.865404 | H | -4.542073 | -1.042513 | 0.706729 |
| H | -0.380955 | -4.768366 | -1.203513 | H | -4.130495 | -0.348393 | 2.308418 |
| H | -0.821259 | -4.405059 | 0.470381 | H | -6.355435 | 0.546398 | 0.920769 |
| C | 0.376071 | -2.270481 | -2.006656 | H | -5.345380 | 1.693865 | 1.826646 |
| H | 1.119861 | -1.468541 | -2.081315 | H | -5.103853 | 0.973537 | -1.148869 |
| H | 0.696982 | -3.085479 | -2.670234 | H | -5.220803 | 2.617088 | -0.457297 |
| H | -0.583576 | -1.895822 | -2.383233 | H | -2.953074 | 2.451523 | 0.445200 |

**Table 8 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.238809 | -3.182141 | -0.288835 | H | -2.775198 | 1.472268 | -1.035186 |
| O | 3.060628 | -0.595886 | -0.464355 | Cl | -3.477198 | -1.529859 | -1.898789 |
| C | 3.855205 | -1.762667 | -0.261202 | | | | |



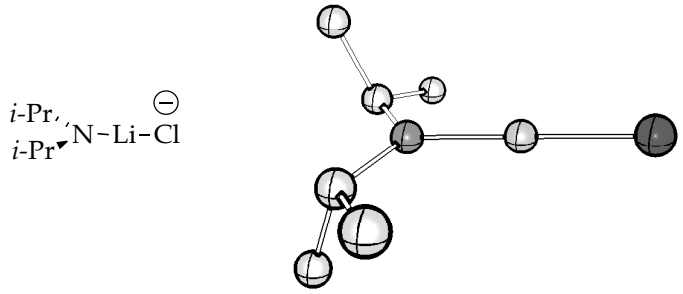



**Q**
$G$ = -1291.089569
$G_{MP2}$ = -1287.473699

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.875668 | -0.000879 | -0.247326 | C | -1.996111 | -1.704697 | 2.117327 |
| N | -0.491629 | 1.698042 | 0.121140 | H | -2.897181 | -1.469112 | 1.538476 |
| C | -0.628084 | 2.625046 | -1.002131 | H | -2.293234 | -2.308381 | 2.987036 |
| C | -0.894549 | 1.891635 | -2.322853 | H | -1.585141 | -0.762903 | 2.503539 |
| H | -1.826115 | 1.315320 | -2.279414 | H | -1.469770 | -3.373992 | 0.924549 |
| H | -0.979356 | 2.600920 | -3.157977 | O | 2.515510 | -0.050533 | 0.584129 |
| H | -0.064790 | 1.210299 | -2.556016 | C | 3.341578 | -1.216145 | 0.465095 |
| C | 0.603561 | 3.549626 | -1.197487 | C | 4.376419 | -0.885166 | -0.635967 |
| H | 1.465430 | 2.957696 | -1.539123 | C | 4.280252 | 0.658223 | -0.788348 |
| H | 0.417175 | 4.333488 | -1.948144 | C | 3.373819 | 1.076756 | 0.378259 |
| H | 0.886265 | 4.049070 | -0.262680 | H | 2.731823 | 1.935102 | 0.176698 |
| H | -1.495567 | 3.300162 | -0.848528 | H | 3.959897 | 1.262549 | 1.292627 |
| Li | 0.515878 | 0.013858 | 0.272285 | H | 3.806752 | 0.921526 | -1.739231 |
| N | -0.564517 | -1.645555 | 0.081369 | H | 5.256619 | 1.152310 | -0.750814 |
| C | -0.265472 | -2.520464 | -1.052414 | H | 4.128242 | -1.387592 | -1.575229 |
| C | -1.519517 | -3.144125 | -1.714833 | H | 5.380107 | -1.209709 | -0.341801 |
| H | -2.174246 | -2.353383 | -2.099431 | H | 3.835740 | -1.406557 | 1.429386 |
| H | -1.247083 | -3.820167 | -2.540658 | H | 2.681495 | -2.052824 | 0.234728 |
| H | -2.106479 | -3.725052 | -0.995115 | C | -0.706469 | 2.414487 | 1.384142 |
| C | 0.520149 | -1.768507 | -2.138741 | C | 0.121469 | 1.810355 | 2.532699 |
| H | 1.451553 | -1.341452 | -1.742734 | H | 1.195835 | 1.892206 | 2.326476 |
| H | 0.782567 | -2.430554 | -2.975069 | H | -0.083252 | 2.313659 | 3.488171 |
| H | -0.080005 | -0.946162 | -2.544136 | H | -0.111027 | 0.746573 | 2.674519 |
| H | 0.380894 | -3.374883 | -0.741055 | C | -2.195290 | 2.491091 | 1.796988 |
| C | -0.968075 | -2.441569 | 1.244436 | H | -2.585459 | 1.495037 | 2.039616 |

**Table 8 (Continued).**

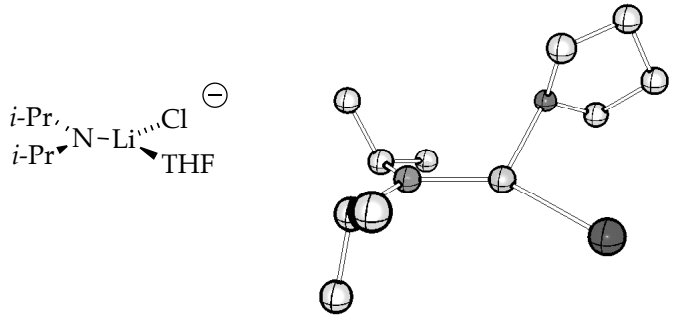
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.232738 | -2.890795 | 2.114752 | H | -2.346962 | 3.140770 | 2.673927 |
| H | 0.726438 | -2.017059 | 2.563248 | H | -2.804636 | 2.878125 | 0.973802 |
| H | -0.068943 | -3.565943 | 2.931145 | H | -0.361631 | 3.465183 | 1.300349 |
| H | 0.975731 | -3.421010 | 1.504936 | Cl | -4.011287 | 0.018832 | -0.951594 |




**32**
$G$ = -759.521337
$G_{MP2}$ = -757.793267

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.291509 | 1.197901 | 0.158166 | H | -0.438698 | -2.519497 | -0.190255 |
| N | 0.500585 | -0.000009 | -0.000101 | H | 2.164322 | -1.040352 | -0.834253 |
| Li | -1.380691 | -0.000102 | -0.000067 | C | 0.446290 | 2.306271 | 0.806056 |
| Cl | -3.567016 | -0.000282 | -0.000042 | H | 0.095684 | 1.990739 | 1.795905 |
| C | 1.291932 | -1.197657 | -0.158029 | H | 1.006538 | 3.246021 | 0.914576 |
| C | 1.883062 | -1.725703 | 1.176791 | H | -0.439509 | 2.519247 | 0.189403 |
| H | 1.068497 | -2.024639 | 1.850050 | C | 1.883128 | 1.726049 | -1.176386 |
| H | 2.549293 | -2.591136 | 1.028364 | H | 1.068801 | 2.024642 | -1.850087 |
| H | 2.462081 | -0.944277 | 1.683857 | H | 2.548970 | 2.591734 | -1.027691 |
| C | 0.447381 | -2.306257 | -0.806414 | H | 2.462687 | 0.944795 | -1.683095 |
| H | 0.097218 | -1.990786 | -1.796438 | H | 2.163596 | 1.040886 | 0.834845 |
| H | 1.007960 | -3.245842 | -0.914655 | | | | |

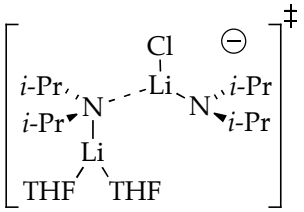
**Table 8 (Continued).**

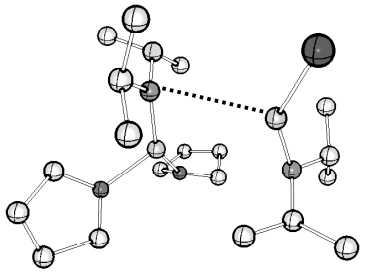



**R**
$G$ = -991.864401
$G_{MP2}$ = -989.363875

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 2.263088 | -1.415273 | -0.455439 | C | 3.600589 | 1.457332 | -0.464303 |
| N | 1.733926 | -0.147812 | -0.011409 | H | 2.963089 | 2.162704 | -1.012523 |
| Li | -0.013959 | 0.522737 | -0.373476 | H | 4.433269 | 2.019020 | -0.008485 |
| Cl | -1.282097 | 2.391671 | -0.757805 | H | 4.030797 | 0.759430 | -1.193685 |
| O | -1.629948 | -0.839192 | -0.085256 | C | 2.109799 | 1.706726 | 1.550924 |
| C | -2.755784 | -0.685464 | -0.977602 | H | 1.611429 | 1.181815 | 2.375702 |
| C | -3.910009 | -0.160191 | -0.119181 | H | 2.852490 | 2.398371 | 1.976203 |
| C | -3.573133 | -0.733747 | 1.265841 | H | 1.352004 | 2.305640 | 1.027764 |
| C | -2.047130 | -0.618914 | 1.277477 | H | 3.473580 | 0.101576 | 1.191656 |
| H | -1.544618 | -1.359762 | 1.906632 | C | 1.384566 | -2.014976 | -1.566745 |
| H | -1.734583 | 0.387549 | 1.584254 | H | 1.356419 | -1.340673 | -2.432034 |
| H | -3.883213 | -1.784747 | 1.339564 | H | 1.750724 | -2.997292 | -1.901077 |
| H | -4.038278 | -0.181089 | 2.089293 | H | 0.356669 | -2.142450 | -1.203159 |
| H | -4.891550 | -0.471449 | -0.494640 | C | 2.407350 | -2.455141 | 0.690613 |
| H | -3.861281 | 0.932870 | -0.096623 | H | 1.414954 | -2.709109 | 1.087030 |
| H | -2.472047 | 0.018624 | -1.763562 | H | 2.899899 | -3.385738 | 0.361194 |
| H | -2.981529 | -1.669414 | -1.414851 | H | 2.998419 | -2.039717 | 1.516049 |
| C | 2.748924 | 0.693995 | 0.585798 | H | 3.283434 | -1.310639 | -0.893966 |

**Table 8 (Continued).**



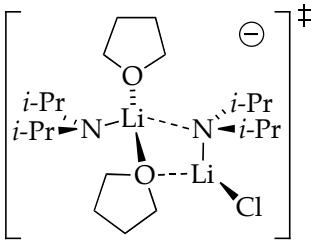
**S**
$G$ = -1523.406885
$G_{MP2}$ = -1519.015314
$\Delta G^{‡}$ = 20.1 kcal/mol*
$\Delta G_{MP2}{}^{‡}$ = 17.7 kcal/mol*

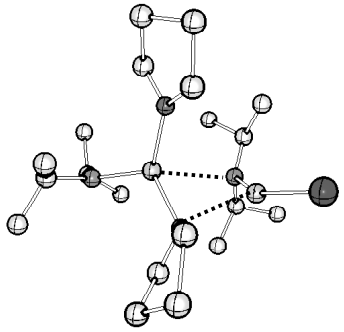
* Activation barrier is measured relative to the ground state energy of open disolvated triple ion xx.

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.776906 | 2.538051 | 0.232587 | H | 0.317279 | 0.559410 | 4.132115 |
| N | 1.227796 | 1.397912 | 0.953630 | H | -0.602377 | 0.361838 | 2.619612 |
| Li | 1.171507 | -0.333737 | 0.205339 | H | 0.656643 | 2.497901 | 2.684432 |
| O | 2.861143 | -0.986656 | -0.777676 | C | 1.259722 | 3.931913 | 0.659149 |
| C | 4.069983 | -0.224680 | -0.561744 | H | 1.552952 | 4.185500 | 1.684987 |
| C | 4.628696 | 0.039880 | -1.958796 | H | 1.680283 | 4.707280 | 0.002944 |
| C | 4.242732 | -1.250069 | -2.702069 | H | 0.166452 | 3.976498 | 0.588718 |
| C | 2.876355 | -1.591502 | -2.088965 | C | 1.492798 | 2.371187 | -1.270152 |
| H | 2.709029 | -2.668654 | -1.982884 | H | 0.420814 | 2.491623 | -1.466647 |
| H | 2.048721 | -1.168413 | -2.669927 | H | 2.032160 | 3.119730 | -1.868126 |
| H | 4.969277 | -2.043825 | -2.488112 | H | 1.793532 | 1.376492 | -1.626697 |
| H | 4.189466 | -1.126622 | -3.788305 | H | 2.894817 | 2.603403 | 0.324985 |
| H | 5.707275 | 0.227739 | -1.952048 | Li | -2.055355 | 1.533886 | -0.220696 |
| H | 4.130176 | 0.906867 | -2.405022 | N | -2.753862 | -0.223038 | -0.697244 |
| H | 3.788068 | 0.667078 | 0.000134 | C | -2.635554 | -0.696075 | -2.063530 |
| H | 4.768912 | -0.827262 | 0.037735 | C | -1.201724 | -0.451214 | -2.563165 |
| O | 0.522265 | -2.198400 | 0.472971 | H | -0.474681 | -0.940094 | -1.902114 |
| C | 1.289193 | -3.150901 | 1.217106 | H | -1.053454 | -0.839319 | -3.581058 |
| C | 0.372771 | -3.638338 | 2.365435 | H | -0.975042 | 0.623379 | -2.578056 |
| C | -1.033352 | -3.113844 | 1.967299 | C | -3.621841 | -0.052501 | -3.072290 |
| C | -0.852830 | -2.646399 | 0.520852 | H | -3.485571 | 1.036591 | -3.088161 |
| H | -1.493153 | -1.803580 | 0.208507 | H | -3.470193 | -0.441444 | -4.090788 |
| H | -0.968312 | -3.485116 | -0.184202 | H | -4.664486 | -0.250115 | -2.798266 |
| H | -1.318655 | -2.265130 | 2.595911 | H | -2.796847 | -1.798092 | -2.151067 |
| H | -1.811714 | -3.877723 | 2.059259 | C | -4.061381 | -0.451493 | -0.099042 |
| H | 0.690487 | -3.229995 | 3.329577 | C | -4.480442 | -1.940574 | 0.030269 |
| H | 0.398882 | -4.730718 | 2.444580 | H | -3.804611 | -2.480382 | 0.707613 |
| H | 1.570587 | -3.984649 | 0.555303 | H | -5.500771 | -2.032044 | 0.430915 |
| H | 2.201612 | -2.652643 | 1.553672 | H | -4.461490 | -2.454486 | -0.938331 |

**Table 8 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.190306 | 1.571874 | 2.394059 | C | -4.104179 | 0.197540 | 1.293993 |
| C | 2.589746 | 1.661021 | 3.058152 | H | -3.942765 | 1.281275 | 1.230549 |
| H | 3.185798 | 2.470682 | 2.620304 | H | -5.073796 | 0.036714 | 1.785606 |
| H | 2.523933 | 1.845859 | 4.141265 | H | -3.321779 | -0.229227 | 1.937884 |
| H | 3.141706 | 0.721412 | 2.903560 | H | -4.881168 | 0.030995 | -0.677561 |
| C | 0.405496 | 0.424573 | 3.045471 | Cl | -2.547082 | 3.683872 | -0.173796 |
| H | 0.908724 | -0.539371 | 2.873054 | | | | |



**31**
$G$ = -1523.421283
$G_{MP2}$ = -1519.035557
$\Delta G^{‡}$ = 11.1 kcal/mol*
$\Delta G_{MP2}{}^{‡}$ = 5.0 kcal/mol*

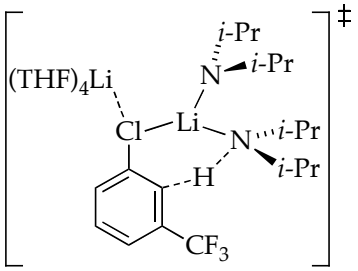
* Activation barrier is measured relative to the ground state energy of open disolvated triple ion xx.

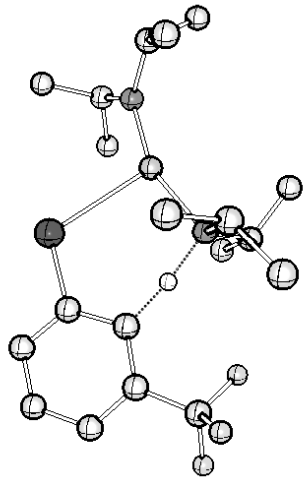
| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 2.482956 | 2.180137 | -1.350140 | Li | -0.612649 | 0.201313 | 0.011151 |
| N | 2.154939 | 1.281835 | -0.249863 | N | -2.379643 | 0.965791 | -0.310221 |
| Li | 2.263919 | -0.620748 | -0.502218 | C | -2.602859 | 2.404053 | -0.346994 |
| O | 0.045637 | -1.327991 | -1.345638 | H | -3.534722 | 2.655735 | -0.897405 |
| C | -0.076458 | -2.766982 | -1.166597 | C | -2.775486 | 3.030891 | 1.062547 |
| C | -0.280434 | -3.331638 | -2.568903 | H | -3.553723 | 2.502639 | 1.628135 |
| C | -1.108305 | -2.224515 | -3.237533 | H | -1.836793 | 2.955094 | 1.626506 |
| C | -0.486540 | -0.954025 | -2.654489 | H | -3.060607 | 4.094308 | 1.018350 |
| H | -1.202433 | -0.142065 | -2.491751 | C | -1.469275 | 3.124587 | -1.090531 |
| H | 0.348173 | -0.600611 | -3.265948 | H | -1.440655 | 2.808223 | -2.139949 |
| H | -2.162311 | -2.306106 | -2.946064 | H | -1.590481 | 4.217332 | -1.062742 |
| H | -1.056745 | -2.239736 | -4.331563 | H | -0.496707 | 2.884108 | -0.643852 |
| H | -0.783022 | -4.304910 | -2.555522 | C | -3.640138 | 0.254535 | -0.221829 |
| H | 0.688135 | -3.451020 | -3.068589 | H | -4.338361 | 0.737787 | 0.502428 |
| H | 0.838403 | -3.111027 | -0.680430 | C | -3.448836 | -1.183764 | 0.283604 |
| H | -0.949513 | -2.966201 | -0.531994 | H | -2.793021 | -1.741017 | -0.397754 |
| Cl | 3.254689 | -2.596275 | -0.175605 | H | -2.981755 | -1.196634 | 1.273866 |
| C | 2.577607 | 1.842529 | 1.030518 | H | -4.404002 | -1.724303 | 0.341283 |

**Table 8 (Continued).**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.554006 | 2.362034 | 0.941275 | C | -4.422235 | 0.193172 | -1.564238 |
| C | 1.600979 | 2.900993 | 1.600239 | H | -5.419870 | -0.259455 | -1.445023 |
| H | 1.407359 | 3.694654 | 0.869494 | H | -4.562225 | 1.194696 | -1.986551 |
| H | 0.635957 | 2.437972 | 1.843960 | H | -3.861237 | -0.400590 | -2.298903 |
| H | 1.994996 | 3.376651 | 2.512417 | O | -0.359192 | -0.755229 | 1.848781 |
| C | 2.794089 | 0.734357 | 2.071422 | C | 0.134696 | -2.058289 | 2.240259 |
| H | 3.572163 | 0.034531 | 1.744831 | C | 0.130224 | -2.053697 | 3.769824 |
| H | 3.085970 | 1.146555 | 3.048101 | C | -1.061601 | -1.134978 | 4.081771 |
| H | 1.867346 | 0.165494 | 2.207605 | C | -0.932323 | -0.073116 | 2.987116 |
| H | 2.138052 | 3.219206 | -1.150685 | H | -0.248329 | 0.729151 | 3.291587 |
| C | 1.780268 | 1.743725 | -2.640625 | H | -1.875965 | 0.372248 | 2.664005 |
| H | 2.005729 | 2.425282 | -3.472336 | H | -1.028714 | -0.701943 | 5.087017 |
| H | 2.122004 | 0.741174 | -2.939629 | H | -2.005821 | -1.683872 | 3.976740 |
| H | 0.696172 | 1.711637 | -2.504260 | H | 1.060240 | -1.615838 | 4.150274 |
| C | 4.002780 | 2.285335 | -1.652535 | H | 0.029502 | -3.060431 | 4.188557 |
| H | 4.210184 | 3.024332 | -2.441979 | H | -0.550317 | -2.821670 | 1.847580 |
| H | 4.576890 | 2.581675 | -0.767970 | H | 1.123345 | -2.207645 | 1.796360 |
| H | 4.385910 | 1.310045 | -1.982880 | | | | |

**Table 8 (Continued).**

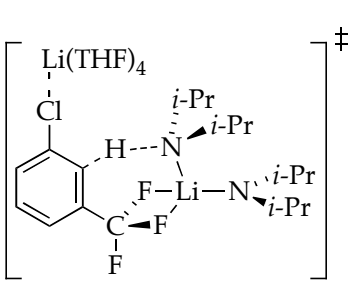


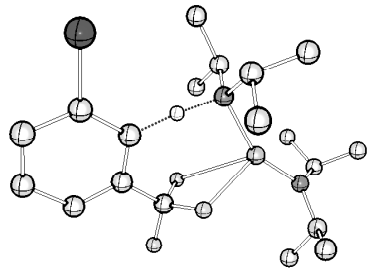



**T**
$G$ = -1619.659781
$G_{MP2}$ = -1615.331737
(calculation does not include $Li(THF)_4^+$ ion)

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 0.060727 | -2.013382 | 1.167439 | H | -0.915399 | -0.443616 | -2.495034 |
| N | -0.036174 | -1.226121 | -0.071550 | C | 1.218349 | -2.983723 | -1.433805 |
| Li | -1.707462 | -0.067164 | -0.020452 | H | 2.162376 | -2.431522 | -1.397084 |
| N | -3.552859 | 0.327947 | 0.131311 | H | 1.238369 | -3.731041 | -0.632587 |
| C | -4.095204 | 1.416629 | 0.918751 | H | 1.175650 | -3.528023 | -2.387563 |
| H | -5.055978 | 1.133218 | 1.404776 | H | 1.004486 | -2.587070 | 1.204265 |
| C | -4.407368 | 2.683730 | 0.078473 | C | 0.091485 | -1.054973 | 2.368470 |
| H | -5.058987 | 2.436946 | -0.768500 | H | 0.213472 | -1.610414 | 3.308028 |
| H | -4.909466 | 3.467255 | 0.669196 | H | 0.919874 | -0.345726 | 2.282386 |
| H | -3.476469 | 3.099543 | -0.328392 | H | -0.843684 | -0.483336 | 2.440480 |
| C | -3.141338 | 1.794138 | 2.063789 | C | -1.084795 | -3.030409 | 1.351646 |
| H | -2.994939 | 0.941370 | 2.737410 | H | -1.101846 | -3.778627 | 0.550628 |
| H | -2.159458 | 2.085142 | 1.665815 | H | -0.977324 | -3.569979 | 2.303351 |
| H | -3.521182 | 2.641386 | 2.652734 | H | -2.056194 | -2.518885 | 1.354936 |
| C | -4.587742 | -0.405942 | -0.567135 | C | 3.291126 | 0.718573 | 0.097751 |
| H | -5.366062 | 0.273544 | -0.983767 | C | 1.902657 | 0.754527 | -0.143459 |
| C | -4.003343 | -1.163167 | -1.769471 | C | 1.425317 | 2.019499 | -0.462357 |
| H | -3.555811 | -0.463682 | -2.485591 | C | 2.195910 | 3.177849 | -0.559558 |
| H | -3.217202 | -1.857344 | -1.439632 | C | 3.566343 | 3.081656 | -0.318796 |
| H | -4.766672 | -1.756103 | -2.293402 | C | 4.118940 | 1.846678 | 0.012733 |
| C | -5.349869 | -1.411470 | 0.337709 | H | 5.183125 | 1.762296 | 0.211005 |
| H | -5.743236 | -0.911400 | 1.230739 | H | 4.194963 | 3.966458 | -0.384331 |
| H | -6.199421 | -1.883204 | -0.182440 | H | 1.738284 | 4.129902 | -0.814111 |
| H | -4.667644 | -2.203458 | 0.673919 | Cl | -0.337279 | 2.234272 | -0.780352 |
| C | 0.007080 | -2.032124 | -1.303359 | C | 3.949297 | -0.599173 | 0.414392 |
| H | -0.892742 | -2.674476 | -1.371487 | F | 4.198993 | -1.333516 | -0.706825 |
| C | -0.036352 | -1.097241 | -2.523273 | F | 3.211518 | -1.381926 | 1.228569 |
| H | 0.852100 | -0.456622 | -2.558012 | F | 5.159104 | -0.444687 | 1.024159 |
| H | -0.077327 | -1.675303 | -3.455883 | H | 0.999858 | -0.290017 | -0.095613 |

**Table 8 (Continued).**

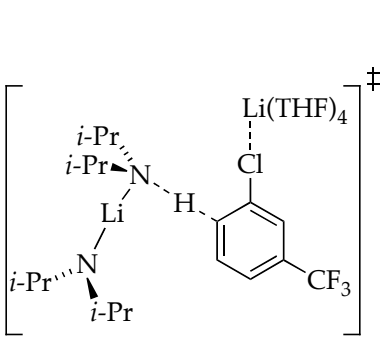


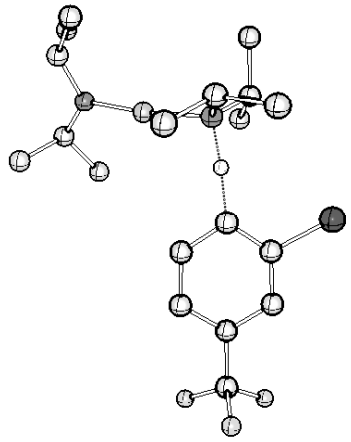



**10**
$G$ = -1619.663984
$G_{MP2}$ = -1615.334181
(calculation does not include $Li(THF)_4^+$ ion)

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -0.623252 | -2.109718 | -0.480839 | H | -0.364569 | 1.711072 | 3.401139 |
| F | -0.458024 | -3.452268 | -0.551905 | H | -1.054472 | 0.463649 | 2.343218 |
| F | 0.189831 | -1.682943 | 0.535875 | H | 0.706325 | 0.632872 | 2.492852 |
| Li | 1.411741 | 0.170956 | 0.045232 | C | 0.924972 | 3.184480 | 1.465743 |
| N | 3.261093 | -0.259004 | 0.112426 | H | 0.916098 | 3.978749 | 0.710491 |
| C | 3.838386 | -1.290861 | 0.952814 | H | 0.865331 | 3.667211 | 2.451492 |
| H | 4.902063 | -1.069534 | 1.190858 | H | 1.889112 | 2.664158 | 1.395079 |
| C | 3.838565 | -2.687060 | 0.274940 | C | -0.209207 | 2.317601 | -1.187305 |
| H | 4.320493 | -2.633762 | -0.708956 | H | 0.729236 | 2.903834 | -1.244051 |
| H | 4.369169 | -3.449433 | 0.869354 | C | -0.255561 | 1.454033 | -2.457256 |
| H | 2.805774 | -3.025803 | 0.121794 | H | -1.182816 | 0.871624 | -2.501386 |
| C | 3.120917 | -1.383814 | 2.309998 | H | -0.205813 | 2.083865 | -3.355422 |
| H | 3.187074 | -0.426978 | 2.840961 | H | 0.582978 | 0.752354 | -2.493663 |
| H | 2.058474 | -1.620534 | 2.170637 | C | -1.359022 | 3.349810 | -1.246257 |
| H | 3.550474 | -2.169705 | 2.948736 | H | -2.334927 | 2.852368 | -1.242648 |
| C | 4.249076 | 0.304742 | -0.783815 | H | -1.338391 | 4.041442 | -0.396862 |
| H | 4.939825 | -0.477469 | -1.175539 | H | -1.282506 | 3.952476 | -2.162145 |
| C | 3.582940 | 0.930726 | -2.017938 | H | -1.299906 | 0.584830 | -0.003008 |
| H | 3.027023 | 0.170204 | -2.579416 | C | -2.314774 | -0.336636 | 0.003766 |
| H | 2.873943 | 1.714166 | -1.715201 | C | -2.054642 | -1.696388 | -0.262701 |
| H | 4.316964 | 1.394410 | -2.692495 | C | -3.046996 | -2.681124 | -0.326532 |
| C | 5.155864 | 1.367298 | -0.106347 | C | -4.376581 | -2.320443 | -0.113606 |
| H | 5.622363 | 0.959563 | 0.798623 | C | -4.690992 | -0.992601 | 0.173274 |
| H | 5.963735 | 1.718252 | -0.769529 | C | -3.655886 | -0.056789 | 0.225705 |
| H | 4.551645 | 2.233802 | 0.193515 | Cl | -4.156628 | 1.622618 | 0.645010 |
| N | -0.190897 | 1.449348 | 0.002600 | H | -5.718547 | -0.691031 | 0.357528 |
| C | -0.237362 | 2.187692 | 1.275468 | H | -5.163904 | -3.068838 | -0.160200 |
| H | -1.175893 | 2.768305 | 1.364828 | H | -2.785688 | -3.714229 | -0.532627 |
| C | -0.240126 | 1.187735 | 2.443709 | F | -0.088752 | -1.595207 | -1.615185 |

**Table 8 (Continued).**

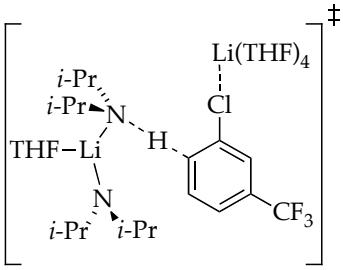


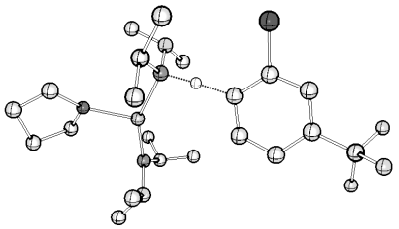



**U**
$G$ = -1619.663694
$G_{MP2}$ = -1615.330688
(calculation does not include $Li(THF)_4^+$ ion)

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -1.491079 | 2.499118 | -0.899219 | H | -1.398463 | 1.463873 | 3.632376 |
| N | -1.312434 | 1.558857 | 0.221351 | C | -0.456644 | 3.319443 | 1.843229 |
| Li | -2.421028 | -0.085776 | -0.009103 | H | -0.602546 | 4.154984 | 1.149673 |
| N | -3.621630 | -1.507209 | -0.131038 | H | -0.597487 | 3.706558 | 2.861701 |
| C | -3.255168 | -2.812076 | -0.641670 | H | 0.580905 | 2.983609 | 1.741416 |
| H | -4.047469 | -3.237901 | -1.297238 | H | -0.710953 | 3.282074 | -0.883118 |
| C | -1.993698 | -2.708565 | -1.512869 | C | -2.853692 | 3.216284 | -0.900957 |
| H | -1.668635 | -3.689194 | -1.886922 | H | -2.991488 | 3.849841 | -0.017517 |
| H | -2.170647 | -2.050817 | -2.372224 | H | -2.951111 | 3.859551 | -1.786027 |
| H | -1.157860 | -2.289052 | -0.933454 | H | -3.673661 | 2.485156 | -0.921093 |
| C | -3.016996 | -3.864767 | 0.471998 | C | -1.309179 | 1.728001 | -2.215432 |
| H | -3.885347 | -3.933828 | 1.137867 | H | -0.344618 | 1.211499 | -2.232218 |
| H | -2.829663 | -4.869950 | 0.062694 | H | -2.102809 | 0.977793 | -2.345074 |
| H | -2.152292 | -3.572660 | 1.082947 | H | -1.349521 | 2.407323 | -3.076743 |
| C | -5.005028 | -1.426700 | 0.286292 | C | 2.440158 | 1.137860 | -0.377292 |
| H | -5.322224 | -2.331207 | 0.852999 | C | 1.251915 | 0.562516 | 0.051401 |
| C | -6.000571 | -1.297023 | -0.896404 | C | 1.390320 | -0.767333 | 0.497556 |
| H | -5.831247 | -0.348440 | -1.423553 | C | 2.604289 | -1.455939 | 0.510045 |
| H | -5.858055 | -2.108076 | -1.620415 | C | 3.761264 | -0.809165 | 0.061773 |
| H | -7.050341 | -1.328173 | -0.563961 | C | 3.685366 | 0.512249 | -0.389897 |
| C | -5.205225 | -0.238303 | 1.239631 | H | 4.572447 | 1.025911 | -0.745511 |
| H | -4.591473 | -0.358792 | 2.140354 | C | 5.086094 | -1.500409 | 0.126554 |
| H | -4.903544 | 0.698752 | 0.748016 | F | 5.696676 | -1.351502 | 1.335133 |
| H | -6.254590 | -0.125535 | 1.545706 | F | 5.965880 | -1.031762 | -0.794851 |
| C | -1.440032 | 2.161748 | 1.561969 | F | 4.982804 | -2.838812 | -0.073628 |
| H | -2.458513 | 2.568374 | 1.696724 | H | 2.659640 | -2.485556 | 0.854063 |
| C | -1.262449 | 1.061083 | 2.620226 | H | 0.502443 | -1.294143 | 0.854087 |
| H | -1.993437 | 0.254177 | 2.481238 | Cl | 2.431352 | 2.842865 | -0.990819 |
| H | -0.260197 | 0.622368 | 2.560244 | H | -0.074787 | 1.129106 | 0.120510 |

**Table 8 (Continued).**



**11**
$G$ = -1851.998595
$G_{MP2}$ = -1846.899014
(calculation does not include $Li(THF)_4^+$ ion)

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -0.829428 | -2.469154 | 1.290779 | H | -4.594894 | -2.480053 | -0.640760 |
| N | -0.759814 | -1.628579 | 0.081532 | C | -0.953930 | -2.384617 | -1.169939 |
| Li | -1.975610 | 0.104943 | 0.186621 | H | -1.976424 | -2.804391 | -1.204669 |
| N | -2.162551 | 2.050643 | 0.503606 | C | -0.830849 | -1.424285 | -2.362146 |
| C | -1.953124 | 2.656795 | 1.810281 | H | -1.565892 | -0.613635 | -2.300901 |
| H | -2.284559 | 3.717552 | 1.821540 | H | 0.164891 | -0.968012 | -2.390697 |
| C | -2.795426 | 1.956601 | 2.890913 | H | -0.991095 | -1.951749 | -3.312155 |
| H | -2.594438 | 2.360600 | 3.893408 | C | 0.005820 | -3.578931 | -1.381833 |
| H | -3.866584 | 2.068374 | 2.683546 | H | -0.097380 | -4.333702 | -0.594936 |
| H | -2.573633 | 0.881499 | 2.920214 | H | -0.205549 | -4.072726 | -2.340796 |
| C | -0.466377 | 2.681698 | 2.247796 | H | 1.049918 | -3.250477 | -1.386235 |
| H | 0.153445 | 3.155423 | 1.477593 | H | -0.041829 | -3.244903 | 1.271781 |
| H | -0.314793 | 3.236839 | 3.187648 | C | -2.172738 | -3.202006 | 1.475348 |
| H | -0.090707 | 1.660617 | 2.387246 | H | -2.367987 | -3.917241 | 0.667341 |
| C | -1.958607 | 3.016839 | -0.559612 | H | -2.179609 | -3.765468 | 2.418776 |
| H | -1.050382 | 3.641166 | -0.389892 | H | -3.001639 | -2.483224 | 1.496056 |
| C | -3.129319 | 4.026191 | -0.725851 | C | -0.538975 | -1.600777 | 2.521723 |
| H | -4.033206 | 3.502550 | -1.067633 | H | 0.407249 | -1.065201 | 2.402344 |
| H | -3.368991 | 4.516144 | 0.224927 | H | -1.331134 | -0.857471 | 2.677850 |
| H | -2.895427 | 4.816666 | -1.456679 | H | -0.474829 | -2.216634 | 3.428611 |
| C | -1.737648 | 2.313548 | -1.906271 | C | 3.047543 | -1.303666 | 0.285050 |
| H | -0.835747 | 1.691850 | -1.884153 | C | 1.833431 | -0.682858 | 0.025547 |
| H | -2.593624 | 1.661385 | -2.135916 | C | 1.957265 | 0.658221 | -0.392939 |
| H | -1.636456 | 3.030098 | -2.733145 | C | 3.182499 | 1.307805 | -0.548799 |
| O | -3.992719 | -0.545694 | -0.170834 | C | 4.366532 | 0.612249 | -0.278532 |
| C | -4.548071 | -1.488146 | -1.105888 | C | 4.304700 | -0.717545 | 0.149048 |
| C | -5.941813 | -0.954728 | -1.498454 | H | 5.211930 | -1.267850 | 0.375870 |
| C | -5.881854 | 0.519572 | -1.061338 | C | 5.695072 | 1.260820 | -0.501507 |
| C | -4.986121 | 0.442930 | 0.171303 | F | 6.145488 | 1.112259 | -1.779416 |
| H | -5.554774 | 0.103368 | 1.052308 | F | 6.667718 | 0.747648 | 0.295460 |
| H | -4.416913 | 1.349404 | 0.406066 | F | 5.666383 | 2.598431 | -0.273479 |
| H | -6.868225 | 0.944961 | -0.847196 | H | 3.226131 | 2.346951 | -0.864826 |
| H | -5.401839 | 1.134919 | -1.831780 | H | 1.047190 | 1.226387 | -0.588260 |
| H | -6.725918 | -1.481967 | -0.941411 | Cl | 3.070187 | -3.020286 | 0.874006 |
| H | -6.148983 | -1.084505 | -2.566113 | H | 0.497549 | -1.204643 | 0.070433 |
| H | -3.870689 | -1.546135 | -1.963828 | | | | |

*References*

I. Completed Reference 15. Gaussian 03, Revision B.04, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

2. *Gaussview*, Version 3.09, Dennington 2, R.; Keith, T.; Millam, J.; Eppinett, K.; Hovell, W. L.; Gilliland, R.; Semichem, Inc.; Shawnee Mission, KS, 2003.