Lithium Diisopropylamide-Mediated Lithiation
of 1,4-Difluorobenzene Under Nonequilibrium Conditions:
Role of Monomer-, Dimer-, and Tetramer-Based Intermediates
and Lessons About Rate Limitation

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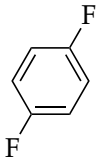
Structures



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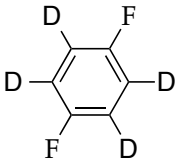
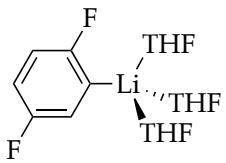


1-d_4



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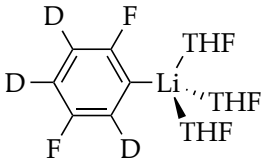

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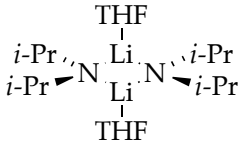

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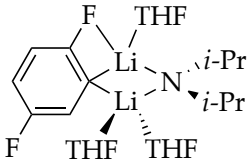


17

Part 1: NMR Spectroscopic Studies

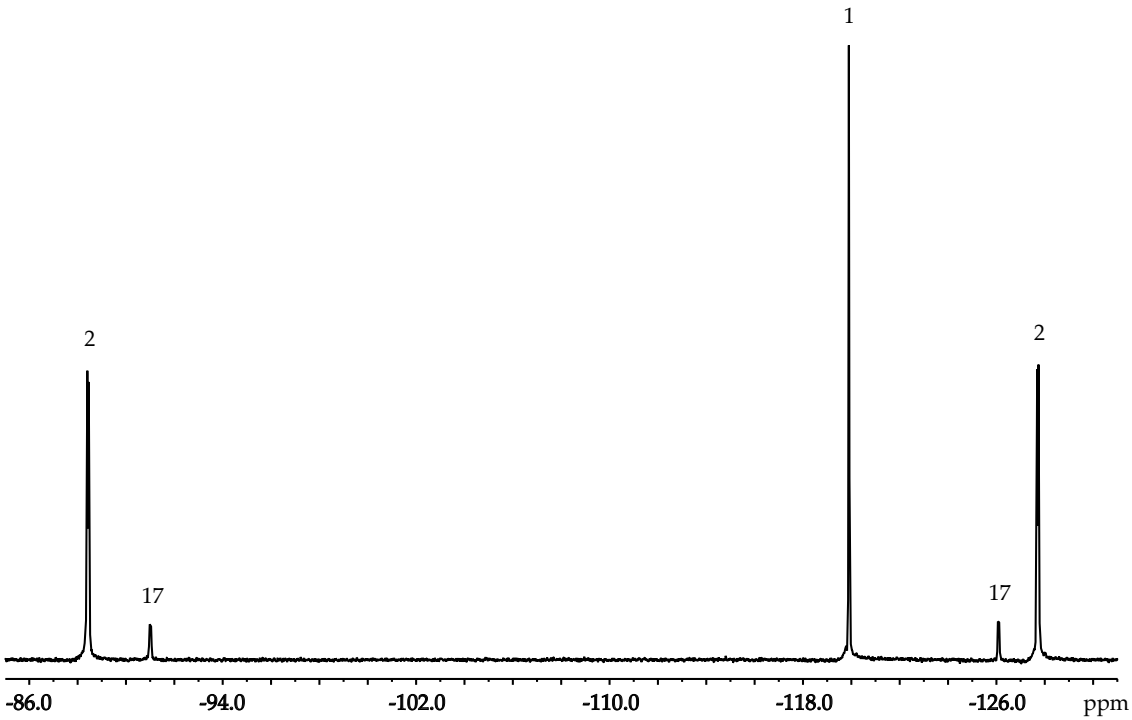


Figure 1. ^{19}F NMR spectrum of LDA (0.10 M) with **1** (0.050 M) and diisopropylamine (0.050 M) in 3.49 M THF/hexanes at –78 °C. **1:** δ -119.90 (s). **2:** δ -127.71 (d, $^{5}J_{F\text{-}F}$ = 31.6 Hz), -88.43 (d, $^{5}J_{F\text{-}F}$ = 31.6 Hz). **17:** δ -126.09 (d, $^{5}J_{F\text{-}F}$ = 31.0 Hz), -91.01 (d, $^{5}J_{F\text{-}F}$ = 31.0 Hz).

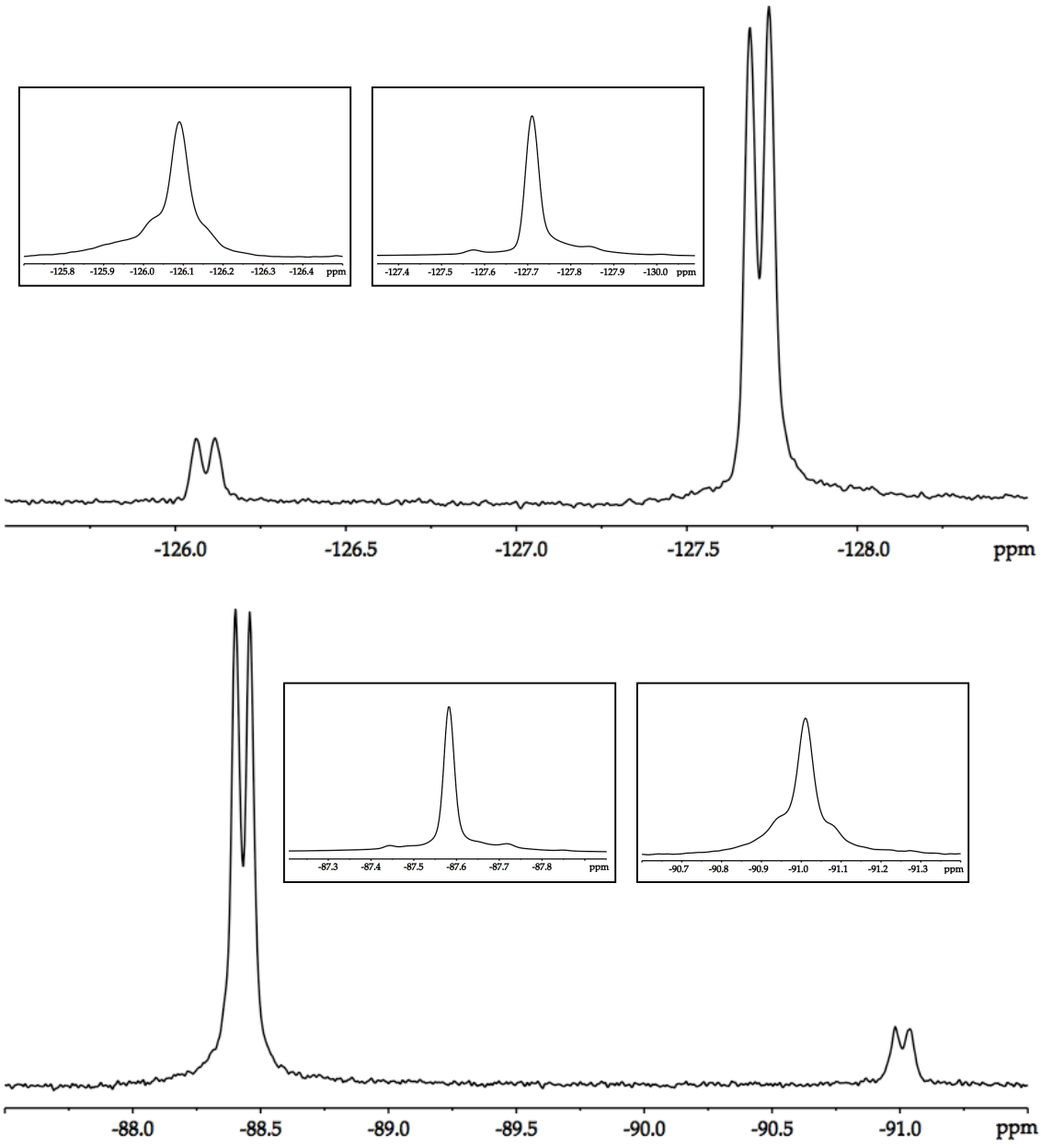


Figure 2. Expansion of ^{19}F NMR spectrum showing four sets of doublets for **2** and **17.** The five-bond ^{19}F –^{19}F coupling was confirmed by single-frequency ^{19}F decoupling (inserts).

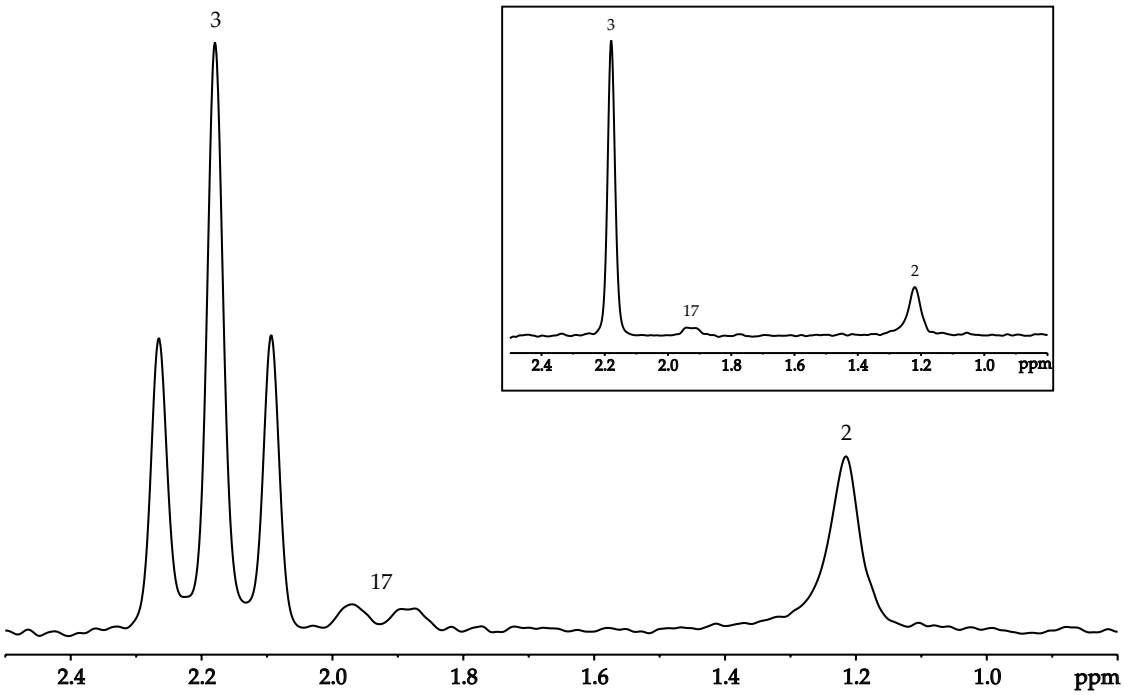


Figure 3. ^{6}Li NMR spectrum of [^{6}Li,^{15}N]LDA (0.10 M) and **1** (0.02 M) in 2.37 M THF/hexanes recorded at –78 °C. **2**: δ 1.22 (s). **17**: δ 1.93 (d, $^{1}J_{\text{Li-N}}$ = 5.1 Hz). **3**: δ 2.18 (t, $^{1}J_{\text{Li-N}}$ = 5.0 Hz). The insert shows ^{15}N decoupled ^{6}Li NMR spectrum. Resonances of **3** and **17** are reduced to singlets.

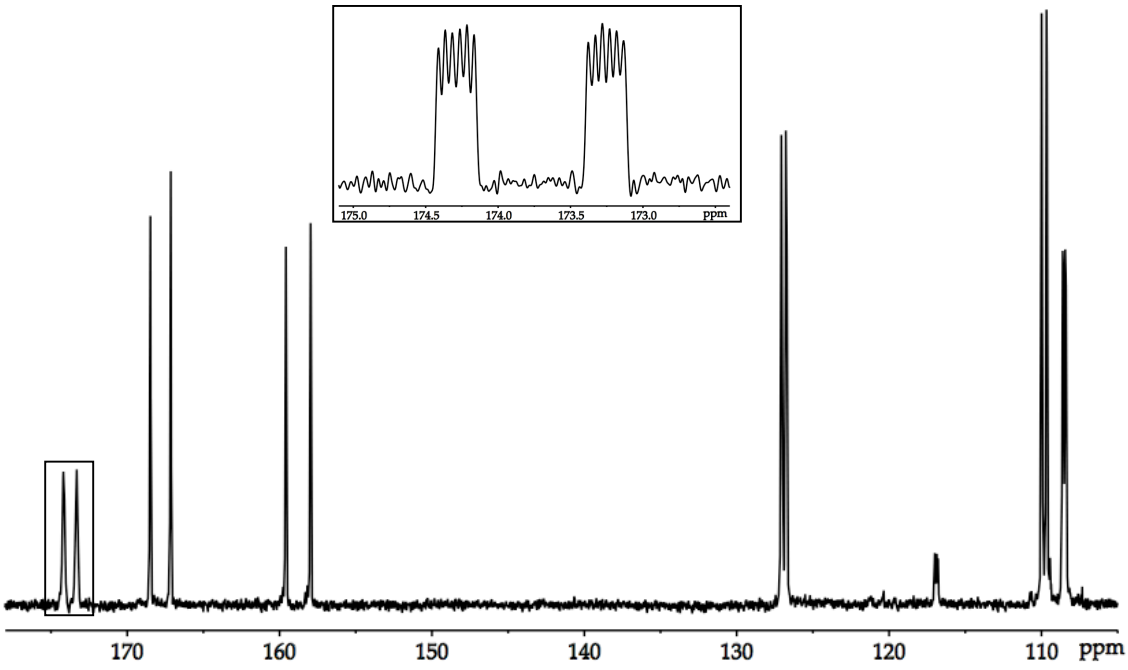


Figure 4. $^{13}C\{^{1}H\}$ NMR spectrum of **2** generated from **1** (0.30 M) with [^{6}Li]LDA (0.40 M) in 12.2 M THF-d_8 at –105 °C: δ 173.75 (ddt, $^{2}J_{C\text{-}F}$ = 130.2 Hz, $^{3}J_{C\text{-}F}$ = 18.6 Hz, $^{1}J_{C\text{-}Li}$ = 6.0 Hz,), 167.81 (d, $^{1}J_{C\text{-}F}$ = 201.7 Hz), 158.77 (d, $^{1}J_{C\text{-}F}$ = 244.7 Hz), 126.90 (dd, $^{2}J_{C\text{-}F}$ = 44.8 Hz, $^{3}J_{C\text{-}F}$ = 8.8 Hz), 109.82 (dd, $^{2}J_{C\text{-}F}$ = 49.3 Hz, $^{3}J_{C\text{-}F}$ = 3.7 Hz), 108.50 (dd, $^{2}J_{C\text{-}F}$ = 25.5 Hz, $^{3}J_{C\text{-}F}$ = 7.2 Hz).

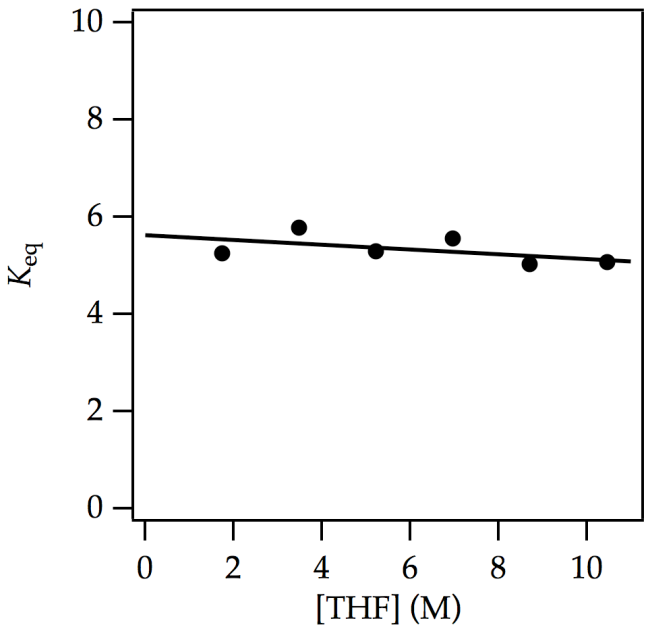


Figure 5. Plot of K_{eq} (derivation 2) versus [THF] in hexanes cosolvent for the equilibration of aryllithium **18** (0.025 M) and arene **1** (0.025 M) measured by ^{19}F NMR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a$[ArH] + b. [a = 5.6$\pm$ 0.2, b = (-5 $\pm$ 4) x 10^{-2}]

[THF] (M)	y_1
1.74	5.26
3.48	5.78
5.23	5.29
6.97	5.55
8.71	5.02
10.46	5.06

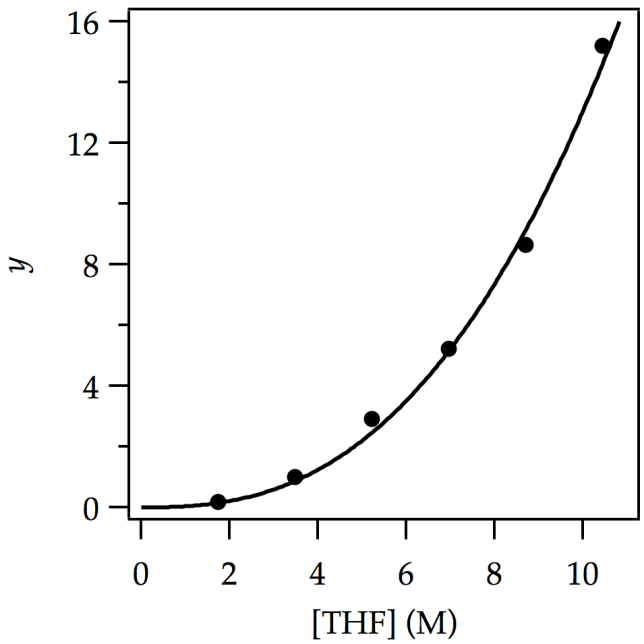


Figure 6. Plot of y (derivation 1) versus [THF] in hexanes cosolvent for the ortholithation of **1** (0.05 M) with LDA (0.10 M) in the presence of added diisopropylamine (0.050 M) measured by ^{19}F NMR at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}]^n$. [$a = (0.03 \pm 0.01) \times 10^{-2}$, $n = 2.6 \pm 0.2$]

[THF] (M)	y_1 (M)
1.74	0.176
3.48	1.01
5.23	2.91
6.97	5.22
8.71	8.65
10.46	15.2

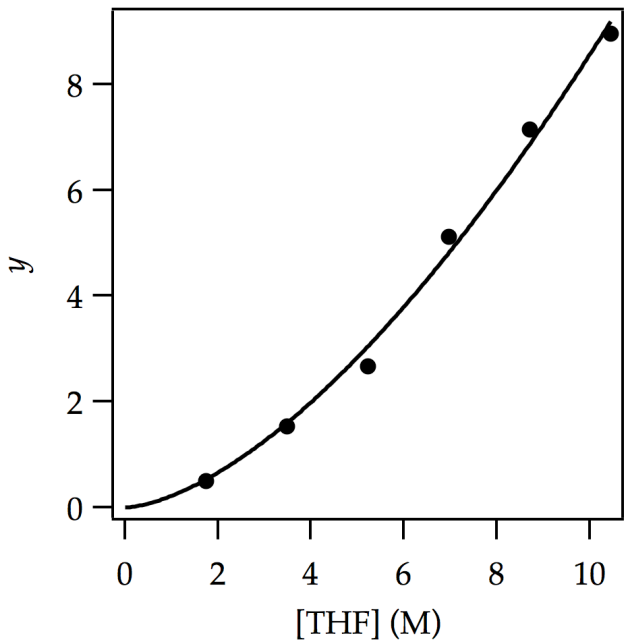


Figure 7. Plot of y (eq 8 in manuscript) versus [THF] in hexanes cosolvent for the ortholithation of **1** (0.050 M) with LDA (0.10 M) in the presence of diisopropylamine (0.05 M) measured by ^{19}F NMR at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\mathrm{THF}]^{4-n}$. [$a = 0.21 \pm 0.05$, $n = 2.4 \pm 0.1$]

[THF] (M)	y_1 (M)
1.74	0.499
3.48	1.52
5.23	2.67
6.97	5.12
8.71	7.14
10.46	8.96

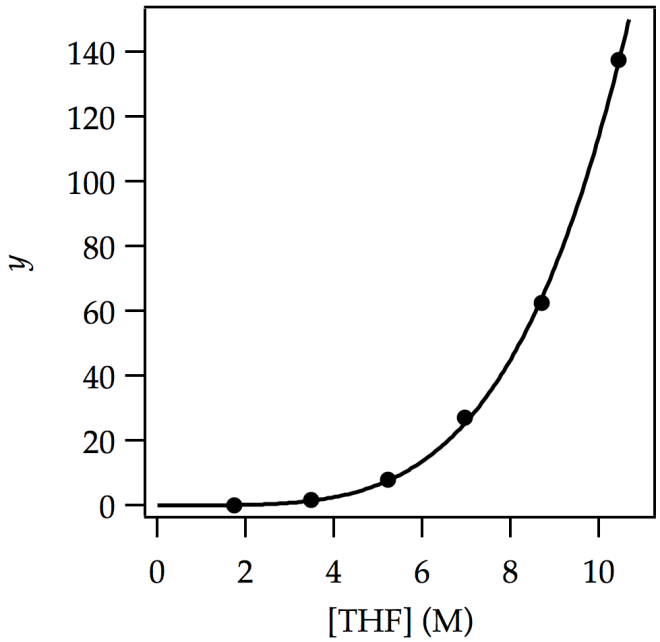


Figure 8. Plot of y (derivation 3) versus [THF] in hexanes cosolvent for the ortholithation of **1** (0.05 M) with LDA (0.10 M) in the presence of diisopropylamine (0.05 M) measured by ^{19}F NMR at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}]^z$. [$a = (8 \pm 1) \times 10^{-3}$, $z = 4.16 \pm 0.08$]

[THF] (M)	y_1 (M)
1.74	9.584
3.48	1.606
5.23	7.976
6.97	27.10
8.71	62.43
10.46	137.4

Part 2: Rate Studies

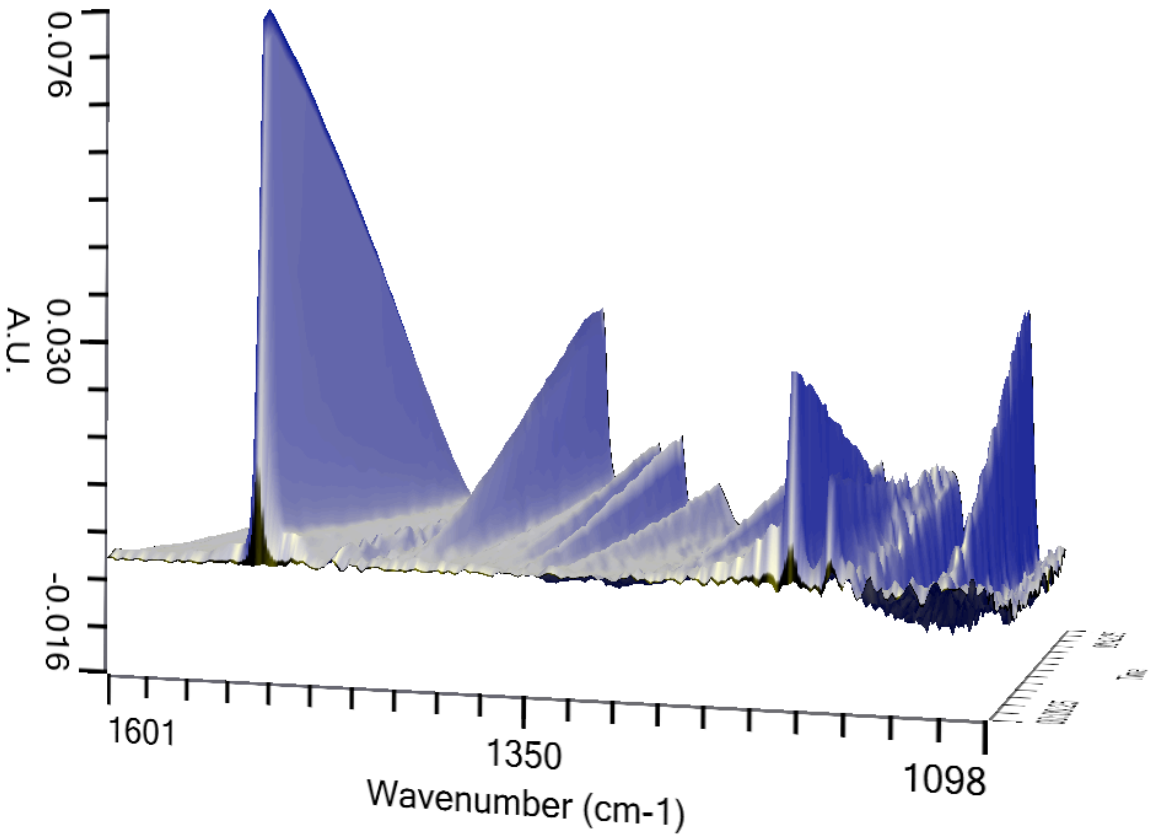


Figure 9. Representative in situ IR traces for the ortholithiation of **1** (0.020 M) by LDA (0.12 M) in THF at –78 °C. IR absorptions for compounds **1** and **2** and their associated isotopomers are listed below. The IR spectra were deconvoluted using ConcIRT®.

1: 1510 cm^{-1}, 1461 cm^{-1}, 1203 cm^{-1}, 1184 cm^{-1}
2: 1586 cm^{-1}, 1551 cm^{-1}, 1421 cm^{-1}, 1380 cm^{-1}, 1363 cm^{-1}, 1279 cm^{-1}, 1223 cm^{-1}, 1125 cm^{-1}

1-d_4: 1428 cm^{-1}, 1136 cm^{-1}, 1121 cm^{-1}
2-d_3: 1381 cm^{-1}, 1342 cm^{-1}, 1318 cm^{-1}, 1257 cm^{-1}, 1218 cm^{-1}, 1186 cm^{-1}

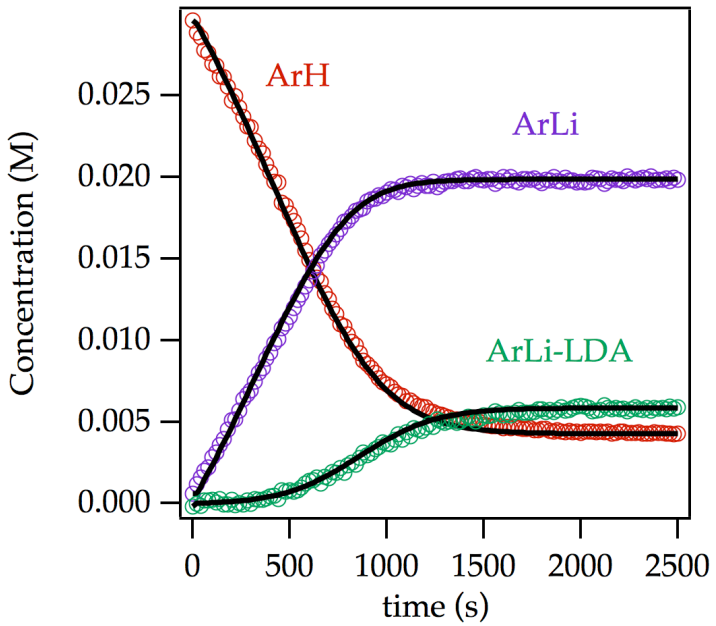


Figure 10. Time-dependent concentrations measured by ^{19}F NMR spectroscopy using 0.10 M LDA and **1** in 3.05 M THF at –65 °C. Legend: ArH = **1**; ArLi = **2**; ArLi-LDA = **17**. The curves represent a parametric fit to reference 39 in the manuscript.

Numerical best-fit parameters:

$k_1 = (2.08 \pm 0.02) \times 10^{-4}$
$k_{-1} = 0.2$
$k_2 = 5 \times 10^{-6}$
$k_{-2} = 90$
$k_3 = (1.5 \pm 0.8) \times 10^{4}$
$k_{-3} = (8 \pm 6) \times 10^{2}$
$k_4 = 16.8 \pm 0.8$
$k_{-4} = (8.7 \pm 0.6) \times 10^{-2}$
$k_5 = (8 \pm 3) \times 10^{3}$
$k_{-5} = 11 \pm 4$
$k_6 = (1.18 \pm 0.04) \times 10^{-2}$
$k_{-6} = (k_{-1}k_6)/k_1$

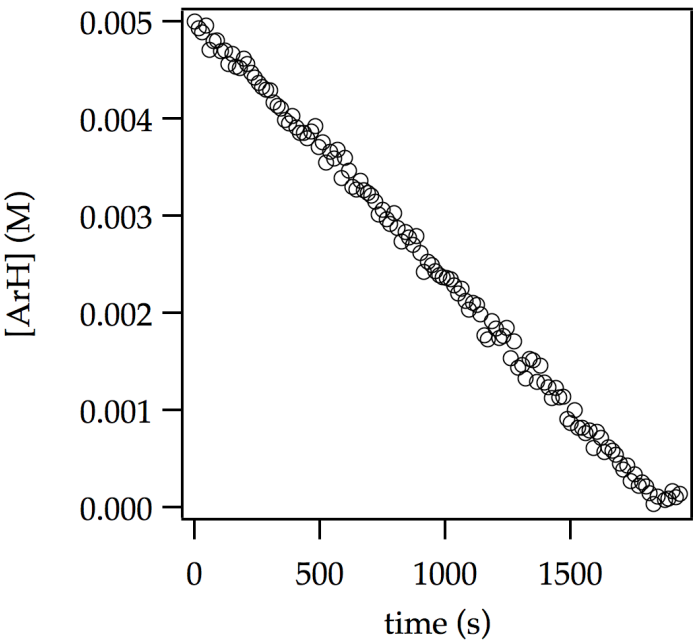


Figure 11. Representative plot showing linear decay for the ortholithiation of **1** (0.005 M) with LDA (0.10 M) in 12.2 M THF monitored using IR spectroscopy at –78 °C.

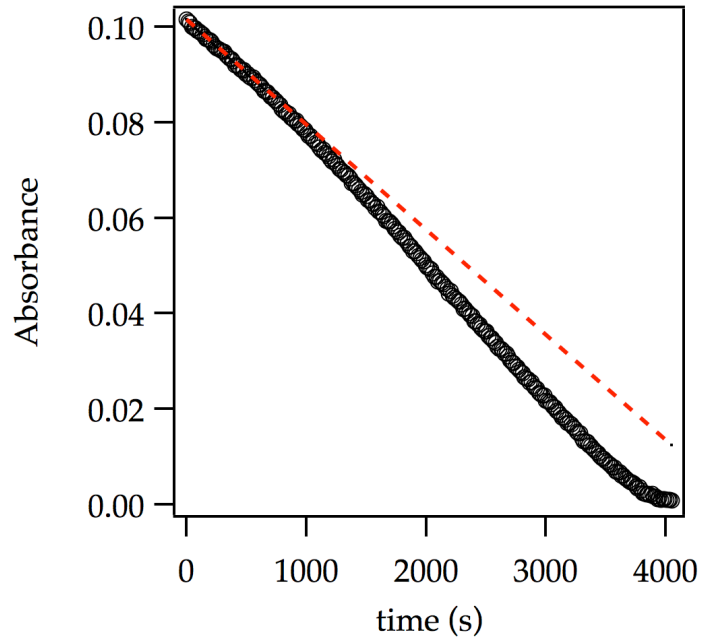


Figure 12. Representative plot showing sigmoidal decay for the ortholithiation of **1** (0.020 M) with LDA (0.10 M) in 12.2 M THF monitored with IR spectroscopy at –78 °C. The red dotted line depicts the time-dependent linear decay extrapolated from initial rate in the absence of autocatalysis.

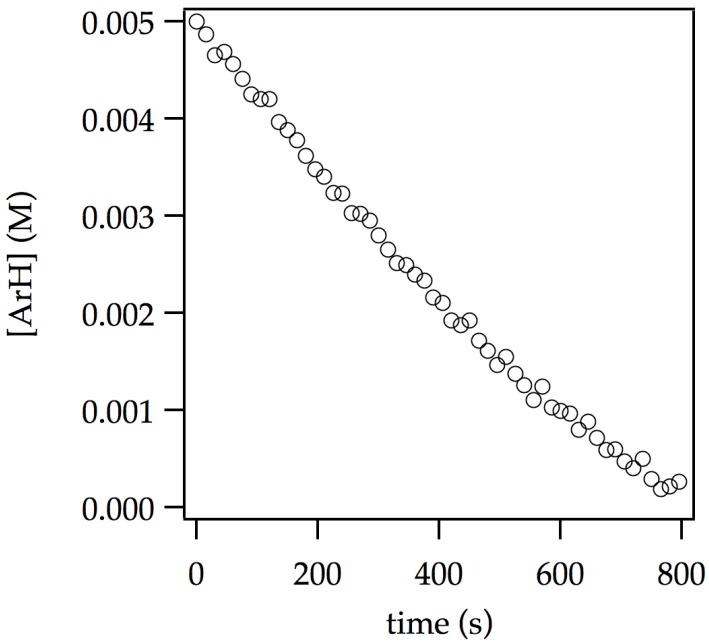


Figure 13. Representative plot showing [**1**] vs time for the ortholiation of **1** (0.005 M) with LDA (0.10 M) and ArLi (0.02 M) in THF (12.2 M) monitored with IR spectroscopy at –78 °C.

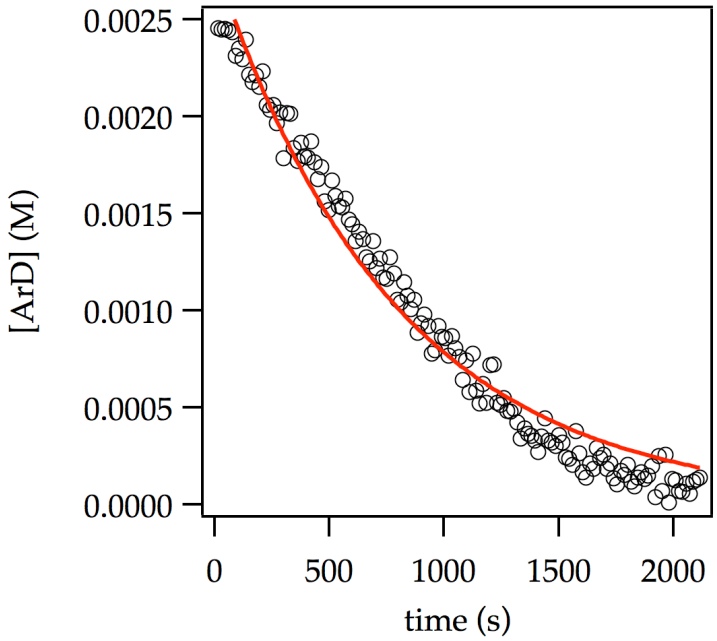


Figure 14. Representative plot showing poor exponential fit (red curve) to the decay for ortholithiation of **1-*d*$_4$** (0.0025 M) with LDA (0.10 M) in THF (12.2 M) monitored with IR spectroscopy at –78 °C.

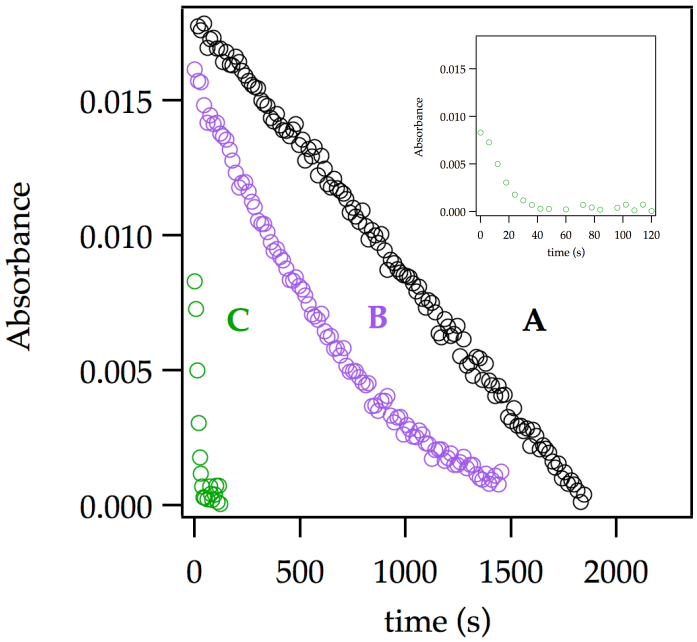


Figure 15. Representative plot showing the absorbance of **1** versus time for the ortholithiation of **1** (0.0050 M) with LDA (0.10 M) in THF (12.2 M) at –78 °C (curve A). Curve B shows the decay under the same conditions as in A but with 0.020 M ArLi. After the lithiation was complete, 0.0010 M LiCl was added and a second aliquot was injected into this mixture (curve C; see inset for expansion). Reactions were monitored with IR spectroscopy.

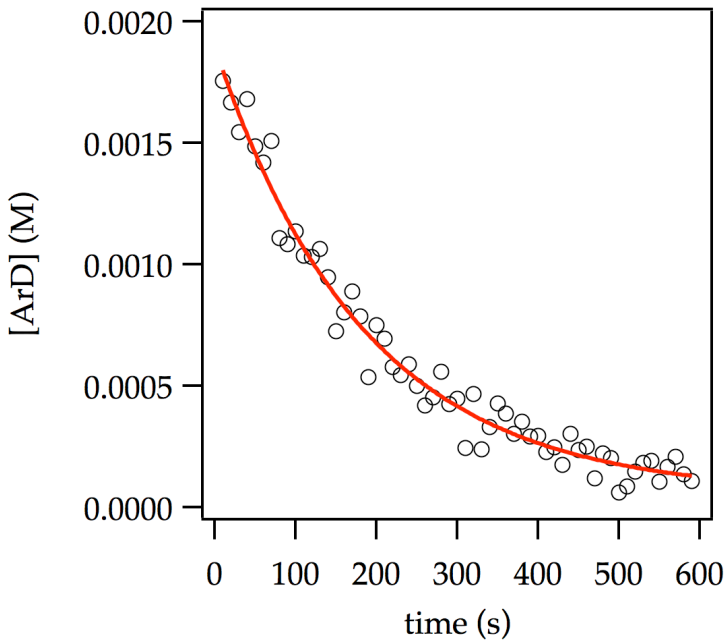


Figure 16. Representative plot showing exponential decay for the ortholithiation of **1-*d*$_4$** (0.002 M) with LDA (0.25 M) in 12.2 M THF monitored with IR spectroscopy at –78 °C.

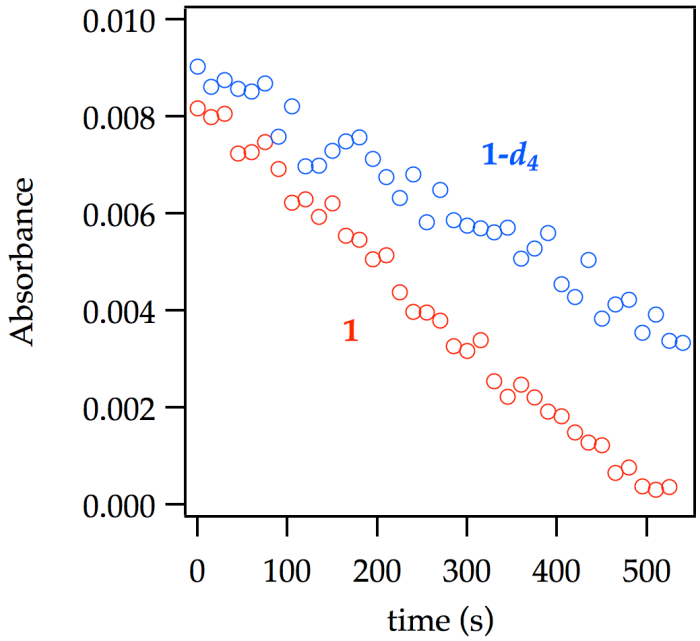


Figure 17. Ortholithiation of **1** (0.0025 M) and **1-*d*$_4$** (0.0025 M) with LDA (0.10 M) in THF (12.2 M) at –78 °C (measured separately). Monitoring the initial rates of both decays by IR spectroscopy afford $k_H/k_D = 1.5$.

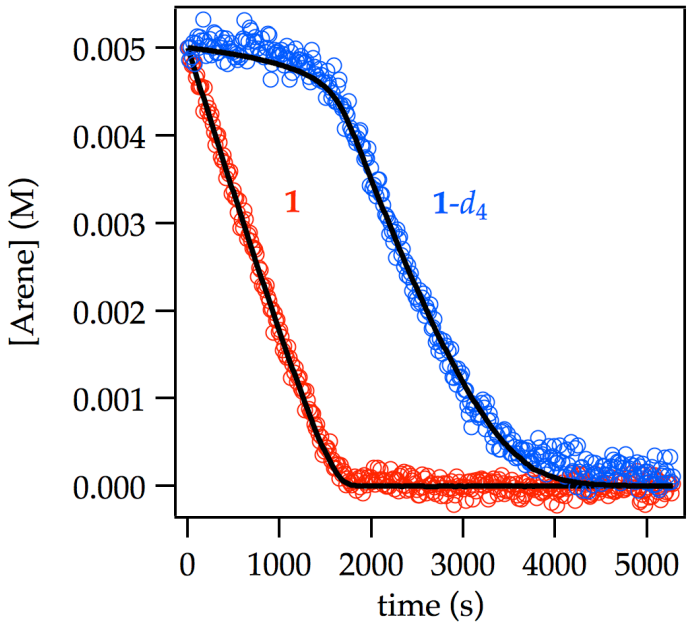


Figure 18. Competitive ortholithiation of **1** (0.005 M) and **1-*d*$_4$** (0.005 M) with LDA (0.10 M) in THF (12.2 M) at –78 °C. The curves result from a best-fit numerical integration to the highly simplified model in Scheme 3 (manuscript) and afford $k_H/k_D = 29$. By contrast, measuring the initial slopes directly affords $k_H/k_D = 40$.

Numerical best-fit parameters:

$k_1 = (3.53 \pm 0.01) \times 10^{-5}$
$k_2 = 0.41 \pm 0.03$
$k_3 = (1.3 \pm 0.1) \times 10^{4}$
$k_4 = (4.4 \pm 0.3) \times 10^{2}$

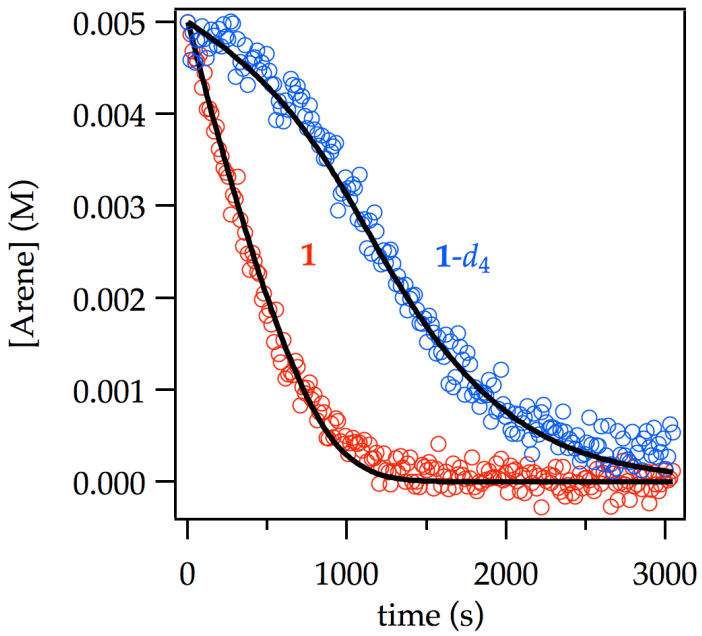


Figure 19. Competitive ortholithiation of **1** (0.0050 M) and **1-*d*$_4$** (0.0050 M) with LDA (0.10 M) in the presence of 0.020 M ArLi in THF (12.2 M) at –78 °C. The curves result from a best-fit numerical integration to the highly simplified model in Scheme 3 (manuscript) and afford $k_H/k_D = 6.3$. Fitting the initial rates of both decays directly affords $k_H/k_D = 40$.

Numerical best-fit parameters:

$k_1 = (8.7 \pm 0.1) \times 10^{-5}$
$k_2 = 24.0 \pm 0.9$
$k_3 = (3.8 \pm 0.2) \times 10^{4}$
$k_4 = (6.0 \pm 0.2) \times 10^{3}$

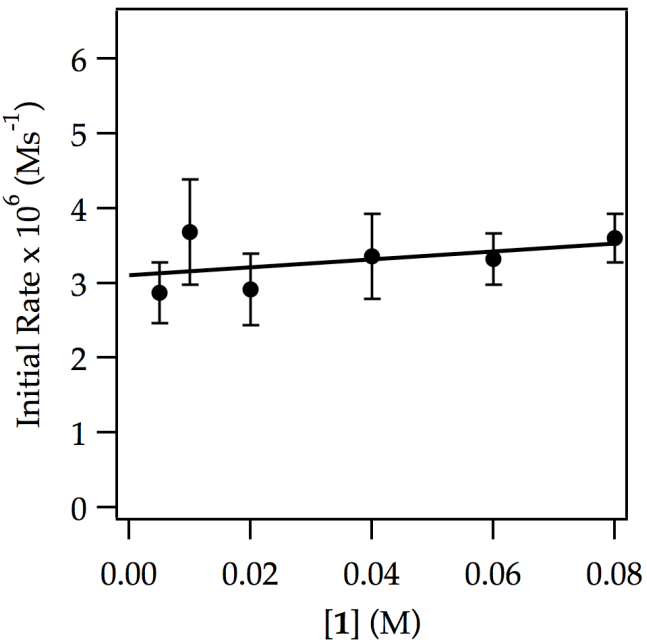


Figure 20. Plot of initial rate vs [ArH] (initial arene concentration) for the ortholithiation of **1** with LDA (0.10 M) in THF (12.2 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\mathrm{ArH}] + b$. [$a = (5 \pm 5) \times 10^{-6}$, $b = (3.1 \pm 0.2) \times 10^{-6}$]

[**1**] (M)	y_1 (M·s^{-1})	y_2 (M·s^{-1})
0.005	3.16e-06	2.58e-06
0.01	4.18e-06	3.18e-06
0.02	3.26e-06	2.58e-06
0.04	3.76e-06	2.96e-06
0.06	3.57e-06	3.08e-06
0.08	3.83e-06	3.37e-06

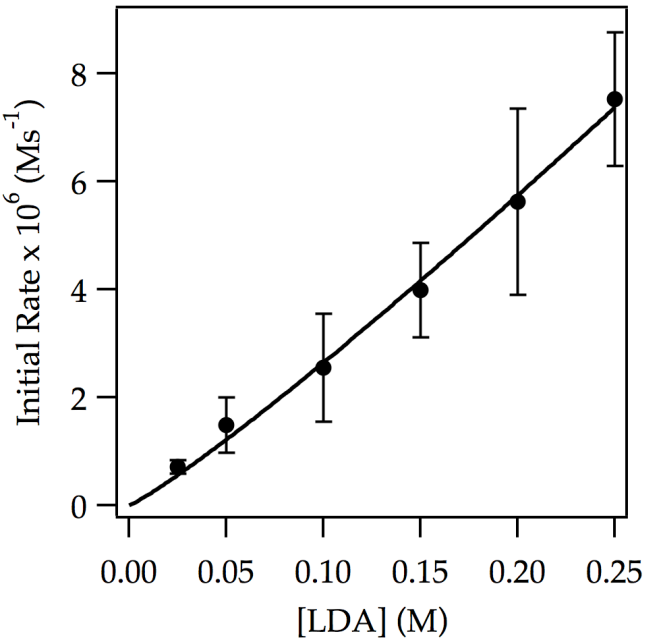


Figure 21. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.005 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (3.5 \pm 0.3) \times 10^{-5}$, $n = 1.12 \pm 0.06$]

[LDA] (M)	y_1 (M•s^{-1})	y_2 (M•s^{-1})	y_3 (M•s^{-1})	y_4 (M•s^{-1})
0.025	5.43e-07	8.21e-07	6.83e-07	7.82e-07
0.05	1.07e-06	1.03e-06	1.89e-06	1.96e-06
0.10	1.34e-06	2.10e-06	3.39e-06	3.36e-06
0.15	2.94e-06	3.83e-06	4.11e-06	5.06e-06
0.20	4.30e-06	6.69e-06	7.51e-06	4.03e-06
0.25	6.18e-06	8.19e-06	8.90e-06	6.85e-06

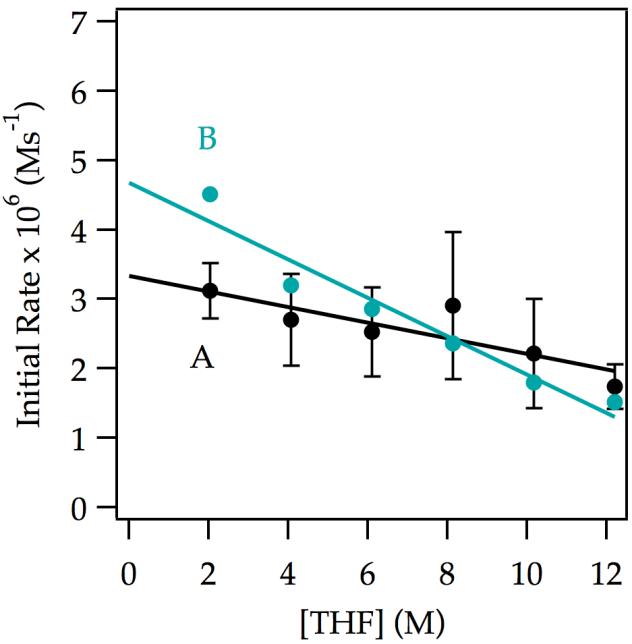


Figure 22. Plot of initial rate versus [THF] in Et_2O (curve A) and in hexanes (curve B) as cosolvent for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at –78 °C. The data was measured with IR spectroscopy. The curves depict unweighted least-squares fits to $y = a[\text{THF}] + b$. Curve A: $a = (-1.1 \pm 0.3) \times 10^{-7}$, $b = (3.3 \pm 0.3) \times 10^{-6}$. Curve B: $a = (-2.8 \pm 0.3) \times 10^{-7}$, $b = (4.7 \pm 0.3) \times 10^{-6}$. The greater slope using hexane as cosolvent compared with that using Et_2O as cosolvent illustrates the influence of long-range medium effects.

[THF] (M)	y_1-A (M•s^{-1})	y_2-A (M•s^{-1})	y_3-B (M•s^{-1})
2.03	2.84e-06	3.40e-06	4.51e-06
4.07	3.17e-06	2.23e-06	3.20e-06
6.00	2.98e-06	2.07e-06	2.86e-06
8.13	3.66e-05	2.16e-05	2.36e-05
10.17	2.77e-05	1.66e-05	1.80e-05
12.2	1.97e-05	1.51e-05	1.52e-05

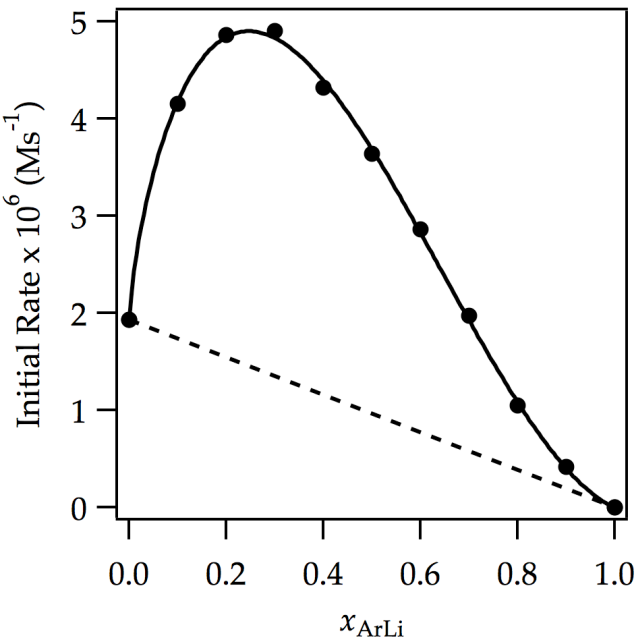


Figure 23. Plot of initial rates versus mole fraction of 2-lithio-1,4-difluorobenzene (X_{ArLi}) for the serial injection of 0.01M aliquots of **1** to 0.10 M LDA in 12.2 M THF monitored with IR spectroscopy at –78 °C. The dotted line depicts the theoretical initial rates in the absence of autocatalysis. The solid line depicts an unweighted least-squares fit to $-d[ArH]/dt = k(X_{ArLi})^n(1-X_{ArLi})^m + k'(1-X_{ArLi})$. [$k = (1.67 \pm 0.09) \times 10^{-5}$, $k' = (1.93 \pm 0.05) \times 10^{-6}$, $n = 0.75 \pm 0.3$, $m = 1.87 \pm 0.05$]

X_{ArLi}	y_1 ($M \cdot s^{-1}$)
0.00	1.93e-06
0.10	4.15e-06
0.20	4.86e-06
0.30	4.90e-06
0.40	4.32e-06
0.50	3.64e-06
0.60	2.86e-06
0.70	1.97e-06
0.80	1.05e-06
0.90	4.14e-07
1.00	0

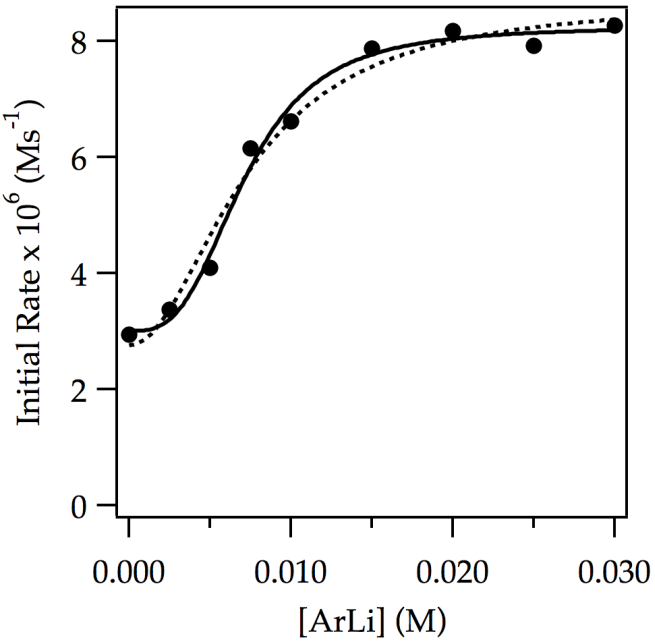


Figure 24. Plot of initial rate versus [ArLi] for the ortholithiation of **1** (0.005 M) by 0.10 M LDA in 12.2 M THF monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to eq 4 in derivation 6. Solid curve: [k_1 = (1.0 ± 0.1) x 10^{-4}, $k_{-1} = 1000k_1$, k_c = (2 ± 5) x 10^3, $k_{-c} = 1000k_c$, k_2 = 3.29 ± 0.08, n = 3.2 ± 0.6]. Dotted curve: [k_1 = (8 ± 1) x 10^{-5}, $k_{-1} = 1000k_1$, k_c = 4.8 ± 0.9, $k_{-c} = 1000k_c$, k_2 = 3.5 ± 0.1, n = 2].

[ArLi] (M)	y_1 (M·s^{-1})
0.00	2.94e-06
0.0025	3.37e-06
0.005	4.09e-06
0.075	6.16e-06
0.01	6.62e-06
0.015	7.88e-06
0.02	8.18e-06
0.025	7.92e-06
0.03	8.27e-06

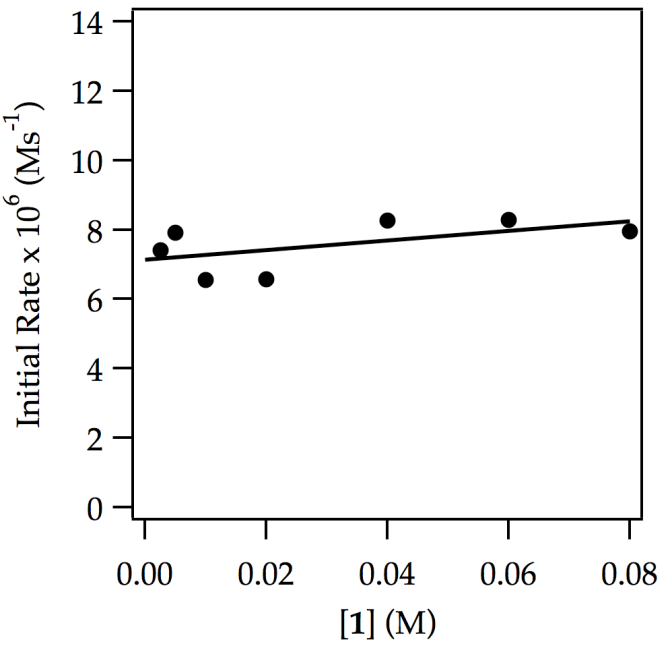


Figure 25. Plot of initial rate vs [ArH] (initial arene concentration) for the ortholithiation of **1** with LDA (0.10 M) in THF (12.2 M) with 0.02 M ArLi monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a$[ArH] + b. [$a = (14 \pm 9) \times 10^{-5}$, $b = (7.1 \pm 0.4) \times 10^{-6}$]

[**1**] (M)	y_1 (M·s^{-1})
0.0025	7.95e-06
0.005	8.29e-06
0.01	8.27e-06
0.02	6.57e-06
0.04	6.56e-06
0.06	7.91e-06
0.08	7.41e-06

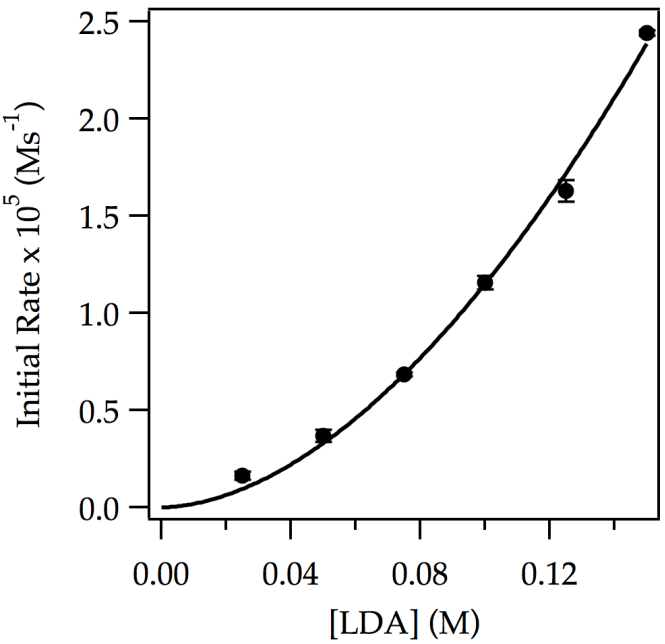


Figure 26. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.005 M) in the presence of 0.020 M ArLi monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (7 \pm 1) \times 10^{-4}$, $n = 1.80 \pm 0.09$]

[LDA] (M)	y_1 (M·s^{-1})	y_2 (M·s^{-1})
0.025	1.77e-06	1.48e-06
0.05	3.48e-06	3.90e-06
0.075	6.77e-06	6.90e-06
0.10	1.13e-05	1.18e-05
0.125	1.59e-05	1.67e-05
0.150	2.45e-05	2.43e-05

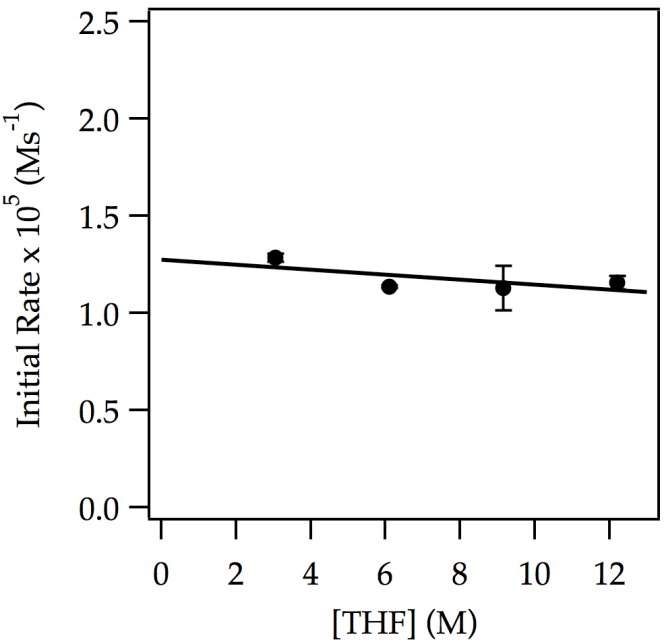


Figure 27. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1** (0.005 M) by LDA (0.10 M) with 0.020 M ArLi monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [a = (-1.3 $\pm$ 0.9) x 10^{-7}, b = (1.28 $\pm$ 0.08) x 10^{-5}]

[THF] (M)	y_1 (M·s^{-1})	y_2 (M·s^{-1})
3.05	1.30e-05	1.27e-05
6.10	1.14e-05	1.13e-05
9.15	1.05e-05	1.21e-05
12.2	1.13e-05	1.18e-05

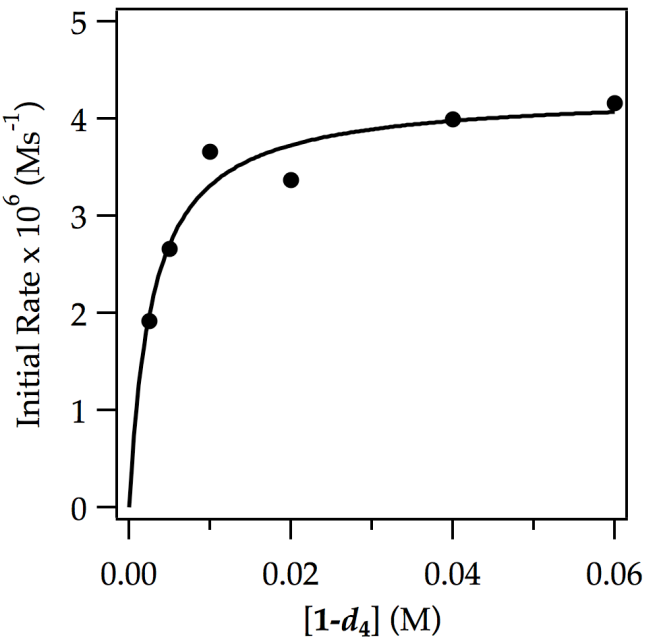


Figure 28. Plot of initial rate vs [ArD] (initial arene concentration) for the ortholithiation of **1-d_4** with LDA (0.10 M) in THF (12.2 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to a first-order saturation function: $-d[\mathrm{ArD}]/dt = (a[\mathrm{ArD}])/(1 + b[\mathrm{ArD}])$. [$a = (1.5 \pm 0.3) \times 10^{-3}$, $b = (3.5 \pm 0.8) \times 10^{2}$]

[**1-d_4**] (M)	y_1 (M·s^{-1})
0.0025	1.92e-06
0.005	2.66e-06
0.01	3.66e-06
0.02	3.37e-06
0.04	3.99e-06
0.06	4.16e-06

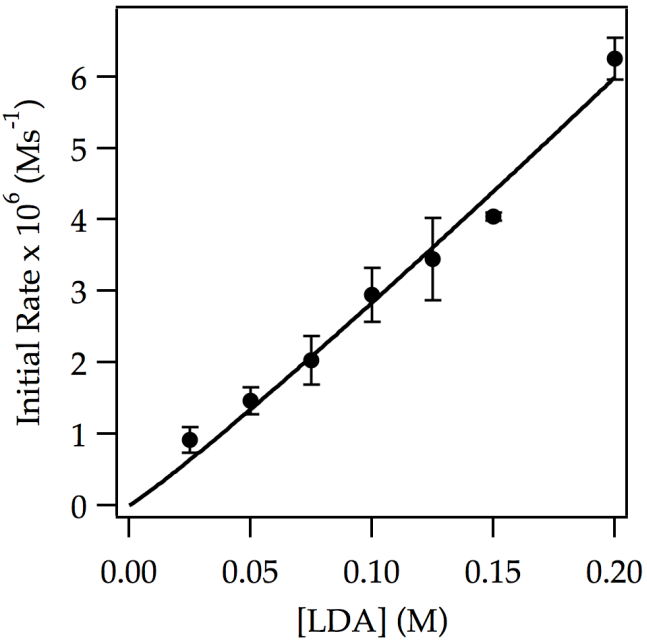


Figure 29. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1-d_4** (0.002 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (3.4 \pm 5) \times 10^{-5}$, $n = 1.08 \pm 0.08$]

[LDA] (M)	y_1 (M·s^{-1})	y_2 (M·s^{-1})
0.025	1.05e-06	9.20e-06
0.05	1.32e-06	1.59e-06
0.075	1.79e-06	2.27e-06
0.10	3.21e-06	2.68e-06
0.125	3.04e-06	3.85e-06
0.150	4.08e-06	4.00e-06
0.20	6.04e-06	6.45e-06

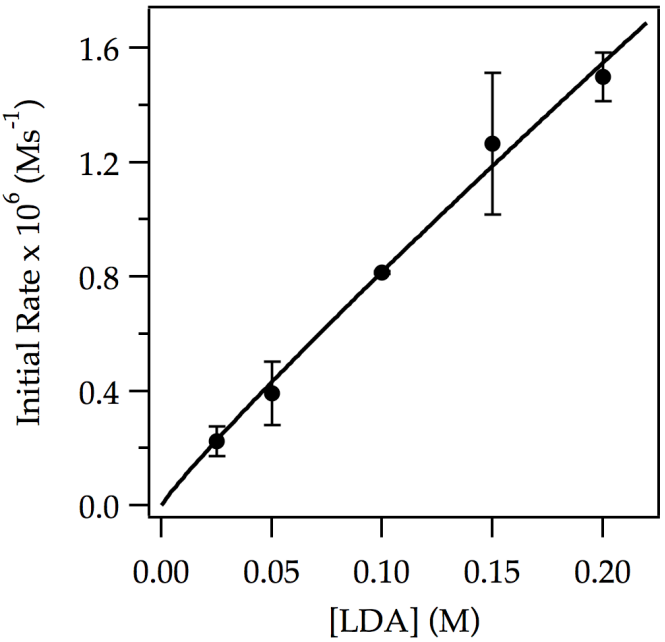


Figure 30. Plot of initial rate versus [LDA] in THF (2.03 M) for the ortholithiation of **1-*d*$_4$** (0.002 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (6.8 \pm 0.9) \times 10^{-6}$, $n = 0.92 \pm 0.07$]

[LDA] (M)	y_1 (M•s^{-1})	y_2 (M•s^{-1})
0.025	1.88e-07	2.61e-07
0.05	4.70e-07	3.13e-07
0.10	8.11e-07	8.19e-07
0.15	1.09e-06	1.44e-06
0.20	1.44e-06	1.56e-06

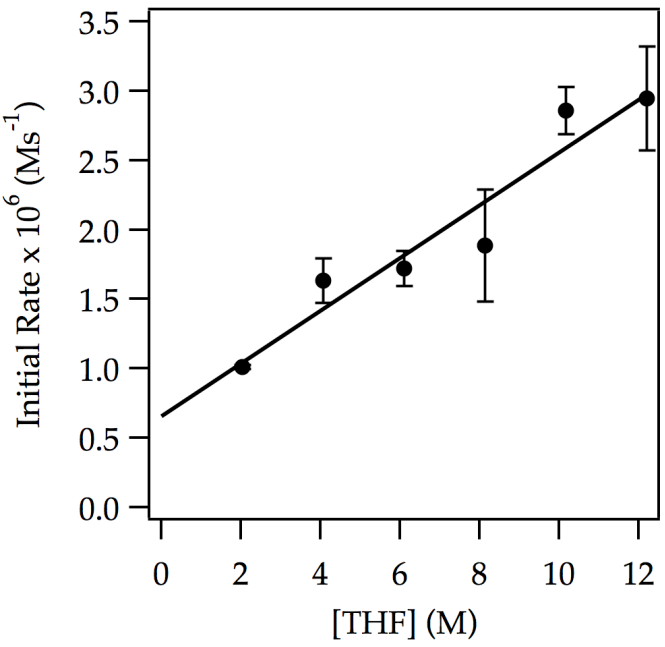


Figure 31. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1-*d*$_4$** (0.002 M) by LDA (0.10 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [$a = (1.9 \pm 0.3) \times 10^{-7}$, $b = (7 \pm 2) \times 10^{-7}$]

[THF] (M)	y_1 (M·s^{-1})	y_2 (M·s^{-1})
2.03	1.02e-06	1.00e-06
4.07	1.75e-06	1.52e-06
6.10	1.81e-06	1.63e-06
8.13	2.17e-06	1.60e-06
10.17	2.98e-06	2.74e-06
12.2	3.21e-06	2.68e-06

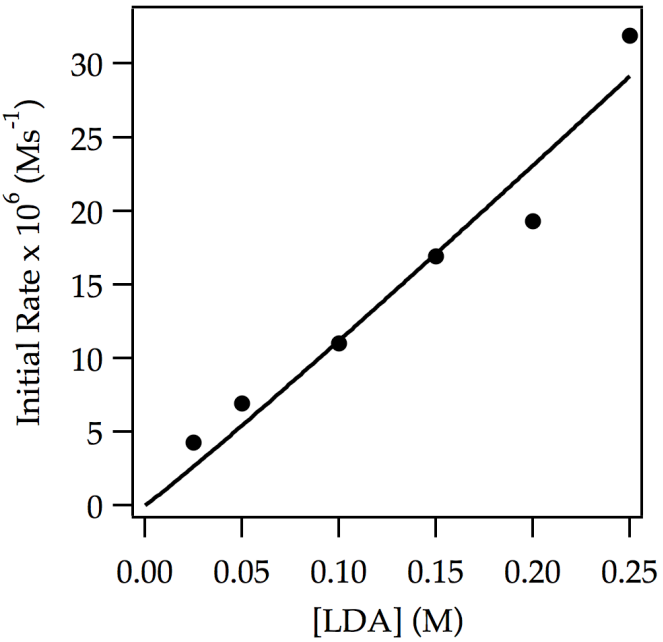


Figure 32. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1-d_4** (0.060 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (1.2 \pm 0.4) \times 10^{-4}$, $n = 1.0 \pm 0.2$]

[LDA] (M)	y_1 (M•s^{-1})
0.025	4.27e-06
0.05	6.94e-06
0.01	1.10e-05
0.15	1.69e-05
0.20	1.93e-05
0.25	3.19e-05

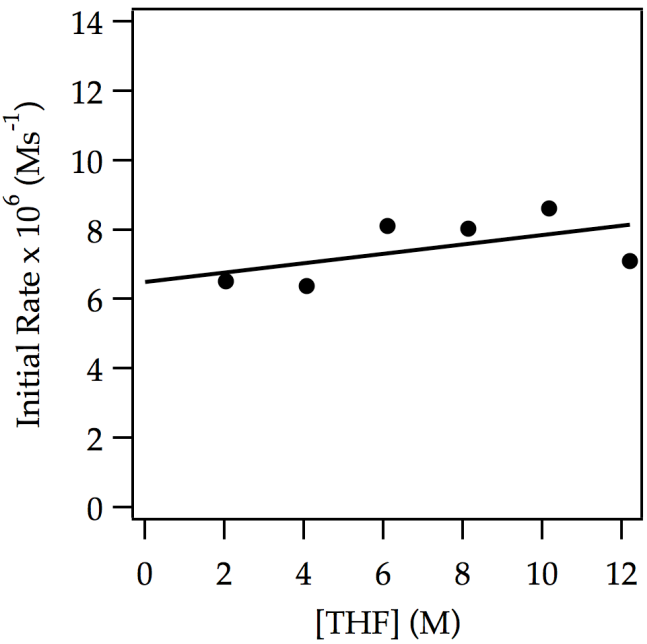


Figure 33. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1-*d*$_4$** (0.060 M) by LDA (0.10 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [$a = (1 \pm 1) \times 10^{-7}$, $b = (6.5 \pm 0.8) \times 10^{-6}$]

[THF] (M)	y_1 (M·s^{-1})
2.03	6.51e-06
4.07	6.37e-06
6.10	8.11e-06
8.13	8.04e-06
10.17	8.62e-06
12.2	7.09e-06

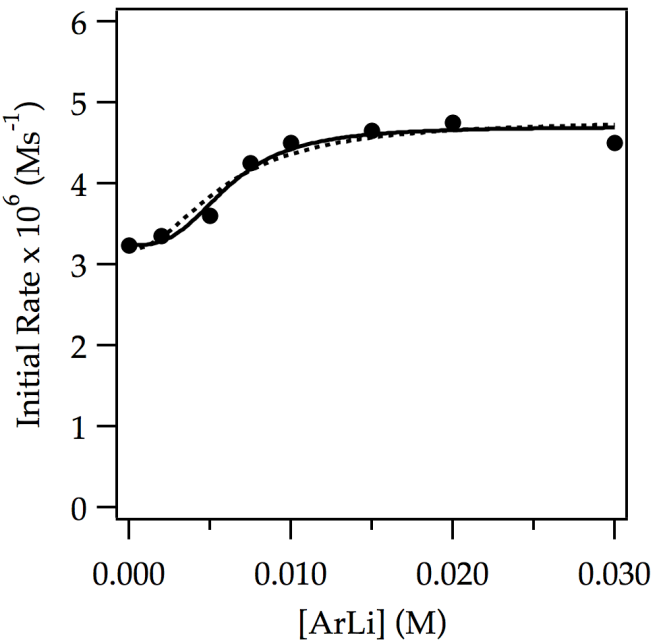


Figure 34. Plot of initial rate versus [ArLi] (specifically, **2–*d*$_3$**) for the ortholithiation of **1-*d*$_4$** (0.002 M) by 0.10 M LDA in 12.2 M THF monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to eq 4 in derivation 6. Solid line: [k_1 = (2.1 ± 0.2) x 10^{-4}, $k_{-1} = 1000k_1$, k_c = (1.3 ± 0.4) x 10^3, $k_{-c} = 1000k_c$, k_2 = 47.0 ± 0.8, n = 3]. Dotted line: [k_1 = (1.9 ± 0.2) x 10^{-4}, $k_2 = 1000k_1$, k_c = 8 ± 3, $k_{-c} = 1000k_c$, k_2 = 47 ± 1, n = 2].

[ArLiD$_3$] (M)	y_1 (M•s^{-1})
0	3.23e-06
0.002	3.35e-06
0.005	3.60e-06
0.0075	4.25e-06
0.01	4.50e-06
0.015	4.65e-06
0.02	4.75e-06
0.03	4.50e-06

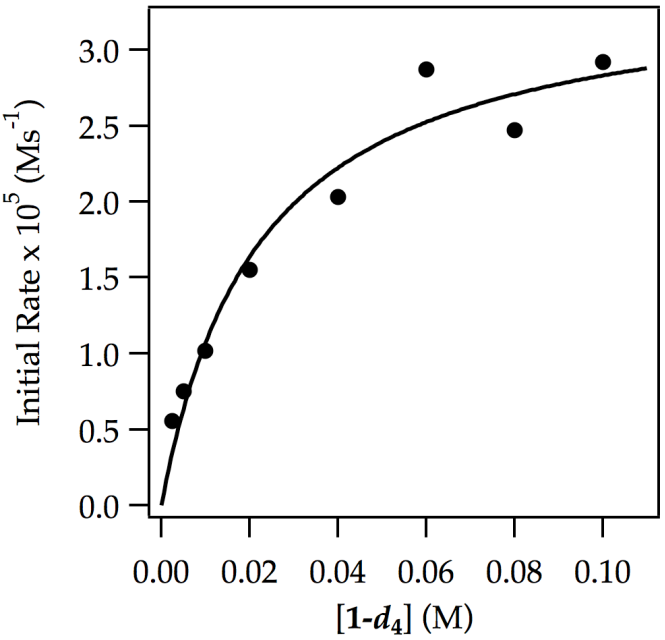


Figure 35. Plot of initial rate vs [ArD] (initial arene concentration) for the ortholithiation of **1-d_4** in the presence of 0.020 M ArLi (**2-d_3**) with LDA (0.10 M) in THF (12.2 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to a first-order saturation function: $-d[\mathrm{ArD}]/dt = (a[\mathrm{ArD}])/(1 + b[\mathrm{ArD}])$. [$a = (1.6 \pm 0.3) \times 10^{-3}$, $b = 40 \pm 10$]

[**1-d_4**] (M)	y_1 (M·s^{-1})
0.0025	5.56e-06
0.005	7.50e-06
0.01	1.02e-05
0.02	1.55e-05
0.04	2.03e-05
0.06	2.87e-05
0.08	2.47e-05
0.10	2.92e-05

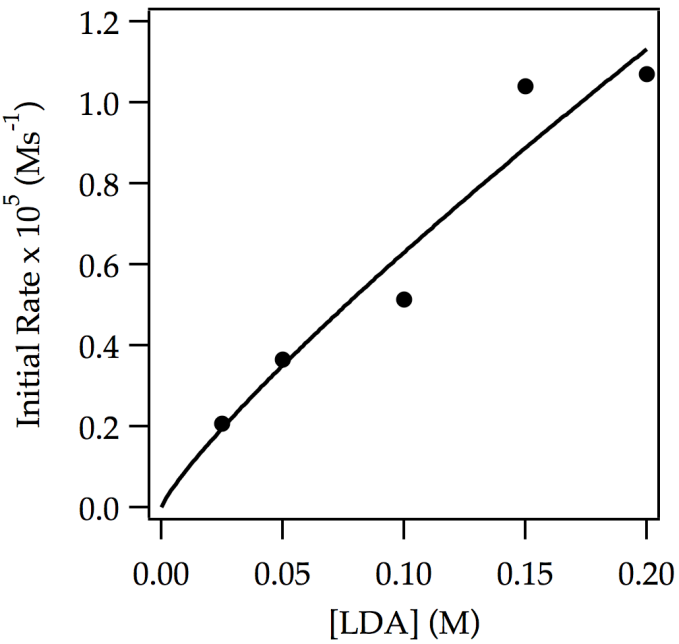


Figure 36. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1-*d*$_4$** (0.002 M) in the presence of 0.020 M ArLi (**2-*d*$_3$**) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (4 \pm 1) \times 10^{-5}$, $n = 0.9 \pm 0.2$]

[LDA] (M)	y_1 (M·s^{-1})
0.025	2.06e-06
0.05	3.65e-06
0.01	5.14e-06
0.15	1.04e-05
0.20	1.07e-05

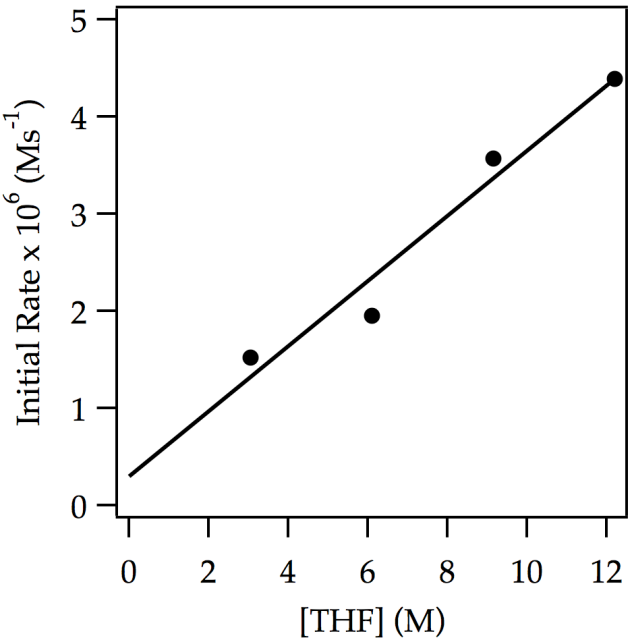


Figure 37. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1-*d*$_4$** (0.002 M) in the presence of 0.020 M ArLi (**2-*d*$_3$**) by LDA (0.10 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [$a = (3.4 \pm 0.5) \times 10^{-7}$, $b = (3 \pm 4) \times 10^{-7}$]

[THF] (M)	y_1 (M·s^{-1})
3.05	1.52e-06
6.10	1.95e-06
9.15	3.57e-06
12.2	4.39e-06

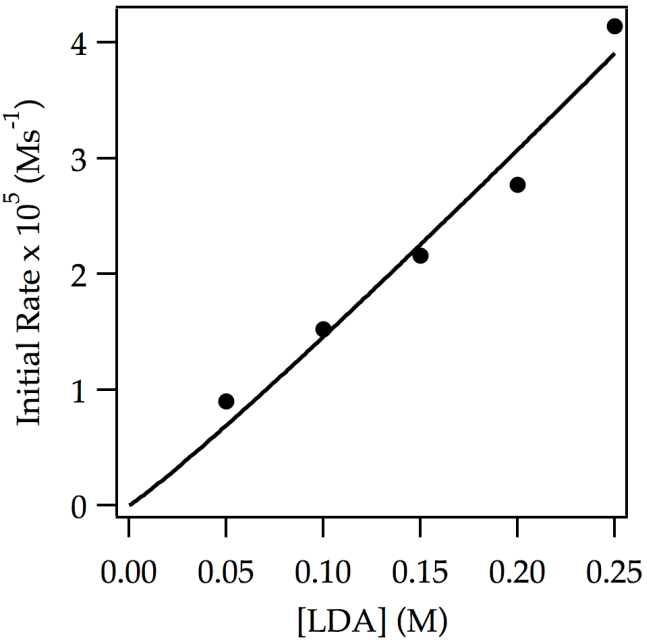


Figure 38. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1-*d*$_4$** (0.08 M) in the presence of 0.020 M ArLi (**2-*d*$_3$**) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (1.7 \pm 0.4) \times 10^{-4}$, $n = 1.1 \pm 0.1$]

[LDA] (M)	y_1 (M·s^{-1})
0.05	9.80e-06
0.01	1.52e-06
0.15	2.16e-05
0.20	2.77e-05
0.25	4.14e-05

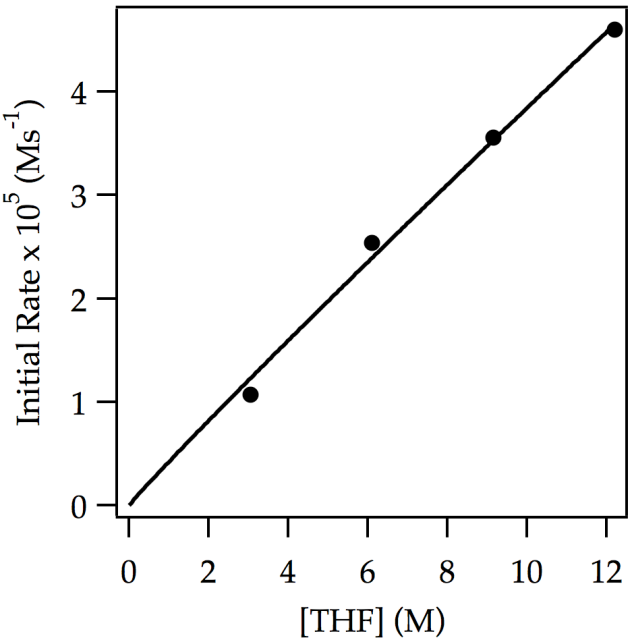


Figure 39. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1-*d*$_4$** (0.08 M) in the presence of 0.020 M ArLi (**2-*d*$_3$**) by LDA (0.10 M) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}]^n$. [$a = (4.2 \pm 0.7) \times 10^{-6}$, $n = 0.96 \pm 0.08$]

[THF] (M)	y_1 (M·s^{-1})
3.05	1.07e-05
6.10	2.54e-05
9.15	3.56e-05
12.2	4.60e-05

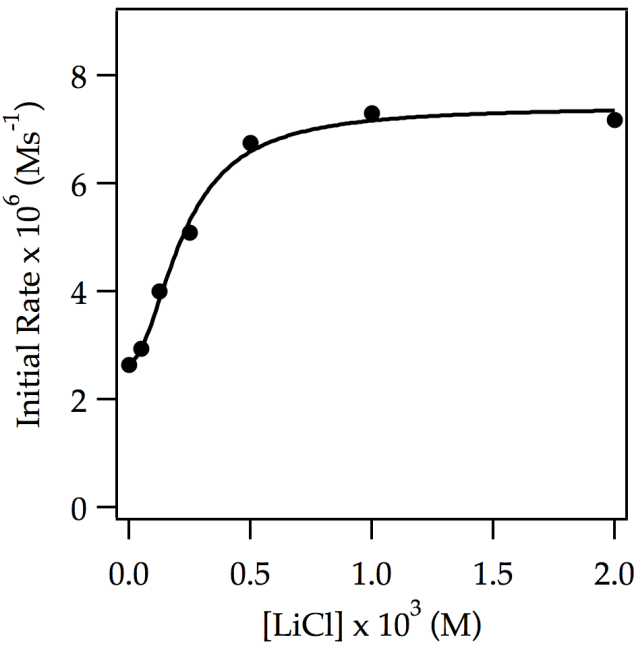


Figure 40. Plot of initial rate versus [LiCl] for the ortholithiation of **1-*d*$_4$** (0.002 M) by 0.10 M LDA in 12.2 M THF monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to eq 4 in derivation 4. [ArD_4] = 0.002 M, [A_2S_2] = 0.05 M. [$k_1 = (3.1 \pm 0.3) \times 10^{-5}$, $k_{-1} = 1000k_1$, $k_c = (3 \pm 7) \times 10^2$, $k_{-c} = 1000k_c$, $k_2 = (5.3 \pm 0.2) \times 10^{-1}$, $n = 1.8 \pm 0.4$]

[LiCl] x 10^3 (M)	y_1 (M·s^{-1})
0	2.64e-06
0.05	2.94e-06
0.125	4.00e-06
0.25	5.08e-06
0.50	6.75e-06
1.0	7.29e-06
2.0	7.18e-06

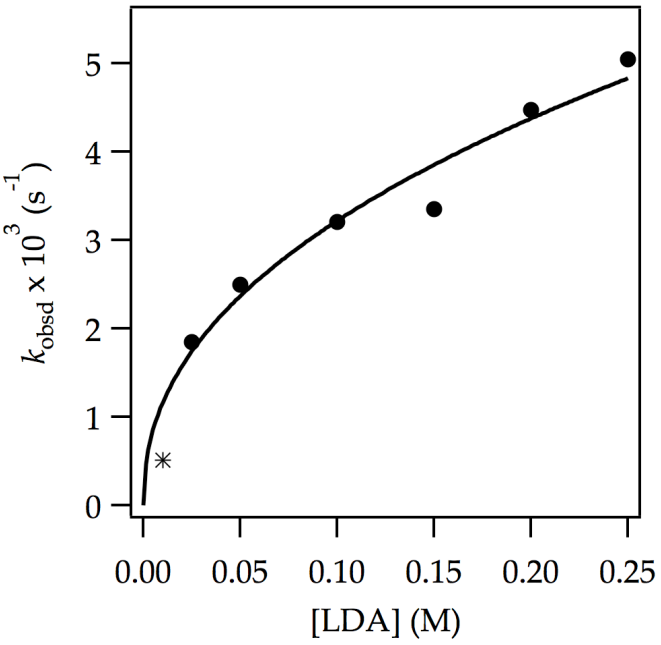


Figure 41. Plot of k_{obsd} versus [LDA] in THF (12.2 M) for the ortholithiation of **1-*d*$_4$** (0.002 M) in the presence of 1.5 mol% LiCl (1.5 mM) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (2.1 \pm 0.2) \times 10^{-2}$, $n = 0.47 \pm 0.04$]. Asterisk is not included in the fit.

[LDA] (M)	y_1 (s^{-1})
0.010*	5.10e-04
0.025	1.85e-03
0.05	2.50e-03
0.01	3.21e-03
0.15	3.35e-03
0.20	4.48e-03
0.25	5.05e-03

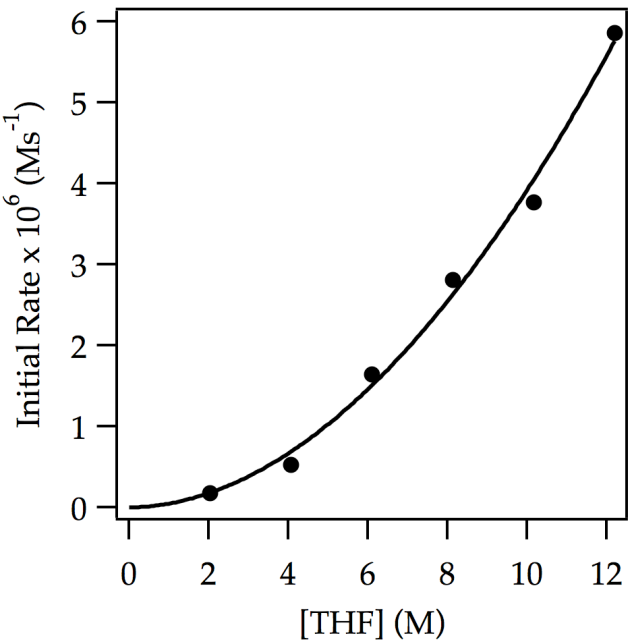


Figure 42. Plot of initial rate versus [THF] in Et_2O for the ortholithiation of **1-*d*$_4$** (0.002 M) by LDA (0.10 M) in the presence of 1.5 mol% LiCl (1.5 mM) monitored with IR spectroscopy at –78 °C. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}]^n$. [$a = (5 \pm 1) \times 10^{-8}$, $n = 1.9 \pm 0.1$]

[THF] (M)	y_1 (M·s^{-1})
2.03	1.74e-07
4.07	5.26e-07
6.10	1.64e-06
8.13	2.81e-06
10.17	3.77e-06
12.2	5.86e-06

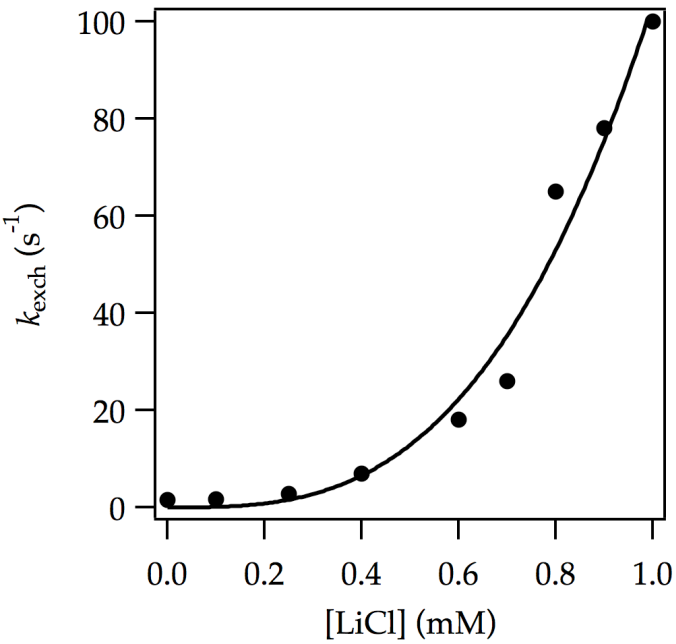


Figure 43. Plot of ^{6}Li nuclear exchange rate versus [LiCl] of [^{6}Li,^{15}N] LDA (0.10 M) at 10 °C in 12.2 M THF. The curve depicts an unweighted least-squares fit to $y = a[\text{LiCl}]^{n}$. [$a = 104 \pm 6$, $n = 3.0 \pm 0.3$]

[LiCl] (mM)	y (s^{-1})
0.00	1.5
0.10	1.7
0.25	2.8
0.40	7.0
0.60	18
0.70	26
0.80	65
0.90	78
1.00	100

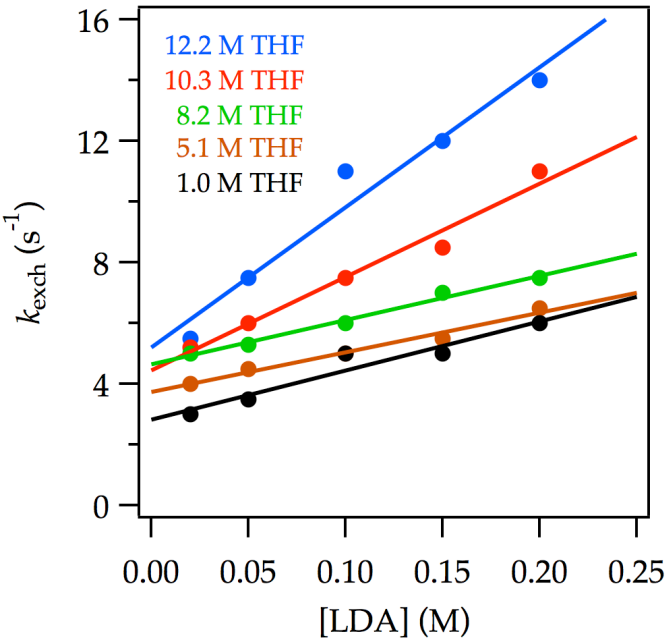


Figure 44. Plot of ^{6}Li nuclear exchange rate at 35 °C versus [LDA] at varying [^{6}Li,^{15}N] LDA and THF concentrations with hexanes as cosolvent. The curve depicts an unweighted least-squares fit to linear functions.

		y_1 (s^{-1})	y_2 (s^{-1})	y_3 (s^{-1})	y_4 (s^{-1})	y_5 (s^{-1})
[LDA] (M)	[THF]	12.2 M	10.3 M	8.2 M	5.1 M	1.0 M
0.02		5.5	5.2	5.0	4.0	3.0
0.05		7.5	6.0	5.3	4.5	3.5
0.10		11	7.5	6.0	5.0	5.0
0.15		12	8.5	7.0	5.5	5.0
0.20		14	11	7.5	6.5	6.0

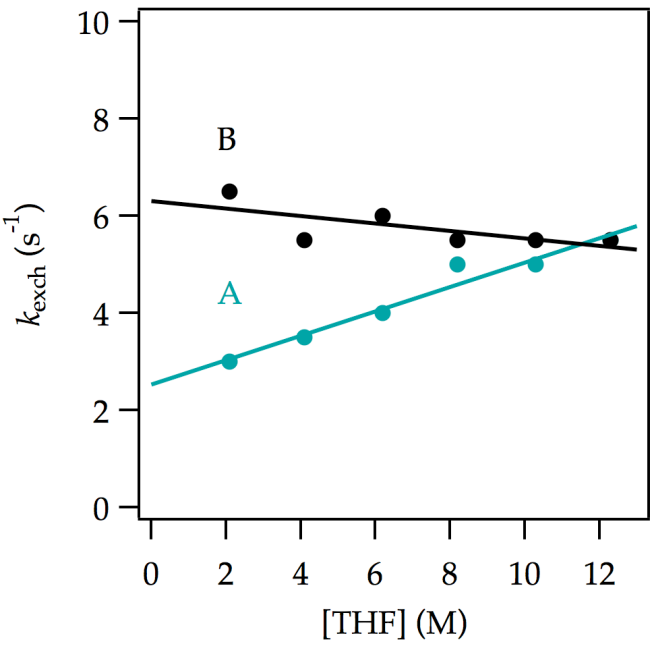
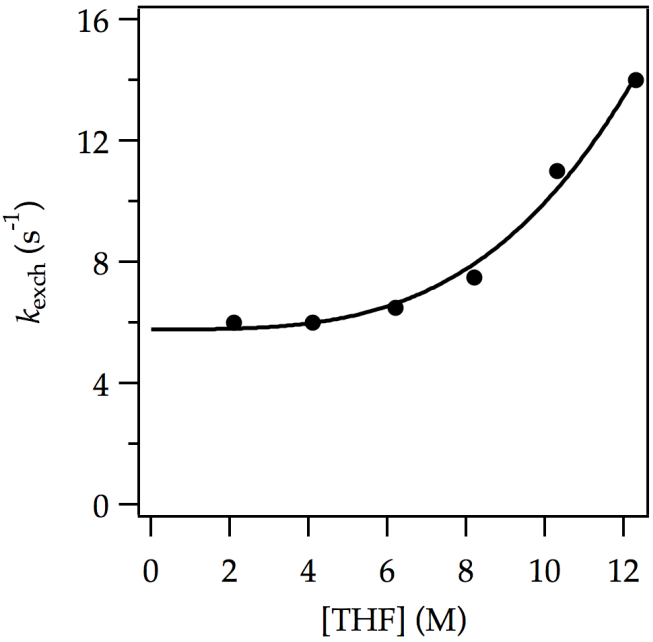


Figure 45. Plot of ^{6}Li nuclear exchange rate of [^{6}Li,^{15}N] LDA (0.02 M) at varying THF concentrations with (A) hexanes (y_1), and (B) 2,5-Me$_2$THF (y_2), as the cosolvent at 35 °C. The curve depicts an unweighted least-squares fit to (A) $y = a$[THF]+b. [a = 0.25± 0.03, b = 2.5 ± 0.2], (B) $y = a$[THF]+b. [a = -0.08± 0.04, b = 6.3 ± 0.3]

[THF] (M)	y_1 (s^{-1})	y_2 (s^{-1})
2.1	3.0	6.5
4.1	3.5	5.5
6.2	4.0	6.0
8.2	5.0	5.5
10.3	5.0	5.5
12.3	5.5	-

(A)



(B)

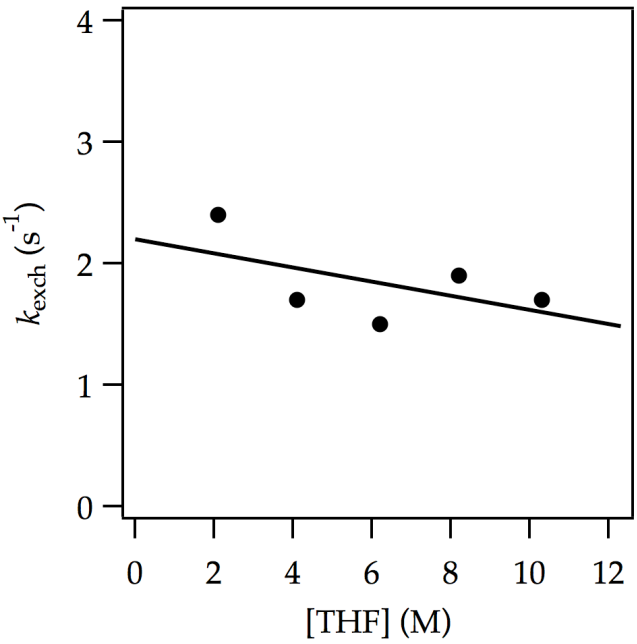
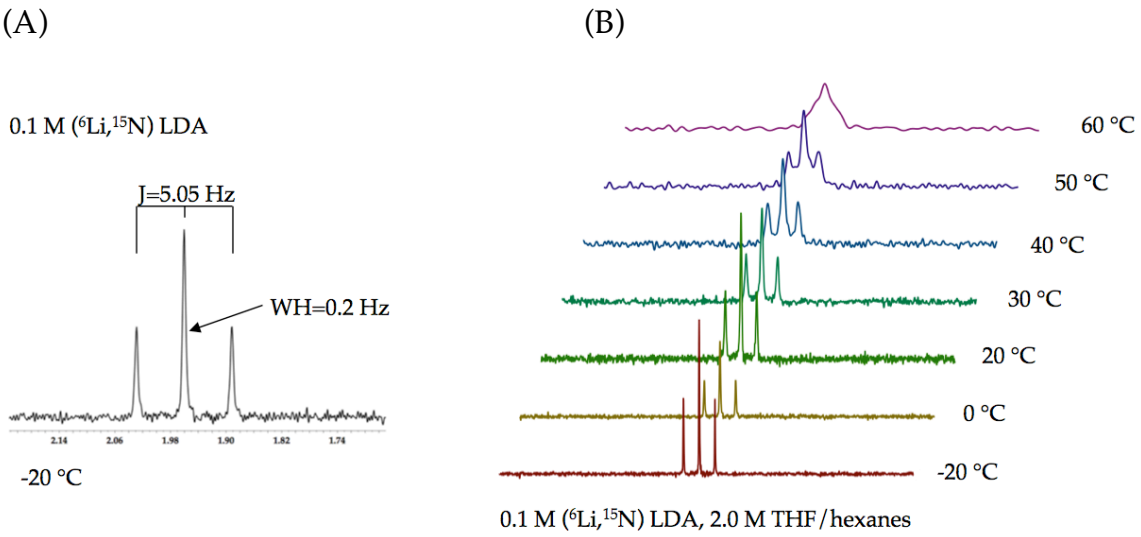


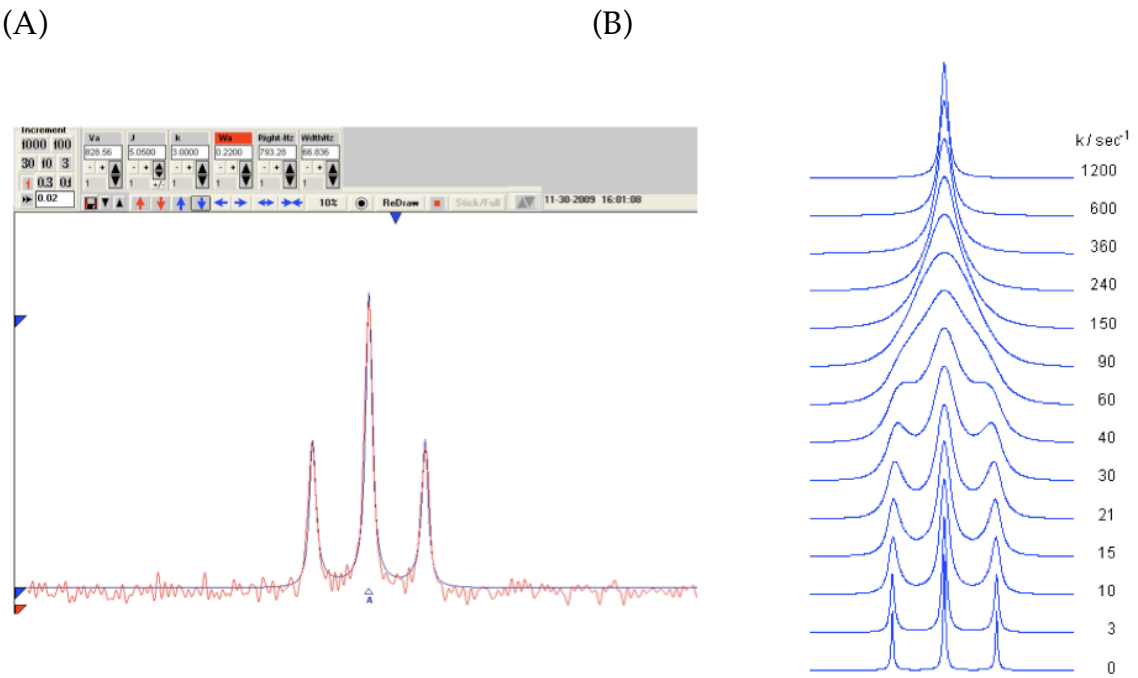
Figure 46. Plot of ^{6}Li nuclear exchange rate of [^{6}Li,^{15}N] LDA (0.20 M) at varying THF concentrations with (A) hexanes, and (B) 2,5-Me_2THF, as the cosolvent at 35 °C. The curve depicts an unweighted least-squares fit to (A) $y = a[\text{THF}]^n+b$. [a = (2 $\pm$ 3) x10^{-3}, n = 3.3 $\pm$ 0.5, b = 5.8 $\pm$ 0.4] (B) $y = a[\text{THF}]+b$. [a = -0.06$\pm$ 0.05, b = 2.2 $\pm$ 0.4]

Figure 46 cont.

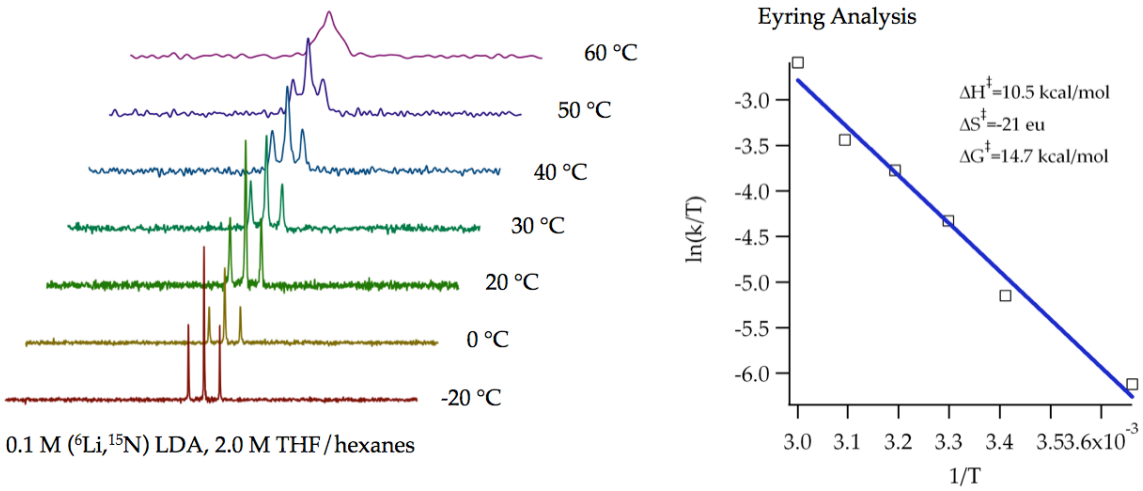
[THF] (M)	y_1 (s^{-1})	y_2 (s^{-1})
2.1	6.0	2.4
4.1	6.0	1.7
6.2	6.5	1.5
8.2	7.5	1.9
10.3	11	1.7
12.3	14	-



Scheme 1. ^{6}Li NMR spectra of [^{6}Li,^{15}N] LDA (0.10 M) in 12.2 M THF at (A) –20 °C, (B) –20 to +60 °C. The coupling constant by ^{15}N and the width at half height are indicated.



Scheme 2. (A) Screenshot of the NMR line shape analysis software *WinDNMR* by Hans Reich. The spectra are handfitted by adjusting the peak frequency (Va), the coupling frequency (*J*), the exchange rate (*k*), and the width at half height (Wa). Wa and *J* are determined at the low exchange limit for which *k* is effectively zero. (B) Simulation of a triplet exchange at varying exchange rates.



Scheme 3. ^{6}Li NMR spectra of [^{6}Li,^{15}N] LDA (0.10 M) in 12.2 M THF at varying temperatures, and the corresponding Eyring plot.

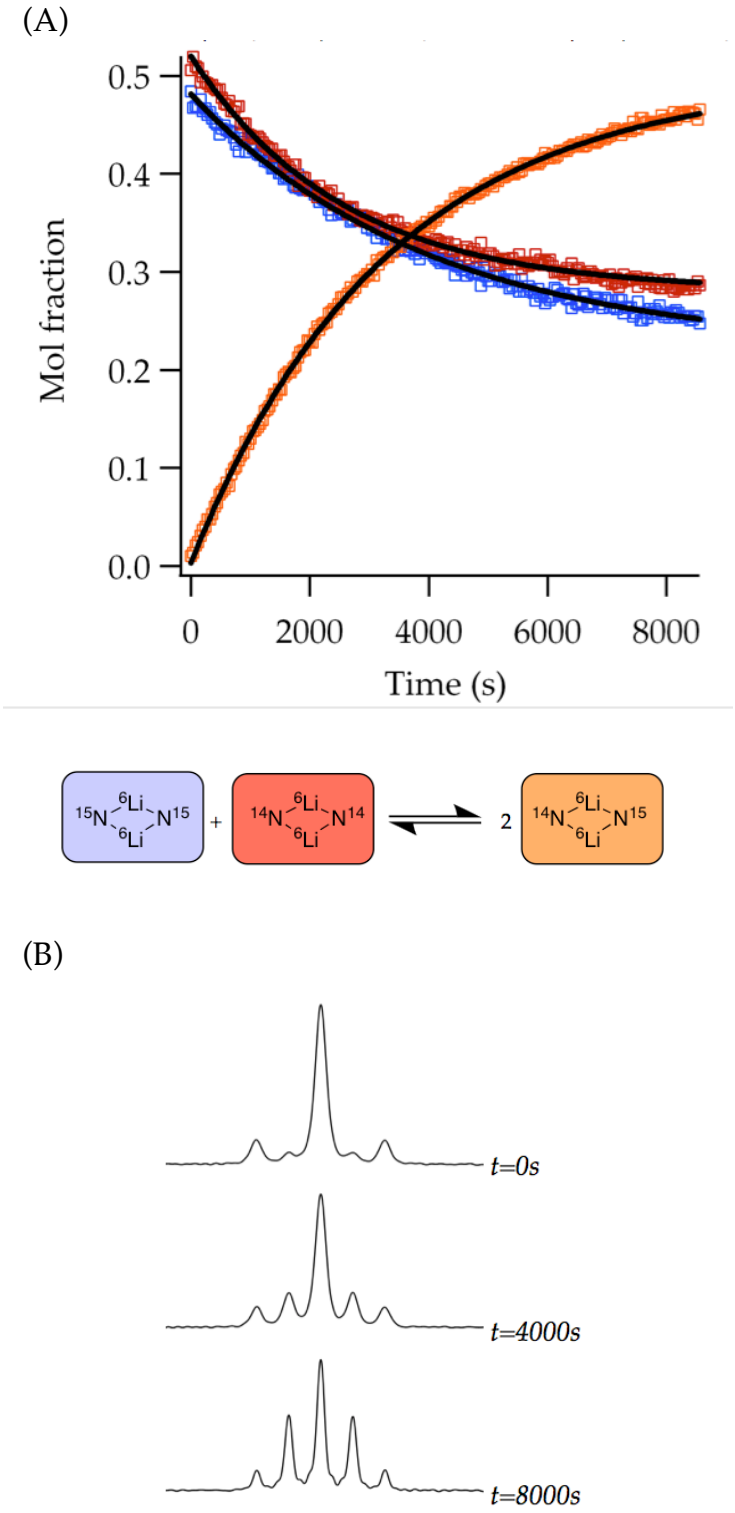


Figure 47. (A) Representative ^{6}Li NMR time trace of the ^{6}Li nuclear exchange of [^{6}Li] LDA (0.10 M) and [^{6}Li,^{15}N] LDA (0.10 M) in 12.2 M THF at –60 °C. (B) Select ^{6}Li NMR spectra at the indicated time point of the time trace in (A).

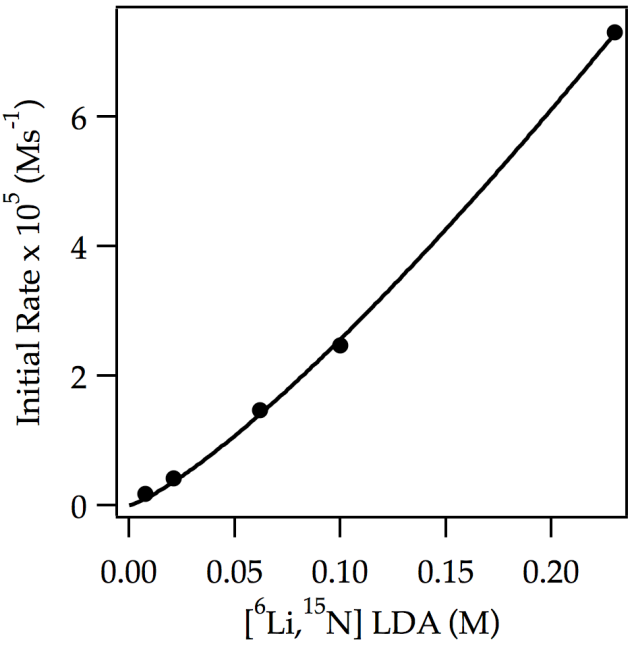


Figure 48. Plot of initial rate versus [^{6}Li,^{15}N] LDA for the subunit exchange in the presence of 0.10M [^{6}Li] LDA at –60 °C in 12.2 M THF. The curve depicts an unweighted least-squares fit to $y = a[\mathrm{LDA}]^{n}$. [$a = (4.6 \pm 0.2)\ \mathrm{x}10^{-4}$, $n = 1.25 \pm 0.03$]

[^{6}Li,^{15}N] LDA (M)	y (M•s^{-1})
0.0076	1.80e-06
0.021	4.20e-06
0.062	1.47e-05
0.10	2.47e-05
0.23	7.30e-05

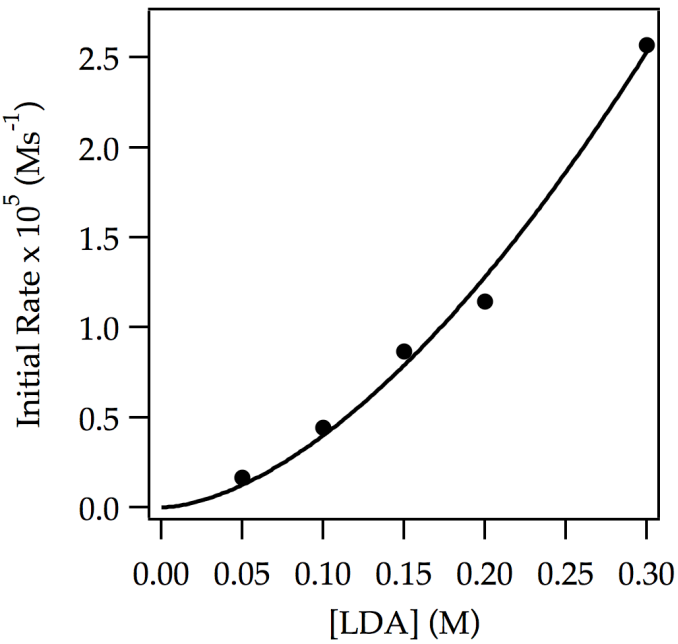
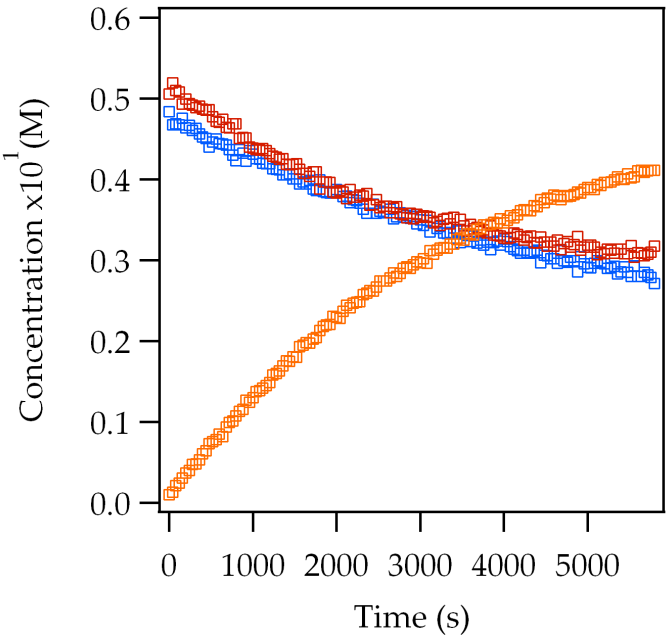


Figure 49. Plot of initial rate for the loss of [^{6}Li,^{15}N] LDA in 1:1 mixtures of [^{6}Li]LDA and [^{6}Li,^{15}N]LDA versus total [LDA] titer at –60 °C in 12.2 M THF. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (1.9 \pm 0.3) \times 10^{-4}$, $n = 1.7 \pm 0.1$]

[LDA] (M)	y (M·s^{-1})
0.05	1.64e-06
0.10	4.43e-06
0.15	8.68e-06
0.20	1.14e-05
0.30	2.57e-05

(A)



(B)

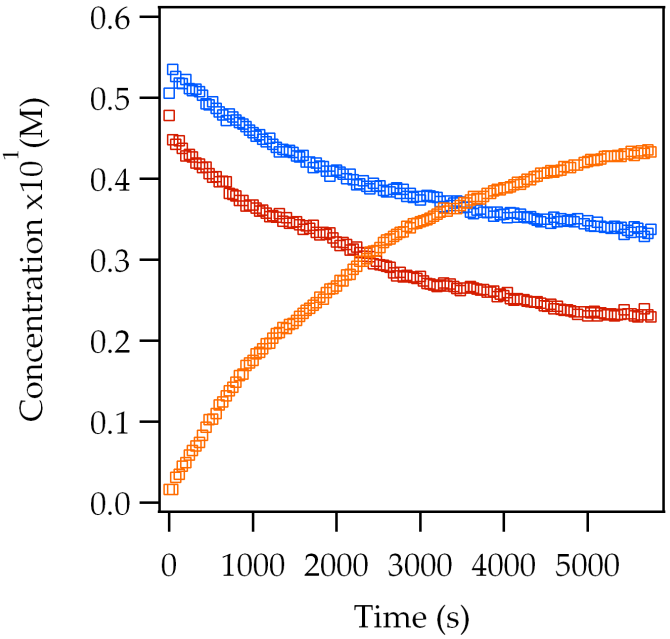


Figure 50. Concentration vs time for the exchange of [^{6}Li]LDA (0.05 M) with [^{6}Li,^{15}N]LDA (0.05 M) at –60 °C in (A) 12.2 M THF and (B) 1.5 M THF/hexanes. The initial rate is measured to be 2.7e-6 M·s^{-1} at 12.2 M THF and 3.2e-6 M·s^{-1} at 1.5 M THF/hexanes indicating a zeroth order dependence on THF.

Part 3: Derivations

Derivation 1. Derivation of fit function for aryllithium solvation.

$$0.5\ A_2S_2 + ArH + nS \quad \underset{}{\overset{K_{eq}}{\rightleftharpoons}} \quad AH + ArLiS_{n+1}$$

The equilibrium expression is defined as:

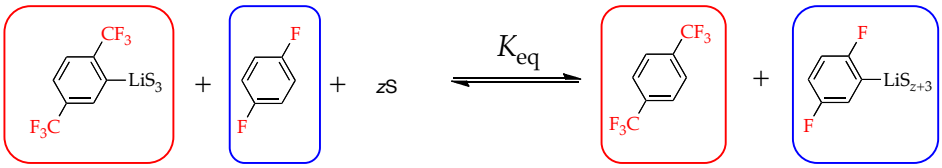
$$K_{eq} = \frac{[AH]\,[ArLiS_{n+1}]}{[A_2S_2]^{0.5}\,[ArH]\,[S]^n} \tag{1}$$

Rearranging the equation gives

$$\frac{[AH]\,[ArLiS_{n+1}]}{[A_2S_2]^{0.5}\,[ArH]} = K_{eq}\,[S]^n \tag{2}$$

Note: Concentrations of [ArH] and [$ArLi_{n+1}$] at equilibrium can be measured by ^{19}F NMR spectroscopy. [AH] and [A_2S_2] are calculated based on the extent of lithiation. K_{eq} and n are the two fitting parameters.

Derivation 2. Derivation of fit function for aryllithium **2** solvation by equilibration with other aryllithium of known solvation number.



$$ArLiS_3(CF_3) + ArH(F) + zS \underset{}{\overset{K_{eq}}{\rightleftharpoons}} ArH(CF_3) + ArLiS_{z+3}(F)$$

The equilibrium expression is defined as:

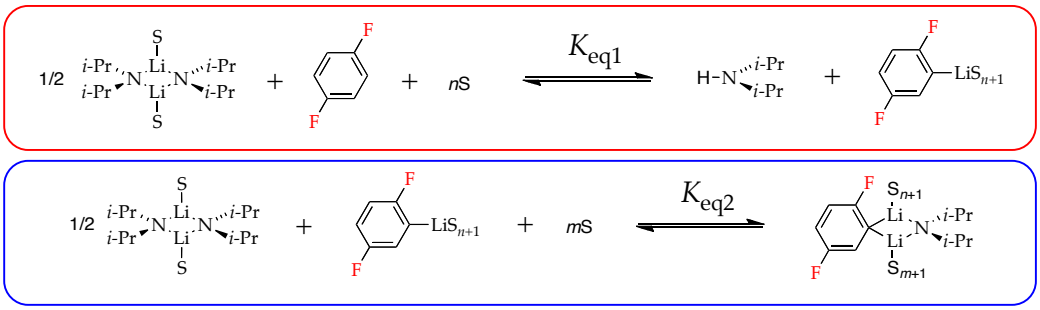
$$K_{eq} = \frac{[ArH(CF_3)]\,[ArLiS_{z+3}(F)]}{[ArLiS_3(CF_3)]\,[ArH(F)]\,[S]^z} \qquad (1)$$

Rearranging the equation gives

$$\frac{[ArH(CF_3)]\,[ArLiS_{z+3}(F)]}{[ArLiS_3(CF_3)]\,[ArH(F)]} = K_{eq}\,[S]^z \qquad (2)$$

Note: Concentrations of all species at equilibrium can be measured by ^{19}F NMR spectroscopy. K_{eq} and z are the two fitting parameters.

Derivation 3. Derivation of fit function for mixed dimer **3** solvation.



$$0.5\ A_2S_2 + ArH + n\mathrm{S} \underset{}{\overset{K_{eq1}}{\rightleftharpoons}} AH + ArLiS_{n+1}$$

$$0.5\ A_2S_2 + ArLiS_{n+1} + m\mathrm{S} \underset{}{\overset{K_{eq2}}{\rightleftharpoons}} ArLiS_{n+1} * AS_{m+1}$$

The equilibrium expressions are defined as:

$$K_{eq1} = \frac{[AH]\,[ArLiS_{n+1}]}{[A_2S_2]^{0.5}\,[ArH]\,[S]^n} \qquad K_{eq2} = \frac{[ArLiS_{n+1} * AS_{m+1}]}{[A_2S_2]^{0.5}\,[ArLiS_{n+1}]\,[S]^m} \tag{1}$$

Rearranging the equations to give

$$[A_2S_2]^{0.5} = \frac{[AH]\,[ArLiS_{n+1}]}{K_{eq1}\,[ArH]\,[S]^n} \qquad [A_2S_2]^{0.5} = \frac{[ArLiS_{n+1} * AS_{m+1}]}{K_{eq2}\,[ArLiS_{n+1}]\,[S]^m} \tag{2}$$

Combining both equations to give

$$\frac{[AH]\,[ArLiS_{n+1}]}{K_{eq1}\,[ArH]\,[S]^n} = \frac{[ArLiS_{n+1} * AS_{m+1}]}{K_{eq2}\,[ArLiS_{n+1}]\,[S]^m} \tag{3}$$

Further rearrangement gives

$$\frac{[AH]\,[ArLiS_{n+1}]}{[ArH]} * \frac{[ArLiS_{n+1}]}{[ArLiS_{n+1} * AS_{m+1}]} = \frac{K_{eq1}\,[S]^n}{K_{eq2}\,[S]^m} \tag{4}$$

Note: Concentrations of all fluorinated species at equilibrium can be measured by ^{19}F NMR spectroscopy. [AH] is calculated based on the extend of lithiation. K_{eq1} / K_{eq2} and (n-m) are the two fitting parameters.

Derivation 4. Derivation of LiCl saturation curve.

$$A_2 \underset{k_{-1}+k_{-c}[LiCl]^n}{\overset{k_1+k_c[LiCl]^n}{\rightleftharpoons}} 2A$$

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

The initial rate of consumption of ArH is defined as:

$$\frac{-d[ArH]}{dt} = k_2[A][ArH] \quad (1)$$

Applying the steady-state approximation to monomer A while denoting $a = (k_1 + k_c[LiCl]^n)$ and $b = (k_{-1} + k_{-c}[LiCl]^n)$

$$\frac{d[A]}{dt} = 2(a)[A_2] - 2(b)[A]^2 - k_2[ArH][A] = 0 \quad (2)$$

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

$$[A] = \frac{1}{4(b)}(\sqrt{k_2^2[ArH]^2 + 16(a)(b)[A_2]} - k_2[ArH]) \quad (3)$$

Substituting eq 3 into eq 1 gives

$$\frac{-d[ArH]}{dt} = \frac{k_2[ArH]}{4(b)}(\sqrt{k_2^2[ArH]^2 + 16(a)(b)[A_2]} - k_2[ArH]) \quad (4)$$

where [ArH] and $[A_2]$ are evaluated at t=0.

In the limit of no catalyst, the equation reduces to

$$\frac{-d[ArH]}{dt} = 2k_1[A_2] \quad (5)$$

In the limit of catalyst saturation, the equation becomes

$$\frac{-d[ArH]}{dt} = k_2\sqrt{\frac{k_1}{k_{-1}}}[ArH][A_2]^{1/2} \quad (6)$$

Derivation 5. Derivation of expression for fitting incremental addition curve (eq 12).

In a serial injection experiment, the amount of [ArH] injected remains constant, but the concentration of LDA and ArLi varies with each successive injection.

Hence, the rate of consumption of arene and its initial rate ($rate_{init}$) are defined as:

$$-d[\mathrm{ArH}]/d\mathrm{t} = k'[\mathrm{ArLi}]^n[\mathrm{LDA}]^m \quad (1)$$

Writing the concentrations in terms of mole fractions:

$$-d[\mathrm{ArH}]/d\mathrm{t} = k[X_{\mathrm{ArLi}}]^n[X_{\mathrm{LDA}}]^m \quad (2)$$

where $X_{\mathrm{ArLi}} = \mathrm{N}_{\mathrm{ArLi}}/(\mathrm{N}_{\mathrm{ArLi}} + \mathrm{N}_{\mathrm{LDA}})$ (N stands for normality)

Also, $X_{\mathrm{LDA}} = 1 - X_{\mathrm{ArLi}}$ (3)

Substituting eq 3 into eq 2 gives

$$-d[\mathrm{ArH}]/d\mathrm{t} = k[X_{\mathrm{ArLi}}]^n[1 - X_{\mathrm{ArLi}}]^m \quad (4)$$

The initial rate in the absence of autocatalysis, assuming an LDA order of 1 is given by:

$$-d[\mathrm{ArH}]/d\mathrm{t} = k'[X_{\mathrm{LDA}}]^1 \quad (5)$$
$$-d[\mathrm{ArH}]/d\mathrm{t} = k'[1 - X_{\mathrm{ArLi}}]^1 \quad (6)$$

To account for the rate in the presence of autocatalysis, we add eq 6 to eq 4. Hence, eq 4 becomes

$$-d[\mathrm{ArH}]/d\mathrm{t} = k[X_{\mathrm{ArLi}}]^n[1 - X_{\mathrm{ArLi}}]^m + k'[1 - X_{\mathrm{ArLi}}]^1 \quad (7)$$

Derivation 6. Derivation of ArLi saturation curve.

$$A_2 \underset{k_{-1} + k_{-c}[\mathrm{ArLi}]^n}{\overset{k_1 + k_c[\mathrm{ArLi}]^n}{\rightleftharpoons}} A_2^*$$

$$A_2 + A_2^* \xrightarrow{k_2} A_4$$

The consumption rate of the reaction is defined as

$$\frac{-d[\mathrm{ArH}]}{dt} = k_2[A_2][A_2^*] \tag{1}$$

Applying steady state approximation to A_2^* gives

$$\frac{d[A_2^*]}{dt} = (k_1 + k_c[\mathrm{ArLi}]^n)[A_2] - (k_{-1} + k_{-c}[\mathrm{ArLi}]^n)[A_2^*] - k_2[A_2][A_2^*] = 0 \tag{2}$$

Solving for A_2^* gives

$$[A_2^*] = \frac{(k_1 + k_c[\mathrm{ArLi}]^n)[A_2]}{(k_{-1} + k_{-c}[\mathrm{ArLi}]^n) + k_2[A_2]} \tag{3}$$

Combining equations 1 and 3 gives

$$\frac{-d[\mathrm{ArH}]}{dt} = \frac{(k_1 + k_c[\mathrm{ArLi}]^n)k_2[A_2]^2}{(k_{-1} + k_{-c}[\mathrm{ArLi}]^n) + k_2[A_2]} \tag{4}$$

In the absence of catalyst and $k_2[A] >> k_{-1}$, the equation reduces to

$$\frac{-d[\mathrm{ArH}]}{dt} = k_1[A_2] \tag{5}$$

In the limit of catalyst saturation, the equation becomes

$$\frac{-d[\mathrm{ArH}]}{dt} = \frac{k_1}{k_{-1}}k_2[A_2]^2 \tag{6}$$

Derivation 7. Saturation equation for dimer based subunit exchange.

$$A_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2A \qquad B_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2B \qquad AB \underset{2k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B$$

The consumption rate of the reaction is defined as:

$$\frac{d[AB]}{dt} = 2k_{-1}[A][B] - k_1[AB] \tag{1}$$

Applying the steady state approximation to [A] and [B] and set [AB] to 0

$$\frac{d[A]}{dt} = 2k_1[A_2] - 2k_{-1}[A]^2 - 2k_{-1}[A][B] + k_1[AB] = 0 \tag{2}$$

$$\frac{d[B]}{dt} = 2k_1[B_2] - 2k_{-1}[B]^2 - 2k_{-1}[A][B] + k_1[AB] = 0 \tag{3}$$

Solving for [A] and [B] using the quadratic equation gives

$$[A] = \sqrt{\frac{[B]^2}{4} + \frac{k_1}{k_{-1}}[A_2]} - \frac{1}{2}[B] \qquad [B] = \sqrt{\frac{[A]^2}{4} + \frac{k_1}{k_{-1}}[B_2]} - \frac{1}{2}[A] \qquad (4) + (5)$$

Adding eq 2 to eq 3 and solving for [A] and [B] gives

$$[A] = \sqrt{\frac{k_1}{k_{-1}}([A_2]+[B_2])} - [B] \qquad [B] = \sqrt{\frac{k_1}{k_{-1}}([A_2]+[B_2])} - [A] \qquad (6) + (7)$$

Substituting eq 7 into eq 4 and eq 6 into eq 5 and solving for [A] and [B]

$$[A] = \frac{[A_2]\sqrt{k_1}}{\sqrt{k_{-1}([A_2]+[B_2])}} \qquad [B] = \frac{[B_2]\sqrt{k_1}}{\sqrt{k_{-1}([A_2]+[B_2])}} \qquad (8) + (9)$$

Substituting eq 8 and 9 into eq 1 and set [AB] to 0 gives

$$\frac{d[AB]}{dt} = \frac{2k_1[A_2][B_2]}{[A_2]+[B_2]} \tag{10}$$

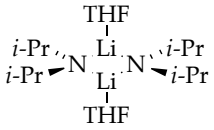
Divide top and bottom by $[A_2]$ and denote $a = 2k_1$ and $b = 1/[A_2]$ produces

$$\frac{d[AB]}{dt} = \frac{a[B_2]}{1+b[B_2]} \tag{11}$$

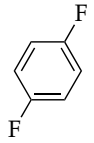
Part 4: DFT Computation

Chart 1

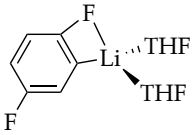
A



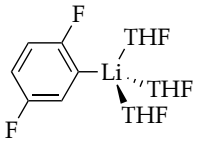
B



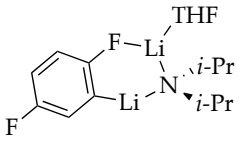
C



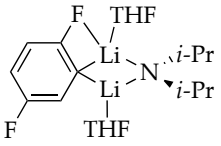
D-1



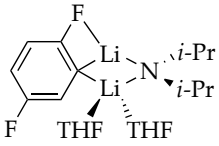
D-2



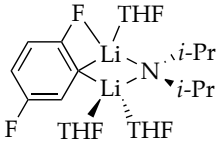
E-1



E-2

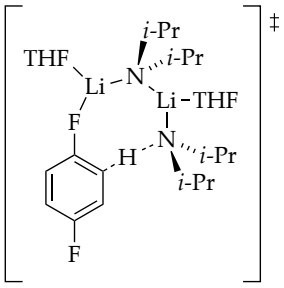


E-3

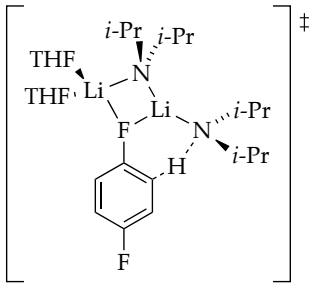


E-4

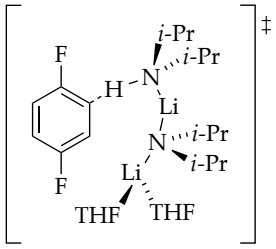
Chart 2



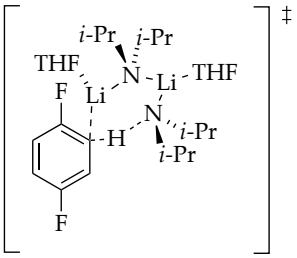
F



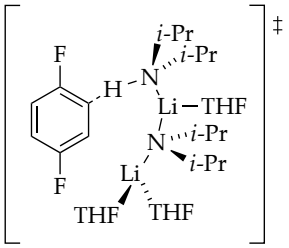
G



H



I



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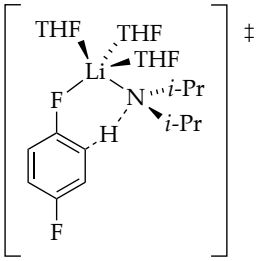
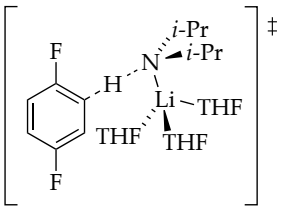


K



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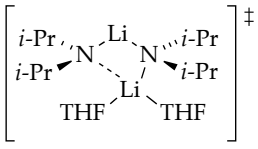

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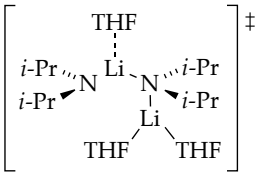
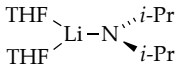


N

Chart 3



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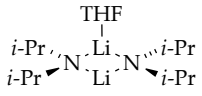

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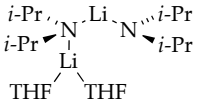

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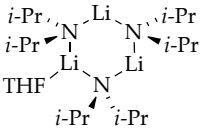

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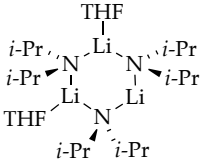

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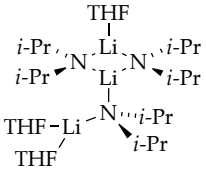
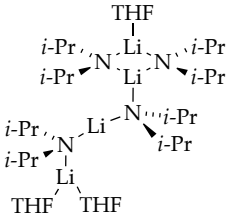


R-3



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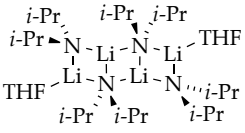

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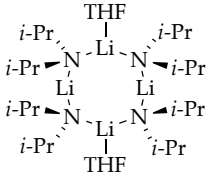

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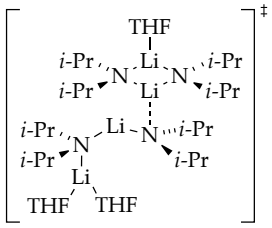

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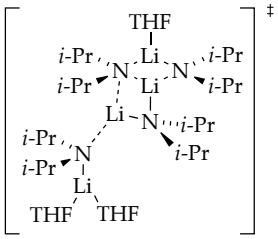
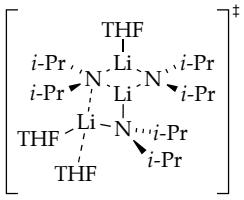
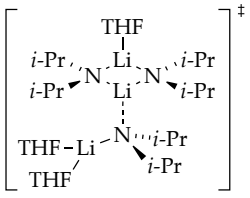


W

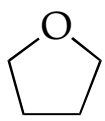


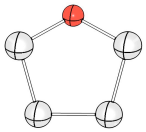
X



Y

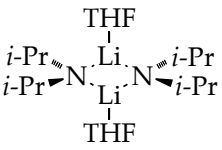
Table 1. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the reactants at –78 °C with free energies (Hartrees) and cartesian coordinates (X,Y,Z) (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

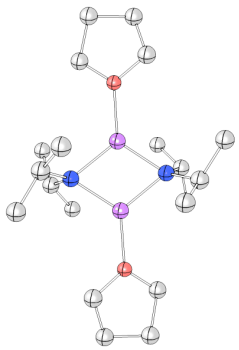




A
G = -232.349367
G_{MP2} = -231.6694404

Atom	X	Y	Z
C	0	0	0
O	1.132807	-0.739653	-0.442032
C	2.264796	-0.012388	0.019216
C	1.92285	1.47444	-0.210686
C	0.368847	1.489728	-0.185167
H	-0.032338	2.108191	0.623792
H	2.365524	2.11958	0.5546
H	2.296315	1.80941	-1.183111
H	2.436349	-0.210295	1.091379
H	3.13745	-0.361827	-0.539569
H	-0.860576	-0.323589	-0.591979
H	-0.206691	-0.218661	1.061467
H	-0.031366	1.878296	-1.126381





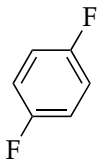
B
G = -1063.135501
G_{MP2} = -1059.937725

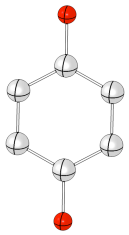
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	2.342273	-2.489712	-3.066295
N	1.208636	1.651497	0.054512	H	1.459639	-1.024712	-2.61925
C	1.39116	2.418143	1.296121	H	2.197266	-3.327267	-0.744239
C	2.354157	1.715455	2.267998	O	4.377659	-0.007833	-0.149374

Table 1 (Continued).

H	3.35351	1.612369	1.827423	C	5.226931	-1.136002	0.177639
H	2.45675	2.272938	3.207825	C	6.632699	-0.75042	-0.292196
H	1.996407	0.710457	2.527911	C	6.60642	0.781703	-0.175985
C	0.062992	2.727638	2.025475	C	5.17888	1.10291	-0.614951
H	-0.404588	1.799198	2.381707	H	5.097869	1.165111	-1.708138
H	0.210938	3.384896	2.894533	H	4.76747	2.017259	-0.182359
H	-0.643891	3.225258	1.35117	H	7.356982	1.27767	-0.79854
H	1.853057	3.400278	1.081215	H	6.765393	1.090722	0.863961
Li	2.389288	0.015575	0.000151	H	6.785755	-1.049705	-1.335767
N	1.18061	-1.635948	0.054545	H	7.414534	-1.219315	0.312467
C	0.997712	-2.402508	1.296154	H	5.185927	-1.29307	1.261339
C	2.325627	-2.711789	2.026056	H	4.82494	-2.023405	-0.318518
H	2.793014	-1.783266	2.382324	C	0.916955	2.561647	-1.058533
H	2.177402	-3.368931	2.895154	C	0.262689	1.821865	-2.23548
H	3.032798	-3.209463	1.352093	H	-0.681409	1.346346	-1.94212
C	0.034251	-1.699838	2.267586	H	0.048061	2.505124	-3.066774
H	-0.96495	-1.596941	1.826616	H	0.930465	1.040099	-2.61936
H	-0.06863	-2.257225	3.207438	C	2.156626	3.319383	-1.592437
H	0.39177	-0.694765	2.527528	H	2.851123	2.61614	-2.071628
H	0.536005	-3.384713	1.081164	H	1.88059	4.081234	-2.33552
C	1.472737	-2.546163	-1.058327	H	2.695608	3.828048	-0.785076
C	0.23331	-3.304044	-1.592589	H	0.192386	3.342833	-0.744747
H	-0.461095	-2.6009	-2.072056	O	-1.988352	0.02346	-0.150036
H	0.509659	-4.065925	-2.335526	C	-2.789454	-1.087285	-0.615741
H	-0.305885	-3.812705	-0.785366	C	-4.216803	-0.766713	-0.175751
C	2.127338	-1.806416	-2.235112	C	-4.24375	0.765406	-0.291896
H	3.071325	-1.330832	-1.941487	C	-2.837739	1.151607	0.176811
H	-4.374893	-1.075857	0.864293	H	-2.796006	1.309332	1.260376
H	-4.967616	-1.262934	-0.7978	H	-2.436368	2.038844	-0.320162
H	-2.709131	-1.148906	-1.709022	H	-5.025285	1.233986	0.313398
H	-2.377444	-2.001694	-0.183863	H	-4.397782	1.064636	-1.335336

Table 1 (Continued).

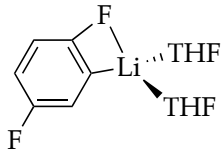


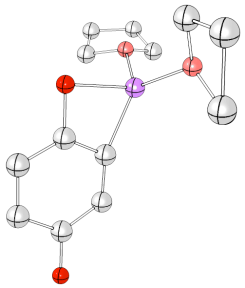


C
G = -430.647552
G_{MP2} = -429.4940576

Atom	X	Y	Z
C	0	0	0
C	0.673675	1.216576	0.000039
C	0.000262	2.433404	0.000081
C	1.395373	2.433304	0.000022
C	2.069264	1.216414	0.000165
C	1.395472	0.000144	0.000152
F	3.419751	1.216878	0.000055
H	1.960835	3.359105	0.000057
H	0.564798	3.359418	0.000189
F	2.024163	1.216878	0.000145
H	0.564873	0.926144	0.000082
H	1.959954	0.926528	-0.00016

Table 2. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of products 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).

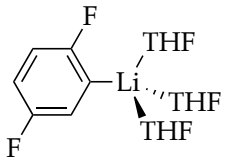


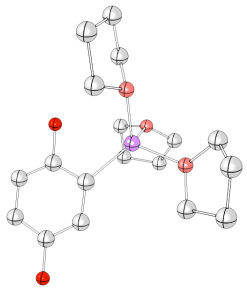


D-1
G = -902.315871
G_{MP2} = -899.7819475

Atom	X	Y	Z	Atom	X	Y	Z
C	0	0	0	H	3.89103	3.029114	-0.521797
O	0.831409	0.268012	1.142115	H	2.797179	4.385512	-0.947988
Li	2.484909	1.297424	0.956078	H	4.717384	4.196871	1.435122
C	4.357348	0.452916	0.665251	H	4.522866	5.573346	0.328766
C	5.473645	-0.062437	-0.023137	H	3.167966	5.625345	2.704464
C	6.618244	-0.476831	0.656577	H	2.303496	6.08275	1.227792
C	6.737111	-0.410682	2.042639	H	0.87188	4.263878	1.842338
C	5.655473	0.09362	2.771309	H	2.173948	3.430242	2.729556
C	4.550118	0.486557	2.031641	C	0.996743	-1.001248	1.811583
F	3.442187	1.006065	2.785818	C	-0.381401	-1.679723	1.721305
H	5.684286	0.170834	3.854916	C	-1.064484	-0.988123	0.506897
H	7.648452	-0.74539	2.527376	H	-1.354302	-1.697512	-0.273564
F	7.671275	-0.967585	-0.052757	H	-1.965987	-0.455405	0.823054
H	5.480733	-0.155223	-1.109504	H	-0.281609	-2.760323	1.584875
O	2.22798	3.208292	0.673585	H	-0.958888	-1.513258	2.635093
C	1.94035	4.025538	1.839579	H	1.773028	-1.576466	1.29001
C	2.838052	5.265385	1.725648	H	1.338894	-0.787665	2.824945
C	3.992617	4.765594	0.84189	H	-0.399648	0.955352	-0.347234
C	3.268133	3.833237	-0.123392	H	0.613239	-0.444486	-0.797456

Table 2 (Continued).

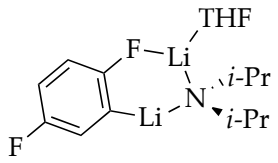


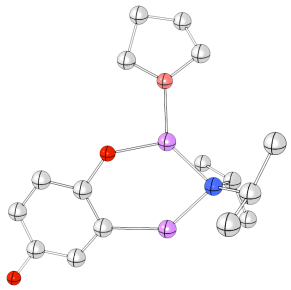


D-2
G = -1134.665978
G_{MP2} = -1131.478216

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	-1.066228	1.266228	3.468569
C	-1.977909	-0.201321	-0.728057	C	-1.879143	-0.00683	3.119493
C	-2.987446	0.670318	-1.193713	C	-0.804927	-0.994998	2.662446
C	-4.24425	0.213724	-1.588177	H	-1.145597	-1.72271	1.925942
C	-4.593724	-1.130726	-1.549237	H	-0.339182	-1.515225	3.513826
C	-3.632819	-2.036155	-1.089978	H	-2.56203	0.188237	2.288331
C	-2.3976	-1.524164	-0.709516	H	-2.460156	-0.384773	3.966263
F	-1.477042	-2.485918	-0.24566	H	-1.544248	2.163509	3.065532
H	-3.842716	-3.101242	-1.032087	H	-0.967902	1.40299	4.550253
H	-5.581532	-1.450236	-1.8655	H	1.089798	0.846098	3.586058
F	-5.170841	1.111509	-2.02897	H	0.649898	1.815163	2.154685
H	-2.820971	1.747117	-1.260492	O	0.910116	1.78117	-0.406082
O	1.428339	-1.293335	-0.685155	C	2.306047	1.876526	-0.754643
C	1.854424	-2.366972	0.171392	C	2.326434	2.515664	-2.141569
C	2.821456	-3.177497	-0.69618	C	1.153516	3.504725	-2.045212
C	2.227992	-3.027042	-2.121611	C	0.140696	2.74308	-1.177823
C	1.187904	-1.890347	-1.979253	H	-0.585521	2.180422	-1.770385
H	0.163209	-2.271723	-1.999772	H	-0.402772	3.392156	-0.483389
H	1.291431	-1.096929	-2.723161	H	0.737862	3.777642	-3.019479
H	1.744598	-3.948757	-2.458736	H	1.476263	4.426548	-1.54726
H	3.005649	-2.779532	-2.850037	H	2.128463	1.757821	-2.908895
H	2.892497	-4.220261	-0.372693	H	3.281822	2.996631	-2.372632
H	3.825004	-2.742023	-0.648502	H	2.823889	2.507783	-0.017616
H	2.30134	-1.919103	1.060743	H	2.71872	0.866274	-0.71855
H	0.980095	-2.961945	0.466448	C	0.318224	1.017759	2.822223
O	0.186711	-0.16958	2.017715				

Table 2 (Continued).

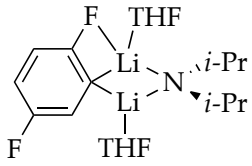


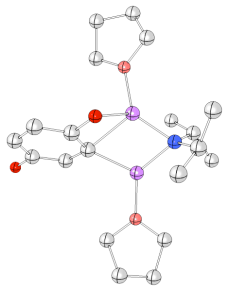


E-1
G = -969.185475
G_{MP2} = -966.3761757

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	-2.288946	5.869997	-1.041841
Li	0.127581	1.961569	-0.215594	H	-1.865965	6.59197	0.521089
Li	1.945511	-0.029353	-0.032954	H	-0.132279	4.939275	0.924211
C	3.469387	1.333381	-0.026367	H	-0.022073	5.03788	-0.849023
C	4.857577	1.202549	0.205354	C	-0.608796	-0.727766	-1.122499
C	5.718012	2.296741	0.153528	C	0.367712	-0.780076	-2.307923
C	5.274382	3.585281	-0.129005	H	1.275392	-1.348456	-2.05758
C	3.909916	3.767229	-0.365021	H	-0.08059	-1.258807	-3.186809
C	3.110693	2.63604	-0.295605	H	0.677543	0.232166	-2.606011
F	1.710531	2.903168	-0.550168	H	-0.820597	-1.776523	-0.842947
H	3.500115	4.746547	-0.5954	C	-1.952555	-0.124538	-1.590373
H	5.9776	4.410711	-0.162703	H	-2.653221	-0.02573	-0.753011
F	7.043257	2.110463	0.38463	H	-1.795914	0.875077	-2.022117
H	5.30294	0.23456	0.432862	H	-2.437032	-0.745469	-2.356073
O	-1.116161	3.436717	-0.118979	C	-0.592005	-0.363359	1.295817
C	-0.690195	4.822258	-0.012505	H	-1.695657	-0.430192	1.222757
C	-1.978575	5.645192	-0.014789	C	-0.104505	-1.728569	1.830876
C	-2.978045	4.68538	0.649478	H	-0.254485	-2.523256	1.091761
C	-2.549782	3.334626	0.076884	H	0.969385	-1.685718	2.066296
H	-3.020748	3.134817	-0.892997	H	-0.633947	-2.023124	2.747091
H	-2.740823	2.487873	0.741288	C	-0.282879	0.723555	2.339064
H	-4.021846	4.920182	0.422355	H	-0.730701	1.68942	2.065094
H	-2.854537	4.697022	1.738656	H	-0.66785	0.455309	3.330137
H	0.802094	0.872748	2.436432				

Table 2 (Continued).

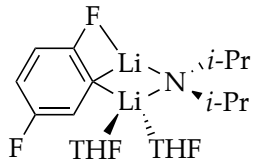


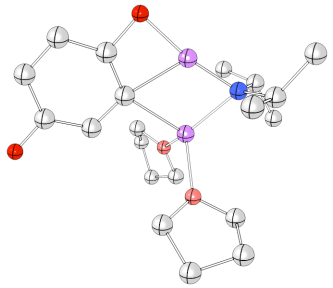


E-2
G = -1201.545187
G_{MP2} = -1198.084676

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	4.365325	0.526541	1.200296
Li	1.305203	1.49154	0.274532	H	3.775428	-0.386323	-0.211698
Li	-1.05799	1.642072	-0.33966	H	6.367023	0.598973	-0.175658
C	0.117779	3.465408	-0.072906	H	5.418401	0.626579	-1.67407
C	-0.230083	4.581967	-0.86814	H	5.694108	2.90312	0.367305
C	0.112954	5.8831	-0.505492	H	5.944103	3.011416	-1.38523
C	0.82473	6.171846	0.655293	H	3.564906	2.774231	-1.832741
C	1.205946	5.103508	1.471052	H	3.481313	3.651076	-0.285106
C	0.826525	3.832166	1.059183	C	-0.309479	-0.747005	1.224229
F	1.267876	2.766485	1.887357	C	-1.076668	0.141393	2.218064
H	1.767522	5.260105	2.387715	H	-2.037414	0.467862	1.796672
H	1.070981	7.199127	0.903123	H	-1.289294	-0.390242	3.154181
F	-0.25938	6.916049	-1.306336	H	-0.498306	1.039384	2.470473
H	-0.783411	4.460217	-1.80006	H	-0.966371	-1.612661	1.010924
O	-2.963357	1.942	-0.638989	C	0.943077	-1.326462	1.924561
C	-3.946362	0.874573	-0.69592	H	1.53427	-1.938336	1.233166
C	-5.283892	1.495254	-0.254748	H	1.586611	-0.514709	2.293848
C	-4.850443	2.772213	0.48537	H	0.679088	-1.960182	2.782876
C	-3.620463	3.188673	-0.314412	C	0.258976	-0.884887	-1.139162
H	-2.900466	3.804144	0.22759	H	0.952346	-1.705717	-0.860903
H	-3.900927	3.704062	-1.243531	C	-1.007813	-1.568817	-1.707015
H	-4.568328	2.546307	1.520177	H	-1.569862	-2.093533	-0.926622
H	-5.625336	3.544309	0.500526	H	-1.674266	-0.818815	-2.155869
H	-5.866951	0.81326	0.370718	H	-0.757161	-2.304352	-2.484098
H	-5.894385	1.752798	-1.127527	C	0.943275	-0.107627	-2.275047
H	-3.977993	0.477227	-1.71523	H	1.905931	0.307406	-1.954593
H	-3.605264	0.08154	-0.024035	H	1.121833	-0.747094	-3.148517
O	3.219077	1.603421	-0.154354	H	0.314087	0.731794	-2.606353
C	3.854804	2.748935	-0.77482	C	5.455631	0.987331	-0.639536
C	5.356943	2.520803	-0.603397	C	4.193593	0.568976	0.117307

Table 2 (Continued).

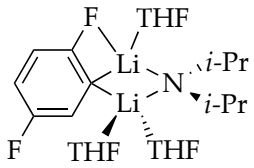


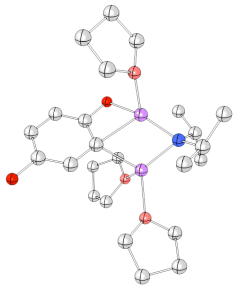


E-3
G = -1201.534585
G_{MP2} = -1198.076993

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	-2.554855	1.214013	-1.201208
N	-1.451067	-1.344955	-0.799489	H	-3.719616	0.703986	-2.444832
Li	0.259201	-2.171783	-1.025234	C	-1.241543	-0.376367	-3.051579
F	1.765657	-3.284262	-1.285997	H	-0.614855	-1.216489	-3.382904
C	2.6186	-2.367018	-0.575295	H	-1.785865	-0.005529	-3.929122
C	2.010025	-1.206407	-0.13467	H	-0.581582	0.426644	-2.702355
C	2.92433	-0.370451	0.545458	O	0.600807	1.762469	-0.866527
C	4.260663	-0.722739	0.725776	C	-0.009275	3.042074	-0.588524
C	4.791659	-1.916558	0.24865	C	0.918886	4.091096	-1.205571
C	3.933501	-2.78143	-0.43505	C	1.510692	3.326401	-2.399223
H	4.278473	-3.729098	-0.837412	C	1.678822	1.92026	-1.823128
H	5.83813	-2.153784	0.408122	H	2.632107	1.802306	-1.296661
F	5.083541	0.131478	1.390389	H	1.592505	1.124051	-2.566143
H	2.614091	0.593248	0.949743	H	2.455922	3.744618	-2.757668
C	-2.287708	-2.072339	0.161025	H	0.801929	3.316807	-3.235673
C	-1.408075	-2.625444	1.294877	H	1.710359	4.367273	-0.498816
H	-0.804023	-1.836986	1.755885	H	0.385855	5.002479	-1.492552
H	-2.016133	-3.095018	2.077973	H	-1.004368	3.064172	-1.052204
H	-0.718989	-3.398893	0.921535	H	-0.123727	3.134558	0.494711
H	-3.035041	-1.406444	0.646615	O	-0.393996	0.762175	1.867801
C	-3.104973	-3.244699	-0.42996	C	-1.748889	1.021434	2.297688
H	-3.851457	-2.91159	-1.15786	C	-1.801514	0.559383	3.751247
H	-2.437792	-3.955981	-0.937439	C	-0.398287	0.94085	4.249874
H	-3.64216	-3.784004	0.361158	C	0.482023	0.672079	3.021122
C	-2.204118	-0.813681	-1.938522	H	0.919602	-0.331363	3.031405
H	-2.849936	-1.588945	-2.390148	H	1.290221	1.401157	2.906162
C	-3.139533	0.362605	-1.576617	H	-0.076852	0.362751	5.120982
H	-3.855052	0.078873	-0.796117	H	-0.36763	2.002607	4.521192
H	-1.954157	2.098609	2.213951	H	-1.947155	-0.525447	3.796766
H	-2.416104	0.478512	1.625811	H	-2.606156	1.039159	4.316448

Table 2 (Continued).

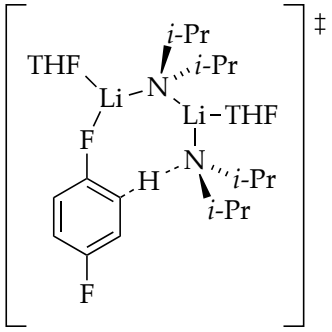


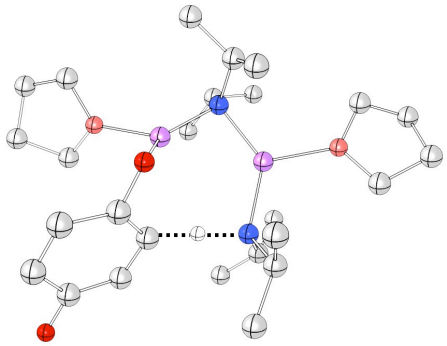


E-4
G = -1433.88825
G_{MP2} = -1429.779748

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	C	-5.594927	1.63566	-0.729663
Li	1.036157	1.765313	-0.379037	C	-4.961515	2.614248	-1.732088
Li	-1.41945	1.328559	-0.340139	C	-3.726271	1.839671	-2.183445
C	-0.576225	3.309926	-0.995372	H	-2.900484	2.470684	-2.519548
C	-0.198628	4.21489	-2.012518	H	-3.97055	1.110438	-2.968086
C	-0.647644	5.535523	-2.034046	H	-4.658972	3.541347	-1.232355
C	-1.506153	6.048814	-1.067174	H	-5.624984	2.870217	-2.563676
C	-1.927728	5.189322	-0.047295	H	-6.254454	2.124269	-0.006435
C	-1.437161	3.889989	-0.078754	H	-6.179864	0.874548	-1.259062
F	-1.902014	3.035819	0.954954	H	-4.503001	-0.057826	0.177095
H	-2.605095	5.524822	0.733574	H	-4.081084	1.53559	0.855089
H	-1.834924	7.081527	-1.120283	O	1.996561	2.98596	1.057099
F	-0.234661	6.360618	-3.033509	C	2.874683	4.012778	0.546807
H	0.459476	3.907655	-2.825462	C	3.058414	5.006437	1.693091
C	0.209479	-0.602523	1.323408	C	1.682912	4.95019	2.372984
C	-0.623813	0.104901	2.403645	C	1.318353	3.468051	2.244994
H	-1.695555	0.007024	2.186454	H	0.247191	3.301137	2.12141
H	-0.441636	-0.315765	3.401719	H	1.676299	2.882707	3.10098
H	-0.390762	1.175047	2.447789	H	0.961624	5.565713	1.823909
H	-0.12873	-1.653673	1.330904	H	1.697558	5.286228	3.414232
C	1.697018	-0.643986	1.746479	H	3.3279	6.006421	1.339485
H	2.29525	-1.170343	0.992492	H	3.842223	4.662162	2.378602
H	2.101071	0.371808	1.84875	H	3.802051	3.534637	0.221681
H	1.840893	-1.16633	2.703556	H	2.395981	4.489427	-0.318659
C	0.04112	-1.022671	-1.052728	O	2.728985	1.705286	-1.587862
H	0.943766	-1.666188	-0.951259	C	3.658222	0.612857	-1.386878
C	-1.173893	-1.985291	-1.051618	C	4.378343	0.431083	-2.72427
H	-1.309519	-2.473688	-0.080754	C	4.379379	1.861489	-3.285337
H	-2.091983	-1.42689	-1.277651	C	3.012039	2.379697	-2.833126
H	-1.05925	-2.778582	-1.804135	H	2.225994	2.12702	-3.556503
C	0.125115	-0.374593	-2.444414	H	2.986976	3.458054	-2.652974
H	1.011224	0.26042	-2.537516	H	4.501881	1.903146	-4.371695
H	0.159412	-1.135256	-3.234785	H	5.183729	2.451288	-2.829564
H	-0.754481	0.255812	-2.63586	H	3.805103	-0.23522	-3.3791
O	-3.278452	1.130147	-1.005579	H	5.381272	0.010701	-2.604426
C	-4.36828	1.002568	-0.057729	H	4.35468	0.890742	-0.584914
H	3.085468	-0.260587	-1.067717				

Table 3. Optimized geometries of dimer-based transition state 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)



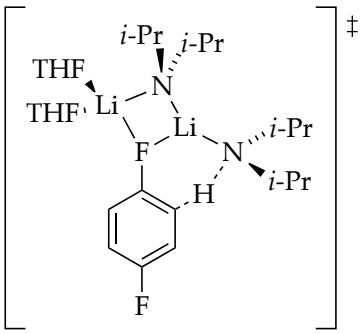


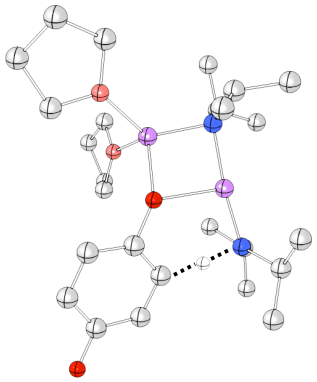
F
G = -1493.742385
G_{MP2} = -1489.417062

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	C	-2.989629	2.812244	-1.35154
Li	0.964914	1.835393	0.016495	C	-4.232279	2.980886	-1.947721
N	0.219992	3.741485	0.264427	C	-5.11067	3.88612	-1.350356
C	0.614788	4.681116	-0.807611	C	-4.684942	4.542655	-0.197288
H	1.675811	4.9622	-0.660878	C	-3.423556	4.342246	0.354429
C	0.519773	4.00604	-2.183357	C	-2.500837	3.44665	-0.223606
H	-0.501795	3.680102	-2.398466	H	-3.164189	4.910877	1.243946
H	0.824537	4.697498	-2.978963	F	-5.536816	5.414102	0.396817
H	1.166832	3.122808	-2.244294	H	-6.096258	4.083718	-1.758478
C	-0.167533	6.014765	-0.834707	H	-4.505373	2.429092	-2.842584
H	-0.086254	6.546997	0.119241	O	-3.594654	0.021812	0.076442
H	0.227664	6.679935	-1.614282	C	-4.07997	-1.218062	-0.497848
H	-1.230406	5.847622	-1.039041	C	-5.447217	-1.473736	0.145282
C	0.570396	4.287275	1.598175	C	-5.919983	-0.052946	0.489674
H	1.218222	5.170717	1.463244	C	-4.616826	0.616919	0.915588
C	-0.640216	4.757416	2.429981	H	-4.377902	0.401682	1.965954
H	-1.334329	3.927694	2.612469	H	-4.594406	1.695775	0.757683
H	-0.321882	5.14664	3.406106	H	-6.679015	-0.028288	1.277069
H	-1.189375	5.551182	1.915541	H	-6.327898	0.445507	-0.397145
C	1.389206	3.287087	2.437606	H	-5.336483	-2.070146	1.058362
H	2.296247	2.971433	1.909627	H	-6.125934	-2.007316	-0.526508
H	1.694442	3.724408	3.397503	H	-4.160093	-1.082309	-1.583224
H	0.80141	2.389562	2.66555	H	-3.346985	-2.003367	-0.295802
O	3.035009	1.847221	-0.365037	C	0.00732	-0.740568	1.274688
C	3.897226	0.688324	-0.413083	H	-0.37228	-1.771142	1.13376
C	5.299917	1.222209	-0.139409	C	1.406066	-0.903795	1.913651
C	5.257894	2.578163	-0.860545	H	1.836446	0.073494	2.170256
C	3.816654	3.044572	-0.612675	H	1.359097	-1.502477	2.833673

Table 3 (Continued).

H	3.384768	3.576208	-1.464217	H	2.096483	-1.413861	1.232377
H	3.737548	3.685237	0.271919	C	-0.941255	-0.084036	2.2916
H	5.440078	2.442107	-1.932901	H	-1.984674	-0.162681	1.965876
H	5.993639	3.294349	-0.483111	H	-0.866617	-0.560565	3.276937
H	6.083409	0.556194	-0.51328	H	-0.707903	0.980097	2.420888
H	5.451723	1.360505	0.937663	C	0.485783	-0.836797	-1.111045
H	3.534749	-0.02396	0.327897	H	1.429056	-1.35114	-0.837749
H	3.831737	0.228913	-1.408935	C	0.801105	0.024789	-2.343808
Li	-1.782541	0.781681	-0.31937	H	-0.085129	0.584767	-2.666841
F	-2.160478	1.829222	-1.943975	H	1.596612	0.749024	-2.137506
H	-0.040528	-2.614375	-2.298574	H	1.128151	-0.595537	-3.187846
H	-0.79744	-2.585252	-0.701861	C	-0.493256	-1.955336	-1.545292
H	-1.169434	3.5204	0.098493	H	-1.399792	-1.519603	-1.989019



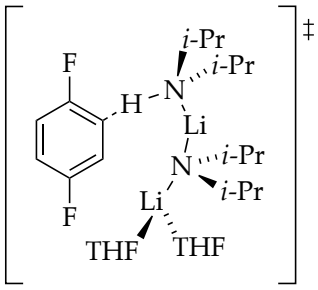


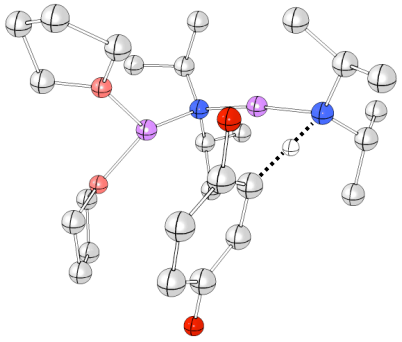
G
G = -1493.745707
G_{MP2} = -1489.410302

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	C	0.740486	3.819534	2.397735
Li	1.928702	0.436552	-0.210132	H	1.68339	3.414819	2.029016
N	3.890328	0.52216	0.159332	H	0.648183	4.85952	2.056904
C	4.694988	-0.143385	-0.884847	H	0.9727	2.761078	4.269824
H	5.192748	-1.026248	-0.446294	H	1.017652	4.525949	4.452922
C	3.784738	-0.667898	-2.00984	H	-1.344148	3.235271	4.951881
H	3.2365	0.160657	-2.482151	H	-1.375519	4.716262	3.981955
H	4.358748	-1.164584	-2.802611	H	-2.336819	3.269248	2.331638
H	3.055714	-1.391726	-1.623595	H	-1.531788	1.830641	3.001766
C	5.793135	0.748369	-1.505799	O	-1.992051	2.828526	-0.692906
H	6.470183	1.145763	-0.744502	C	-2.06788	4.242618	-0.985464
H	6.393277	0.185091	-2.232837	C	-3.541072	4.524791	-1.284451
H	5.347327	1.60277	-2.028307	C	-3.998209	3.195957	-1.906142
C	4.325846	0.199113	1.526116	C	-3.225982	2.170498	-1.074777
H	4.242111	-0.894968	1.683422	H	-2.970809	1.258009	-1.617629
C	5.785849	0.571356	1.869119	H	-3.770659	1.896621	-0.162171
H	5.952383	1.650109	1.75438	H	-3.695758	3.142478	-2.958385

Table 3 (Continued).

H	6.020765	0.299916	2.90688	H	-5.080035	3.042639	-1.855277
H	6.500445	0.04759	1.226568	H	-3.674102	5.383808	-1.948416
C	3.392595	0.879293	2.539558	H	-4.09074	4.723632	-0.356622
H	2.342988	0.612838	2.36469	H	-1.676067	4.788779	-0.122914
H	3.643227	0.581907	3.564978	H	-1.434346	4.454155	-1.856675
H	3.486265	1.969753	2.473604	C	-0.308195	-0.584741	1.320533
Li	-0.373356	1.965856	0.113398	C	0.555553	-1.799124	1.752088
F	1.365218	2.577261	-0.791525	H	0.416927	-2.014764	2.821168
C	2.375639	3.600205	-0.736105	H	0.305957	-2.709295	1.198722
C	1.976421	4.861449	-1.150924	H	1.620211	-1.594619	1.589155
C	2.938169	5.874255	-1.091253	H	-0.051728	0.205291	2.050096
C	4.210942	5.546364	-0.629859	C	-1.79936	-0.905913	1.568633
C	4.554617	4.254641	-0.238272	H	-2.146312	-1.749962	0.961436
C	3.613506	3.212466	-0.281344	H	-1.970988	-1.171682	2.619659
H	5.575915	4.075054	0.096217	H	-2.436449	-0.043866	1.329202
F	5.142684	6.530614	-0.570027	C	-0.644782	-0.637355	-1.155565
H	2.71698	6.890987	-1.398376	C	-0.317623	0.167904	-2.426676
H	0.97168	5.057522	-1.514882	H	-0.606765	1.220876	-2.329782
O	-0.335875	3.037128	1.822904	H	0.758063	0.138033	-2.646071
C	-1.411707	2.89746	2.784616	H	-0.837783	-0.245432	-3.299673
C	-0.984659	3.69302	4.025819	H	-1.751133	-0.618097	-1.056195
C	0.547731	3.703394	3.905961	C	-0.28983	-2.119584	-1.425526
H	0.796958	-2.252231	-1.504039	H	-0.650347	-2.780641	-0.632743
H	3.847704	1.860382	-0.01825	H	-0.742945	-2.463282	-2.365704





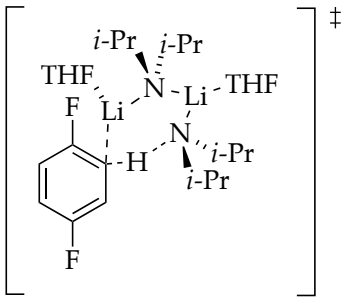
H
G = -1493.738102
G_{MP2} = -1489.408464

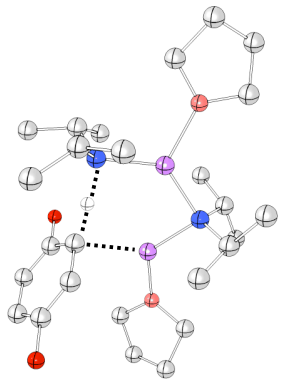
Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	3.833656	1.705623	3.25059
Li	-1.656097	0.905947	0.633139	O	2.971787	2.029818	0.313192
N	-3.205031	2.023551	1.157528	C	3.767692	1.654598	-0.827177
C	-3.888418	1.740974	2.439449	C	4.011676	2.961542	-1.601117
H	-4.78652	1.132596	2.236317	C	3.821907	4.07548	-0.533232
C	-2.994219	0.908374	3.367347	C	3.482416	3.305411	0.75419
H	-2.071568	1.450095	3.598852	H	2.711763	3.777206	1.365201

Table 3 (Continued).

H	-3.500198	0.699869	4.318604	H	4.379105	3.133313	1.367118
H	-2.738215	-0.056306	2.912498	H	3.003151	4.745463	-0.804161
C	-4.363224	3.011001	3.180618	H	4.722074	4.683204	-0.401813
H	-4.959951	3.658697	2.528966	H	3.281249	3.073497	-2.406764
H	-4.989203	2.747735	4.043805	H	5.00862	2.974959	-2.051101
H	-3.508265	3.587636	3.544671	H	4.710637	1.21418	-0.47214
C	-4.190889	2.360935	0.111621	H	3.208777	0.898778	-1.381961
H	-5.028245	2.928294	0.55364	C	0.17785	0.128423	-1.460491
C	-3.592133	3.263615	-0.973699	C	-0.931709	-0.544109	-2.303195
H	-2.74114	2.778802	-1.470467	H	-1.898101	-0.052511	-2.126464
H	-4.337493	3.481165	-1.748248	H	-0.711001	-0.472177	-3.376492
H	-3.245462	4.212829	-0.555776	H	-1.051161	-1.606041	-2.066216
C	-4.803675	1.101725	-0.534212	H	1.131348	-0.343902	-1.780271
H	-5.230851	0.431691	0.220471	C	0.256684	1.604119	-1.87205
H	-5.603143	1.360155	-1.241776	H	1.04241	2.142033	-1.332915
H	-4.036782	0.53961	-1.085101	H	0.44813	1.704847	-2.947544
Li	1.339759	1.134307	1.0169	H	-0.689906	2.116508	-1.66314
O	1.869871	1.092149	2.944122	C	0.201819	-1.400542	0.424457
C	3.233953	0.790232	3.326116	C	-0.564925	-1.7065	1.71608
C	3.154369	0.294565	4.76839	H	-0.281404	-1.009948	2.515696
C	1.991341	1.130622	5.321432	H	-1.647613	-1.620544	1.560925
C	1.029476	1.173171	4.133402	H	-0.362539	-2.723152	2.0758
H	0.436397	2.085695	4.076582	H	-0.194616	-2.095682	-0.333987
H	0.355525	0.309202	4.132076	C	1.691542	-1.780334	0.604557
H	2.332963	2.140411	5.577118	H	2.124156	-1.254424	1.467322
H	1.527659	0.694755	6.210953	H	1.820802	-2.856927	0.780237
H	4.093721	0.439783	5.310136	H	2.277598	-1.520338	-0.285267
H	2.90579	-0.772903	4.792761	C	0.294281	5.296512	2.917768
H	3.630634	0.050944	2.62495	C	0.840091	5.922389	1.793258
F	-1.122443	3.697829	3.88036	C	0.404918	5.492735	0.5457
H	-0.847689	4.240549	-0.625158	C	-0.548432	4.490222	0.390763
F	0.954009	6.067689	-0.566142	C	-1.12355	3.83405	1.49671
H	1.569761	6.721475	1.876875	C	-0.645288	4.288031	2.72136
H	0.582194	5.591834	3.923231	H	-2.242381	2.950164	1.347369

Table 3 (Continued).



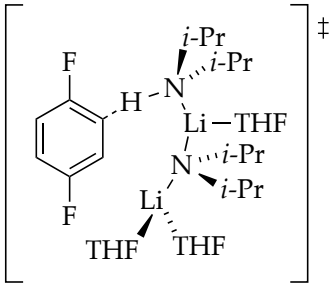


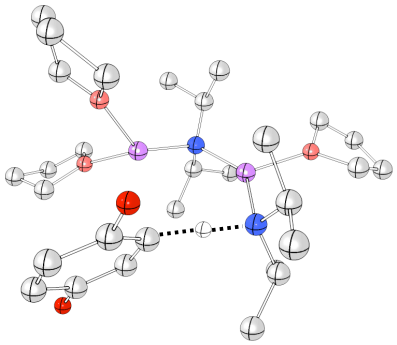
I
G = -1493.734144
G_{MP2} = -1489.410234

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	5.403198	0.466256	1.038726
Li	-1.192693	-1.695058	-0.063952	H	5.743783	2.019033	0.24517
N	-0.675301	-3.675555	-0.137412	H	3.562048	2.00221	-0.878403
C	-1.148543	-4.376495	-1.350143	H	3.131317	1.336763	0.713322
H	-2.22586	-4.605173	-1.220472	C	0.140186	0.620646	1.329106
C	-1.037033	-3.466724	-2.581355	C	-1.197586	0.879091	2.061197
H	0.002476	-3.183786	-2.767809	H	-1.702578	-0.068544	2.292019
H	-1.405538	-3.980097	-3.478343	H	-1.040196	1.415054	3.007181
H	-1.629062	-2.553358	-2.459959	H	-1.875896	1.485654	1.452126
C	-0.479822	-5.735454	-1.661976	H	0.632356	1.610421	1.252378
H	-0.615862	-6.451724	-0.84627	C	1.041618	-0.224649	2.242108
H	-0.926545	-6.179908	-2.561775	H	2.058563	-0.327537	1.840363
H	0.592109	-5.616726	-1.846255	H	1.133636	0.223763	3.238821
C	-1.045372	-4.425753	1.083509	H	0.632435	-1.233338	2.372176
H	-1.907134	-5.075219	0.839933	C	-0.468786	0.9808	-0.994582
C	0.045503	-5.352308	1.669429	C	-0.929603	0.274657	-2.276728
H	0.866831	-4.771015	2.10151	H	-0.123408	-0.345235	-2.692892
H	-0.37121	-5.978265	2.470086	H	-1.791818	-0.375469	-2.093508
H	0.476594	-6.012039	0.912729	H	-1.218613	0.99939	-3.048041
C	-1.52163	-3.481228	2.203366	H	-1.34855	1.538031	-0.612968
H	-2.369148	-2.864223	1.881319	C	0.566878	2.060824	-1.389999
H	-1.833198	-4.041369	3.09461	H	1.406673	1.605415	-1.931031
H	-0.712591	-2.808496	2.51381	H	0.115237	2.818401	-2.044714
O	-3.229971	-1.436471	-0.186793	H	0.96957	2.58574	-0.517296
C	-3.988817	-0.213087	-0.024911	C	4.125078	-4.314803	-1.276906
C	-5.391026	-0.521364	-0.551294	C	4.795021	-4.242968	-0.053098
C	-5.5325	-2.014431	-0.220202	C	4.116755	-3.693858	1.029947
C	-4.122861	-2.533664	-0.503311	C	2.798877	-3.257338	0.931631
H	-3.994481	-2.795269	-1.560657	C	2.084295	-3.319733	-0.283016
H	-3.833222	-3.392965	0.104776	C	2.819115	-3.839196	-1.350422
H	-6.291575	-2.52393	-0.821096	F	2.229974	-3.898686	-2.58718
H	-5.787847	-2.149322	0.837646	H	2.322372	-2.886587	1.836971

Table 3 (Continued).

H	-5.438256	-0.365205	-1.63555	F	4.762831	-3.591272	2.219033
H	-6.157453	0.10391	-0.083718	H	5.813249	-4.599367	0.06442
H	-4.005621	0.048921	1.039538	H	4.605266	-4.726264	-2.160084
H	-3.47543	0.581401	-0.571856	H	0.74717	-3.411744	-0.251461
Li	1.662541	-0.996964	-0.434338	C	4.554852	-0.679694	-1.386618
O	3.384134	-0.072406	-0.768623	H	4.697438	-1.658461	-0.925902
C	3.758271	1.189332	-0.167906	H	4.3555	-0.813792	-2.454713
C	5.247885	1.0512	0.124789	H	6.66286	-0.271745	-0.939426
C	5.728541	0.271017	-1.108837	H	5.883853	0.954586	-1.951406





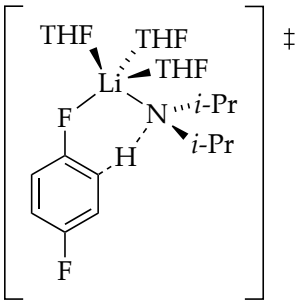
J
G = -1726.079261
G_{MP2} = -1721.100781

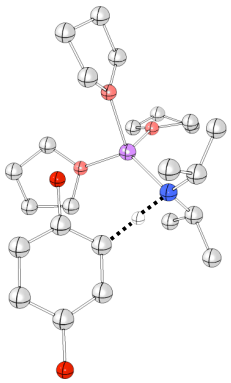
Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	C	3.548958	1.837012	4.353121
Li	-1.37906	1.57084	0.246915	C	2.374992	1.956319	3.382055
N	-1.384291	3.647861	0.289643	H	2.196647	2.970224	3.027833
C	-1.864966	4.161012	1.591151	H	1.451211	1.561629	3.821883
H	-2.964498	4.034964	1.635217	H	4.327934	2.567721	4.105483
C	-1.271671	3.330209	2.736971	H	3.245967	2.00207	5.391228
H	-0.184518	3.437948	2.762106	H	5.078561	0.237589	4.393276
H	-1.664251	3.666276	3.704952	H	3.406539	-0.320247	4.593835
H	-1.516149	2.266438	2.636767	H	3.671801	-0.717007	2.221386
C	-1.613379	5.659952	1.878931	H	4.747955	0.687593	2.034924
H	-2.107774	6.303605	1.145058	O	3.481877	0.407254	-0.573112
H	-2.01796	5.925474	2.865166	C	3.752938	-0.919797	-1.088087
H	-0.543813	5.889079	1.881086	C	5.049733	-0.804915	-1.895466
C	-2.062364	4.324953	-0.839545	C	5.758097	0.374803	-1.211692
H	-3.032247	4.714078	-0.476535	C	4.58231	1.295564	-0.896128
C	-1.303305	5.527719	-1.448673	H	4.308735	1.907593	-1.760978
H	-0.396029	5.19613	-1.964419	H	4.739716	1.955388	-0.03964
H	-1.933369	6.048434	-2.182524	H	6.506475	0.857769	-1.84674
H	-0.99922	6.250886	-0.688903	H	6.251765	0.045062	-0.289217
C	-2.385806	3.342703	-1.979872	H	4.830794	-0.55974	-2.94105
H	-2.982318	2.491531	-1.630278	H	5.630644	-1.731877	-1.879579
H	-2.945241	3.836937	-2.784953	H	3.864631	-1.601055	-0.23595

Table 3 (Continued).

H	-1.463824	2.949553	-2.424055	H	2.89481	-1.243453	-1.682408
O	-3.366057	0.943296	0.61015	C	-0.022899	-0.49092	-1.391829
C	-4.486801	1.831111	0.772088	C	-1.417735	-0.915778	-1.913327
C	-5.68336	1.104499	0.127392	H	-2.109281	-0.062726	-1.921175
C	-5.251584	-0.387903	0.119355	H	-1.352446	-1.304116	-2.938601
C	-3.893977	-0.373229	0.83848	H	-1.861731	-1.706879	-1.299487
H	-3.171642	-1.091531	0.45445	H	0.615069	-1.3912	-1.504896
H	-4.015826	-0.530468	1.920948	C	0.553971	0.557929	-2.351992
H	-5.135732	-0.751655	-0.905962	H	1.592641	0.802085	-2.107609
H	-5.969547	-1.040369	0.625271	H	0.525598	0.202992	-3.389919
H	-5.85676	1.464666	-0.890785	H	-0.025679	1.486284	-2.306112
H	-6.601837	1.271853	0.697832	C	-0.241095	-1.102366	0.947269
H	-4.655207	2.002979	1.844929	C	-0.5552	-0.560337	2.347923
H	-4.225949	2.777452	0.301652	H	0.275324	0.051751	2.718576
Li	1.76139	0.940398	0.430647	H	-1.456816	0.061447	2.346234
O	2.727065	1.126447	2.238892	H	-0.714977	-1.376236	3.064476
C	3.869135	0.301546	2.566097	H	-1.121468	-1.703679	0.646327
C	4.043965	0.409804	4.081194	C	0.917912	-2.123174	1.069041
C	1.349096	4.022723	0.074704	H	1.808698	-1.643572	1.496155
C	2.148475	4.736903	0.9615	H	0.643699	-2.960246	1.725436
F	1.676903	4.961161	2.245097	H	1.195159	-2.548686	0.098915
H	1.399141	3.322832	-1.984171	C	3.407917	5.264278	0.693704
F	3.730643	4.105577	-2.729802	C	3.953997	5.064741	-0.577819
H	4.929716	5.452524	-0.852396	C	3.196469	4.350596	-1.496367
H	3.942941	5.824648	1.455855	C	1.934572	3.846207	-1.19369
H	-0.037327	3.804473	0.232869				

Table 4. Optimized geometries of monomer-based transition state 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)



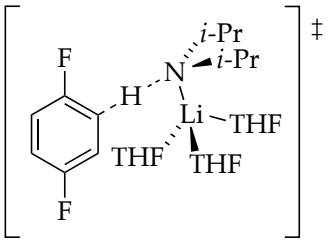


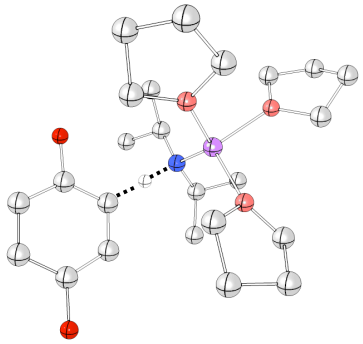
K
G = -1426.871146
G_{MP2} = -1422.815045

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	-2.492091	0.310904	-1.991576
N	1.160162	1.522202	0.85362	H	-1.780564	0.58542	-2.77892
C	1.06774	1.622684	2.327489	H	-2.618481	-0.77569	-2.00617
H	1.479617	2.585934	2.672278	H	-4.081046	1.270281	-3.16178
C	-0.390283	1.580151	2.827681	H	-4.628858	0.52218	-1.651037
H	-0.850367	0.613347	2.586684	H	-2.931233	3.062451	-1.932302
H	-0.44448	1.722318	3.915981	H	-4.407923	2.872561	-0.969473
H	-0.993629	2.369047	2.363556	H	-3.275767	1.478062	0.664299
C	1.899144	0.533126	3.021507	H	-1.922299	2.537111	0.204099
H	1.64837	-0.461171	2.638303	O	-0.882126	-1.582113	1.127516
H	2.968491	0.681258	2.850024	C	-0.221883	-2.469859	2.061275
H	1.718775	0.5405	4.104056	C	-1.153532	-3.671285	2.176462
C	1.060379	2.852823	0.221592	C	-2.531435	-2.991613	2.140137
H	0.183689	3.38898	0.634182	C	-2.309282	-1.818584	1.169423
C	0.840785	2.719562	-1.292175	H	-2.815636	-0.902456	1.487988
H	0.730584	3.705509	-1.761607	H	-2.637162	-2.059276	0.152019
H	1.700648	2.225867	-1.758168	H	-2.793701	-2.619781	3.137088
H	-0.054571	2.130624	-1.51741	H	-3.335561	-3.655723	1.809273
C	2.283434	3.770674	0.457394	H	-0.982805	-4.251145	3.088394
H	3.167309	3.37212	-0.052428	H	-1.025182	-4.339774	1.316551
H	2.094251	4.779035	0.065783	H	0.768318	-2.684309	1.660988
H	2.527579	3.87268	1.519545	H	-0.111563	-1.960955	3.02796
O	0.372403	-0.946668	-1.811034	C	5.937692	-1.259109	-0.140916
C	0.097566	-2.349342	-1.98339	C	5.952136	0.131053	-0.164366
C	1.399805	-2.954984	-2.498369	C	4.795252	0.891121	-0.005485
C	1.922939	-1.834715	-3.412279	C	3.53859	0.289191	0.180843
C	1.461386	-0.55601	-2.694521	C	3.582041	-1.095326	0.197282
H	1.090153	0.206004	-3.388374	C	4.707536	-1.896484	0.04604
H	2.246185	-0.122527	-2.070535	H	4.634674	-2.980822	0.07864

Table 4 (Continued).

H	1.468626	-1.90891	-4.407445	F	2.370238	-1.781612	0.364709
H	3.009265	-1.860111	-3.534719	H	4.902821	1.975977	-0.025881
H	1.246157	-3.903162	-3.023212	F	7.144191	0.761642	-0.346484
H	2.083652	-3.116027	-1.661657	H	6.860412	-1.817036	-0.263215
H	-0.229165	-2.736218	-1.016485	H	2.309823	0.983985	0.512862
H	-0.717119	-2.475724	-2.714252	C	-3.509155	2.358362	-1.322587
O	-1.93465	0.688083	-0.712732	C	-3.80897	1.07998	-2.119269
C	-2.653825	1.82069	-0.174033				





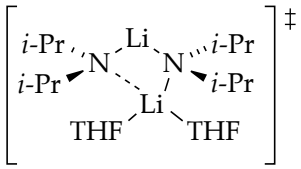
L
G = -1426.867251
G_{MP2} = -1422.810814

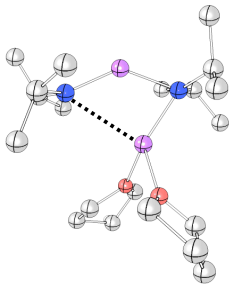
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	2.499832	4.408857	1.024973
N	0.886732	-1.219237	-1.411148	H	1.062254	2.660908	1.916424
C	0.741567	-0.757156	-2.807456	H	2.183354	1.672558	0.935369
H	1.04291	-1.556136	-3.506369	O	0.266204	-0.205678	2.054772
C	-0.717125	-0.406743	-3.168102	C	-0.770897	0.198991	2.974926
H	-1.070377	0.451224	-2.580739	C	-0.276676	-0.165701	4.386357
H	-0.815497	-0.15194	-4.232426	C	0.818808	-1.207366	4.10672
H	-1.389264	-1.24959	-2.968915	C	1.408403	-0.688791	2.799702
C	1.655592	0.43657	-3.111846	H	1.912378	-1.440029	2.19499
H	1.50236	1.239306	-2.381011	H	2.103277	0.143511	2.980441
H	2.707914	0.145856	-3.069367	H	0.382955	-2.201689	3.955547
H	1.450614	0.840816	-4.111154	H	1.561658	-1.276165	4.906911
C	0.613558	-2.673274	-1.330923	H	-1.083411	-0.543826	5.021504
H	-0.289521	-2.898221	-1.929267	H	0.154295	0.711659	4.882175
C	0.315617	-3.118965	0.107766	H	-0.954917	1.273944	2.85881
H	0.038305	-4.180849	0.132706	H	-1.684605	-0.337433	2.701083
H	1.202033	-2.993756	0.733472	C	6.012699	-0.019506	0.705583
H	-0.506404	-2.546678	0.551923	C	5.368652	0.82875	-0.185629
C	1.755135	-3.553182	-1.892383	C	4.110418	0.539643	-0.709362
H	2.639956	-3.479205	-1.253691	C	3.400462	-0.62603	-0.361198
H	1.450637	-4.607711	-1.933715	C	4.088176	-1.434906	0.536103
H	2.041605	-3.254858	-2.906669	C	5.346351	-1.189892	1.077602
O	-2.095467	0.005678	0.053985	H	5.793972	-1.898093	1.770046
C	-2.949032	1.166788	0.028053	F	3.480364	-2.604224	0.976438

Table 4 (Continued).

C	-4.368431	0.641716	0.240516	H	3.694849	1.257474	-1.415994
C	-4.301898	-0.720108	-0.467291	F	5.992023	1.983671	-0.554835
C	-2.888472	-1.194916	-0.118305	H	6.996331	0.230231	1.090033
H	-2.423645	-1.804983	-0.895282	H	2.100962	-0.97171	-0.941954
H	-2.872675	-1.755565	0.82517	C	0.741836	4.400572	-0.314714
H	-4.406883	-0.591969	-1.550792	C	-0.024314	3.17266	-0.816364
H	-5.070738	-1.422607	-0.132666	H	0.249013	2.918773	-1.846844
H	-5.128997	1.311117	-0.172266	H	-1.110683	3.293262	-0.764358
H	-4.573	0.509887	1.309762	H	0.951438	5.11387	-1.117291
H	-2.608265	1.856796	0.804995	H	0.16812	4.922361	0.460851
H	-2.852779	1.660251	-0.94856	H	2.733138	3.528759	-0.495001
O	0.359799	2.076675	0.046218	C	2.005543	3.769385	0.287668
C	1.456669	2.485876	0.906324				

Table 5. Optimized geometries of dimer-based deaggregation transition state structures of LDA 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)



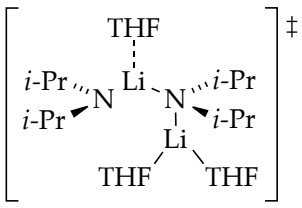


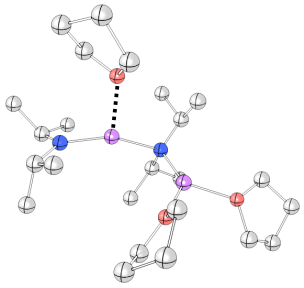
M
G = -1063.113138
G_{MP2} = -1059.914778

Atom	X	Y	Z	Atom	X	Y	Z
C	0	0	0	C	3.321573	-0.562069	5.874681
N	-0.086375	0.248713	1.43741	H	4.194396	-1.159861	5.587908
Li	0.476016	-1.014773	2.724545	H	3.269569	-0.552599	6.972743
N	2.138128	-1.279129	3.772572	H	3.497472	0.467446	5.534423
Li	2.503654	0.456333	2.713605	H	1.864103	-2.113578	5.707163
O	4.188355	0.779148	1.581	C	2.815518	-2.559001	3.486633
C	5.37711	1.142108	2.32174	C	1.83041	-3.751466	3.449856
C	6.463722	1.370813	1.270717	H	1.222611	-3.784152	4.361881
C	6.063604	0.366196	0.179428	H	2.346175	-4.717753	3.356511
C	4.535377	0.440423	0.216395	H	1.147073	-3.659353	2.59187
H	4.1503	1.226979	-0.443671	H	3.541764	-2.786577	4.288659
H	4.045636	-0.501902	-0.039364	C	3.631923	-2.532551	2.189454
H	6.467125	0.612726	-0.807057	H	4.401326	-1.755005	2.232552
H	6.405074	-0.641	0.444514	H	2.991672	-2.331203	1.322646
H	6.416126	2.396203	0.884895	H	4.124597	-3.497449	2.01308
H	7.469242	1.20287	1.667689	C	-1.166122	1.190216	1.736546
H	5.635506	0.316928	2.998032	C	-2.585773	0.5927	1.568951
H	5.140613	2.025672	2.919472	H	-2.739853	0.17485	0.568726
O	2.52989	2.437526	3.310016	H	-3.366342	1.349284	1.73273
C	2.5151	3.159012	4.564058	H	-2.737295	-0.218396	2.294919
C	2.576658	4.641315	4.19128	C	-1.049528	1.737147	3.164053
C	1.835537	4.661018	2.845345	H	-1.196206	0.936463	3.901054
C	2.301532	3.353513	2.205813	H	-1.811408	2.501877	3.362518
H	1.568674	2.891354	1.540712	H	-0.060742	2.172735	3.33861
H	3.246961	3.482046	1.663679	H	-1.125068	2.073656	1.063815
H	0.751896	4.642554	3.005453	C	0.706389	1.130825	-0.787323
H	2.075568	5.53355	2.23051	H	0.233109	2.101165	-0.596934
H	2.11638	5.279458	4.951366	H	0.675249	0.958044	-1.87267
H	3.616919	4.963587	4.061334	H	1.758879	1.205665	-0.483494
H	3.363344	2.819745	5.165453	C	0.702643	-1.330503	-0.292682
H	1.588768	2.917666	5.098605	H	1.728104	-1.318927	0.097898

Table 5 (Continued).

C	2.032262	-1.127061	5.234221	H	0.764447	-1.532404	-1.369675
C	0.833133	-0.262547	5.639443	H	0.169187	-2.166927	0.178112
H	0.883335	0.729323	5.175844	H	-1.007396	-0.090339	-0.449933
H	0.788757	-0.119683	6.7266	H	-0.112084	-0.728423	5.329526





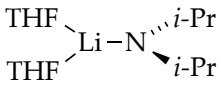
N
G = -1295.456439
G_{MP2} = -1291.595118

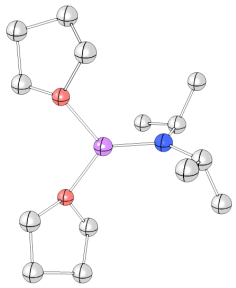
Atom	X	Y	Z	Atom	X	Y	Z
C	0	0	0	C	5.948311	1.07573	-0.249706
N	0.231281	0.82555	1.200346	H	6.381895	2.075788	-0.364667
Li	-0.922353	2.39411	1.193924	H	5.992563	0.812125	0.815805
O	-2.836904	2.454698	1.733351	H	6.591337	0.372991	-0.799418
C	-3.835183	3.161251	0.963905	C	3.920643	-0.375683	-0.48896
C	-5.039848	2.224737	0.912707	H	2.928644	-0.493957	-0.939725
C	-4.979343	1.563123	2.298333	H	4.57409	-1.160099	-0.892517
C	-3.471485	1.417498	2.534541	H	3.825177	-0.550987	0.592848
H	-3.086167	0.453066	2.192427	C	3.888033	3.370072	-0.674588
H	-3.181138	1.563292	3.578578	H	4.975295	3.604372	-0.676727
H	-5.496625	0.600429	2.338467	C	3.23914	4.423153	0.237295
H	-5.428394	2.2191	3.053055	H	2.15554	4.243156	0.308104
H	-4.906139	1.477232	0.122415	H	3.644763	4.365684	1.251926
H	-5.977244	2.757208	0.726878	H	3.38791	5.443225	-0.144194
H	-4.080578	4.105027	1.470072	C	3.413412	3.611135	-2.132062
H	-3.406096	3.389509	-0.015	H	3.709192	4.603743	-2.504017
O	-0.696455	4.264401	0.614359	H	3.833857	2.865637	-2.815663
C	-0.583776	5.336419	1.581899	H	2.318841	3.530384	-2.195563
C	-0.810647	6.621968	0.787926	H	0.759785	-0.800508	-0.093641
C	-0.193601	6.264339	-0.57357	C	0.144669	0.872946	-1.256104
C	-0.574671	4.79072	-0.734881	H	0.028735	0.276434	-2.169583
H	0.175498	4.201998	-1.267183	H	-0.634577	1.653196	-1.281191
H	-1.545095	4.672384	-1.234544	H	1.12503	1.363707	-1.290141
H	0.895318	6.36944	-0.53795	C	-1.369598	-0.71722	-0.056047
H	-0.571308	6.880438	-1.394592	H	-1.466524	-1.299134	-0.981684
H	-0.340981	7.489772	1.259947	H	-1.51548	-1.410877	0.779002
H	-1.883279	6.826629	0.686757	H	-2.19013	0.016056	-0.033712
H	-1.326579	5.159712	2.365695	O	3.022723	2.770745	3.337815

Table 5 (Continued).

H	0.419403	5.305933	2.024023	C	2.869218	3.894967	4.215297
C	0.14168	0.063213	2.454972	C	4.198653	4.046127	4.967658
H	-0.805735	-0.510356	2.510513	C	5.201225	3.463821	3.958303
C	1.270788	-0.972044	2.658101	C	4.396085	2.320315	3.340244
H	1.322205	-1.68204	1.825913	H	4.471449	1.407573	3.950363
H	2.246531	-0.472337	2.73202	H	4.654086	2.091623	2.302323
H	1.12096	-1.551614	3.579255	H	6.132831	3.122801	4.420448
C	0.12859	1.026131	3.653192	H	5.452386	4.20876	3.193948
H	-0.707581	1.738934	3.589445	H	4.190105	3.445691	5.885312
H	0.014746	0.480622	4.598927	H	4.407531	5.084327	5.245296
H	1.061439	1.59813	3.698923	H	2.651776	4.789838	3.612973
Li	2.123565	1.626121	0.935432	H	2.016314	3.713229	4.88081
N	3.614951	2.037711	-0.170474	H	4.546263	1.124202	-1.861082
C	4.483007	1.027814	-0.754776				

Table 6. Optimized geometries of LDA Monomer and Dimer intermediates at B3LYP level of theory with 6-31G(d) basis set 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)

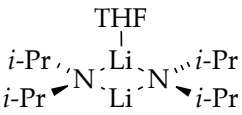


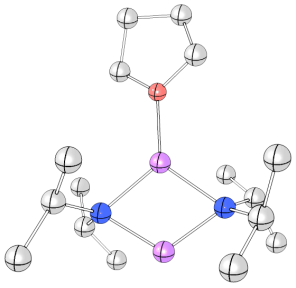


O
G = -763.909491
G_{MP2} = -761.6322164

Atom	X	Y	Z	Atom	X	Y	Z
C	0	0	0	H	-4.600416	-5.275712	-2.065516
N	-0.552097	-0.791733	-1.08216	H	-2.277069	-4.73069	-2.421557
C	-1.100726	0.003952	-2.163167	H	-2.054509	-5.85731	-1.062374
H	-0.42462	0.838047	-2.452483	O	0.928677	-3.84446	-1.600313
C	-1.261764	-0.861954	-3.422722	C	1.430248	-4.933118	-0.788525
H	-1.922259	-1.719434	-3.214761	C	2.950846	-4.9556	-0.995241
H	-1.708423	-0.303457	-4.255299	C	3.255616	-3.502185	-1.393799
H	-0.292451	-1.254225	-3.754666	C	2.032631	-3.142063	-2.231704
C	-2.463159	0.663803	-1.830387	H	2.13068	-3.498223	-3.266133
H	-2.802676	1.338115	-2.630223	H	1.769306	-2.081255	-2.227245
H	-3.232374	-0.1078	-1.684469	H	4.191584	-3.396235	-1.950228
H	-2.403086	1.250892	-0.90701	H	3.308556	-2.859385	-0.507448
Li	-0.554552	-2.660513	-1.083367	H	3.216417	-5.6368	-1.811959
O	-2.040768	-3.840775	-0.566936	H	3.485002	-5.28118	-0.097692
C	-2.544624	-4.929889	-1.376656	H	1.162279	-4.731873	0.255882
C	-4.065111	-4.949637	-1.168831	H	0.938866	-5.86023	-1.101727
C	-4.367295	-3.495144	-0.772206	H	-0.672433	0.836632	0.290479
C	-3.14313	-3.135747	0.064289	C	1.365347	0.654309	-0.33183
H	-3.241005	-3.490326	1.099282	H	1.707479	1.326654	0.468548
H	-2.878003	-2.075394	0.058276	H	2.131354	-0.120443	-0.477981
H	-5.302683	-3.386912	-0.215241	H	1.308012	1.242189	-1.254875
H	-4.419918	-2.853576	-1.659473	C	0.157181	-0.868367	1.258346
H	-4.331203	-5.629195	-0.350914	H	0.814037	-1.728384	1.049267
H	-0.813839	-1.256932	1.58963	H	0.606163	-0.312969	2.091742

Table 6 (Continued).

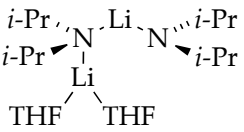


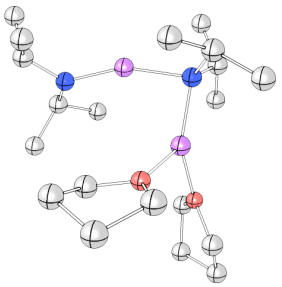


P
G = -830.781351
G_{MP2} = -828.2368513

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	1.629998	5.253231	-0.973867
Li	1.055816	1.628316	0.006298	C	-1.107815	3.490471	-2.194308
N	-0.000752	3.256107	0.012202	H	-2.079779	3.153228	-1.812989
Li	-1.263992	1.627801	0.006004	H	-1.296414	4.16856	-3.035649
O	-3.236325	1.627449	0.005869	H	-0.580032	2.614526	-2.595291
C	-4.064991	2.727409	0.458429	H	-0.885496	5.034735	-0.743763
C	-5.480265	2.394865	-0.01548	C	-0.277878	-0.919445	1.108398
C	-5.479759	0.858724	0.027435	C	-1.10751	-0.23505	2.206206
C	-4.064418	0.527156	-0.446904	H	-2.079514	0.101731	1.824586
H	-4.003634	0.47322	-1.540595	H	-1.296043	-0.913309	3.047426
H	-3.658459	-0.396839	-0.027697	H	-0.580321	0.641135	2.607453
H	-6.247246	0.406149	-0.607121	C	0.999641	-1.516298	1.742168
H	-5.633406	0.505027	1.053705	H	1.591091	-0.721205	2.216957
H	-5.634469	2.748446	-1.041706	H	0.766335	-2.270459	2.507056
H	-6.247854	2.846945	0.619302	H	1.631579	-1.996288	0.986427
H	-4.003956	2.781752	1.552079	H	-0.883908	-1.779154	0.755706
H	-3.659702	3.651517	0.038814	C	0.320874	-0.742282	-1.226831
C	0.319438	3.998626	1.239077	C	1.341495	0.023724	-2.088242
C	-0.928935	4.336924	2.082978	H	2.296429	0.137595	-1.553096
H	-1.399739	3.416616	2.455837	H	1.55771	-0.493165	-3.031326
H	-0.690261	4.97018	2.949206	H	0.969794	1.024158	-2.354464
H	-1.667621	4.870725	1.473441	C	-0.927114	-1.080946	-2.07116
C	1.340049	3.233067	2.100901	H	-1.398145	-0.160766	-2.444047
H	2.295242	3.119556	1.566136	H	-0.687948	-1.714016	-2.937388
H	1.555695	3.750092	3.044041	H	-1.665774	-1.615086	-1.46189
H	0.968653	2.232497	2.367031	H	0.800445	-1.707153	-0.981465
H	0.798758	4.963636	0.993772	H	1.590422	3.97816	-2.204443
C	-0.278877	4.175379	-1.09629	H	0.764923	5.526996	-2.494661
C	0.998465	4.772931	-1.729749				

Table 6 (Continued).

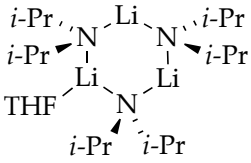


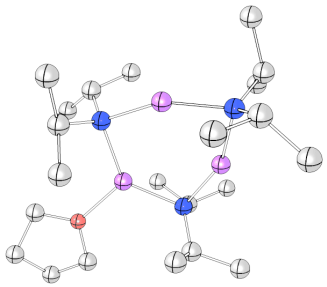


Q
G = -1063.11763
G_{MP2} = -1059.913141

Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	1.013566	-4.608918	-1.607685
Li	-1.524323	-0.913264	-0.958264	O	2.824175	-1.567241	-1.79498
N	-2.416496	-2.13582	-2.069113	C	2.918494	-1.274852	-3.213947
C	-3.633338	-2.83569	-1.677259	C	4.044204	-2.164986	-3.737922
C	-3.613251	-3.182217	-0.182693	C	4.98415	-2.236533	-2.524837
H	-2.748355	-3.808297	0.066417	C	3.994712	-2.301189	-1.359861
H	-3.553507	-2.268271	0.425102	H	4.370024	-1.836363	-0.442485
H	-4.523129	-3.714816	0.122135	H	3.692782	-3.331319	-1.137198
H	-3.73242	-3.803458	-2.213703	H	5.59461	-1.328534	-2.460122
C	-4.929971	-2.044	-1.980975	H	5.657361	-3.09843	-2.545751
H	-4.965162	-1.133002	-1.367765	H	4.519924	-1.749311	-4.630738
H	-4.974767	-1.73781	-3.031912	H	3.66211	-3.161716	-3.987492
H	-5.832504	-2.63605	-1.769976	H	1.945387	-1.477376	-3.667045
C	-2.214651	-2.180273	-3.510086	H	3.150101	-0.210574	-3.336437
H	-3.165775	-2.019714	-4.057977	C	0.197785	1.383	-0.475737
C	-1.279283	-1.051514	-3.960533	C	1.020782	1.431286	-1.769051
H	-1.707075	-0.069215	-3.725346	H	2.027774	1.030111	-1.602891
H	-0.313853	-1.133122	-3.437843	H	0.541908	0.842581	-2.561944
H	-1.073874	-1.087992	-5.038427	H	1.123113	2.45882	-2.140228
C	-1.655756	-3.530509	-4.02786	H	0.77277	1.960827	0.272188
H	-1.640221	-3.573856	-5.126686	C	-1.133852	2.141058	-0.679612
H	-0.628128	-3.683432	-3.668953	H	-0.972209	3.19906	-0.92884
H	-2.261657	-4.371834	-3.672843	H	-1.713566	1.692133	-1.499193
Li	1.255858	-1.41748	-0.572615	H	-1.750834	2.103971	0.226192
O	1.176476	-3.319601	0.022002	C	-0.151937	0.002689	1.467792
C	0.386848	-4.250039	-0.779451	C	-1.026873	-1.162473	1.948467
C	0.02824	-5.383739	0.175908	H	-2.061476	-1.045761	1.603947
C	1.267678	-5.448704	1.081976	H	-0.654589	-2.119093	1.561376
C	1.6414	-3.970464	1.229048	H	-1.051854	-1.227437	3.043799
H	2.719871	-3.802948	1.323528	H	-0.664971	0.925587	1.79546
H	1.139029	-3.507909	2.086093	C	1.206244	-0.013721	2.208878
H	2.074179	-6.002702	0.586929	H	1.855435	0.793374	1.849308
H	1.076299	-5.922778	2.049142	H	1.090071	0.108304	3.294981
H	-0.172411	-6.321525	-0.350081	H	1.730769	-0.966692	2.039234
H	-0.862534	-5.121649	0.757788	H	-0.474491	-3.703127	-1.18328

Table 7. Optimized geometries of LDA Trimer intermediates at B3LYP level of theory with 6-31G(d) basis set 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)



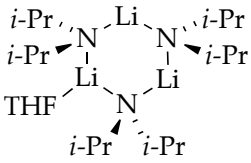


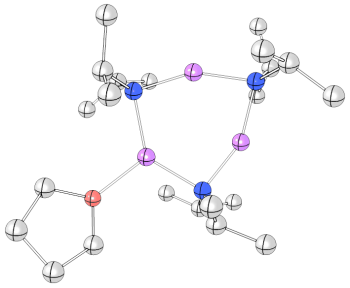
R-1$_a$
G = -1129.995901
G_{MP2} = -1126.529703

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	-3.387124	-1.826488	3.168147
Li	-2.705154	1.333703	0.301623	H	-3.588751	-0.186344	2.520526
N	-1.842967	3.235262	0.410489	H	-4.112525	-1.593059	1.573184
C	-2.17202	4.105492	-0.731863	C	-0.885997	-0.791009	2.587209
H	-3.220116	4.460131	-0.644646	H	-0.972938	0.292686	2.738092
C	-2.082663	3.327978	-2.051792	H	-0.99117	-1.267871	3.569325
H	-2.367682	3.958351	-2.902891	H	0.132857	-1.00247	2.235153
H	-1.058946	2.978299	-2.238906	O	-4.747745	1.451446	0.011674
H	-2.737688	2.449276	-2.052352	C	-5.427603	2.696396	-0.29375
C	-1.323203	5.393769	-0.858178	C	-6.925244	2.385248	-0.232039
H	-0.255479	5.153629	-0.973252	C	-6.9622	0.90038	-0.621893
H	-1.626929	5.985486	-1.732467	C	-5.708733	0.369345	0.069804
H	-1.428698	6.034015	0.022817	H	-5.264242	-0.501831	-0.416064
C	-2.191141	3.890284	1.689365	H	-5.903848	0.12485	1.12115
H	-2.914977	4.704505	1.495473	H	-6.878476	0.786157	-1.709209
C	-0.995774	4.532915	2.433305	H	-7.870006	0.386081	-0.29282
H	-0.438365	5.218836	1.787227	H	-7.509027	3.026333	-0.899036
H	-1.322201	5.095625	3.31895	H	-7.305267	2.520357	0.787476
H	-0.30084	3.757982	2.784581	H	-5.103584	3.450479	0.427236
C	-2.885164	2.91525	2.658963	H	-5.120969	3.017698	-1.295695
H	-2.225442	2.070123	2.895891	N	1.444339	1.338627	-0.138644
H	-3.13962	3.400321	3.610204	Li	0.034882	2.667266	0.261845
H	-3.810974	2.513235	2.230761	C	2.512914	1.325012	0.879686
N	-1.846894	-0.588857	0.302932	C	2.03328	1.928415	2.206611
C	-2.380519	-1.433335	-0.781579	H	1.791619	2.99376	2.093066
H	-3.329367	-1.915352	-0.469279	H	1.140291	1.410552	2.580831
C	-2.706426	-0.596595	-2.026788	H	2.802128	1.853449	2.985285
H	-3.07492	-1.227052	-2.84565	H	3.357146	1.956644	0.546164
H	-3.471841	0.159195	-1.816713	C	3.098076	-0.083675	1.123659
H	-1.812063	-0.076518	-2.392259	H	2.345245	-0.743176	1.577401
C	-1.434739	-2.587103	-1.196122	H	3.420782	-0.542554	0.18182

Table 7 (Continued).

H	-1.135103	-3.195747	-0.335869	H	3.966411	-0.057204	1.796227
H	-1.907634	-3.258626	-1.925629	C	2.04363	1.389518	-1.487174
H	-0.520868	-2.187644	-1.659863	H	3.002169	0.840268	-1.491836
C	-1.942425	-1.297983	1.595745	C	1.155594	0.696282	-2.529265
H	-1.73422	-2.375147	1.460144	H	1.044864	-0.374334	-2.30799
C	-3.338385	-1.2214	2.252523	H	0.153506	1.1436	-2.559969
H	1.442336	3.408715	-2.083277	H	1.576812	0.778112	-3.53876
H	2.979431	3.346879	-1.199022	C	2.366179	2.828665	-1.945738
H	2.913799	2.84694	-2.898097				



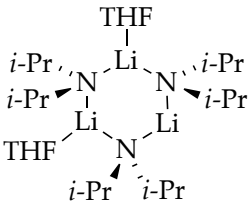


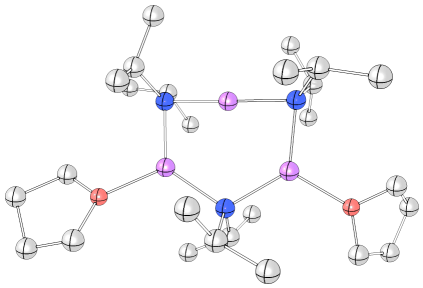
R-1$_b$
G = -1129.995057
G_{MP2} = -1126.528457

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	-6.804798	0.899427	-0.849272
Li	-2.695004	1.340324	0.368957	C	-5.698552	0.351589	0.068995
N	-1.830083	3.247066	0.426154	H	-5.16707	-0.512618	-0.32871
C	-2.226756	4.090102	-0.713337	H	-6.091835	0.100305	1.064169
H	-3.270649	4.446813	-0.574224	H	-6.616815	0.619239	-1.889849
C	-2.216099	3.282211	-2.01737	H	-7.786128	0.503618	-0.571701
H	-2.550055	3.8933	-2.864537	H	-6.473774	2.927916	-1.619257
H	-1.205395	2.925256	-2.254996	H	-7.632858	2.880023	-0.287845
H	-2.873984	2.408397	-1.957183	H	-5.923692	2.682642	1.363275
C	-1.39692	5.380537	-0.923188	H	-4.903882	3.471216	0.131646
H	-0.334401	5.144767	-1.085219	N	1.439408	1.338618	-0.191178
H	-1.751092	5.938984	-1.800203	Li	0.043649	2.677686	0.218128
H	-1.463288	6.051207	-0.061179	C	2.530911	1.303673	0.802071
C	-2.098866	3.92854	1.709769	C	2.088886	1.896294	2.146541
H	-2.861057	4.715393	1.551749	H	1.858665	2.965681	2.051048
C	-0.871281	4.626949	2.345174	H	1.197434	1.385698	2.534187
H	-0.376917	5.30387	1.641594	H	2.87384	1.801318	2.906787
H	-1.151033	5.211198	3.232814	H	3.373808	1.930099	0.455654
H	-0.133951	3.881601	2.673517	C	3.1063	-0.113973	1.016942
C	-2.681084	2.959663	2.754927	H	2.356645	-0.770722	1.480363
H	-1.97853	2.140555	2.956171	H	3.402888	-0.565851	0.06319
H	-2.872652	3.461902	3.71186	H	3.989596	-0.104815	1.670156

Table 7 (Continued).

H	-3.626056	2.520277	2.415306	C	2.008764	1.395017	-1.552638
N	-1.840205	-0.586245	0.339429	H	2.963912	0.840854	-1.582042
C	-2.385208	-1.435876	-0.735054	C	1.094655	0.714963	-2.580406
H	-3.332222	-1.914236	-0.410785	H	0.978409	-0.35555	-2.362157
C	-2.718431	-0.608635	-1.984339	H	0.09619	1.171246	-2.588946
H	-3.101079	-1.243769	-2.792991	H	1.49681	0.798805	-3.597514
H	-3.474856	0.156573	-1.775827	C	2.328278	2.836007	-2.00753
H	-1.824972	-0.0984	-2.364639	H	2.855935	2.859331	-2.970955
C	-1.446091	-2.5953	-1.149483	H	1.403815	3.420516	-2.122398
H	-1.140913	-3.198188	-0.287216	H	2.958667	3.346506	-1.269841
H	-1.926508	-3.270797	-1.870341	H	-4.108168	-1.531281	1.649703
H	-0.534975	-2.201405	-1.623429	C	-0.846213	-0.803692	2.608762
C	-1.931031	-1.288082	1.637036	H	-0.905125	0.282102	2.756922
H	-1.750678	-2.370007	1.501439	H	-0.945593	-1.274156	3.594603
C	-3.314506	-1.176602	2.315606	H	0.160747	-1.040562	2.238972
H	-3.362629	-1.778336	3.233445	O	-4.75129	1.42708	0.197769
H	-3.537785	-0.135767	2.584678	C	-5.549769	2.617043	0.330742
C	-6.706372	2.440126	-0.66829				





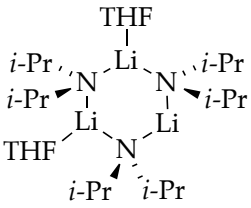
R-2$_a$
G = -1362.338194
G_{MP2} = -1358.219791

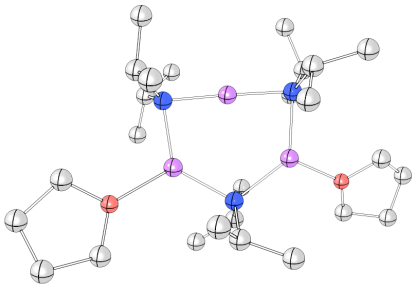
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	5.281677	-4.310928	-1.174317
Li	1.844654	-1.982372	0.165167	C	5.828197	-2.864555	-1.044757
N	0.060237	-3.128876	0.010099	C	4.972559	-2.258477	0.073007
C	0.264497	-4.053587	-1.126559	H	4.785455	-1.190263	-0.021639
H	0.887121	-4.915826	-0.813934	H	5.405736	-2.458632	1.064217
C	1.01404	-3.385756	-2.288456	H	5.67699	-2.31075	-1.976497
H	1.151454	-4.087128	-3.121642	H	6.895341	-2.832203	-0.806057
H	0.454099	-2.527789	-2.672516	H	5.0384	-4.548135	-2.213866
H	2.008163	-3.03359	-1.991511	H	6.00268	-5.057166	-0.827249
C	-1.036969	-4.675064	-1.690509	H	4.205433	-4.816366	0.672814
H	-1.672053	-3.902648	-2.145979	H	3.1447	-4.766988	-0.755711
H	-0.820807	-5.424894	-2.464058	N	-1.928025	-0.002237	-0.495715
H	-1.618915	-5.171865	-0.907618	Li	-1.750905	-2.02915	-0.251418

Table 7 (Continued).

C	-0.154139	-3.916884	1.244113	O	-3.585426	-2.97447	-0.025763
H	-0.81065	-4.78651	1.040081	C	-4.759028	-2.365995	-0.624135
C	-0.86168	-3.092645	2.326642	C	-5.963265	-3.087055	-0.014089
H	-1.858936	-2.768632	2.013569	C	-5.389549	-4.480984	0.278904
H	-0.983168	-3.671886	3.250809	C	-3.97252	-4.140904	0.737141
H	-0.285519	-2.19534	2.573958	H	-3.242655	-4.930471	0.547639
C	1.135878	-4.512214	1.858179	H	-3.948868	-3.889931	1.805791
H	1.812364	-3.713933	2.195245	H	-5.361918	-5.085717	-0.635376
H	0.910281	-5.14434	2.728056	H	-5.951993	-5.03368	1.037409
H	1.678354	-5.13233	1.138142	H	-6.823366	-3.10234	-0.689901
N	1.951566	0.065123	0.334348	H	-6.271732	-2.59881	0.917832
C	2.640155	0.818467	-0.731718	H	-4.72965	-1.295002	-0.417118
H	3.670009	1.077498	-0.420372	H	-4.706992	-2.516356	-1.709629
C	2.784719	-0.010849	-2.014725	C	-2.735349	0.756388	0.47387
H	3.300288	0.558844	-2.798034	C	-2.834907	0.011912	1.811479
H	3.350465	-0.931961	-1.838382	H	-3.303564	-0.969878	1.68129
H	1.804858	-0.296445	-2.41557	H	-1.847045	-0.145884	2.261615
C	1.954438	2.162201	-1.082541	H	-3.435559	0.579513	2.533084
H	1.80097	2.779801	-0.19071	H	-3.779113	0.860645	0.121363
H	2.551695	2.75059	-1.792806	C	-2.233966	2.197521	0.731009
H	0.971092	1.988927	-1.543427	H	-1.229234	2.187008	1.178504
C	2.270985	0.650915	1.650233	H	-2.175982	2.779732	-0.195131
H	2.189051	1.755081	1.613651	H	-2.898627	2.736879	1.419207
C	3.698979	0.350932	2.163074	C	-2.0227	0.568029	-1.854193
H	3.900525	0.879782	3.104532	H	-1.526566	1.561179	-1.913124
H	3.821145	-0.724738	2.347192	C	-1.282648	-0.333367	-2.848012
H	4.467967	0.662663	1.447921	H	-0.248765	-0.512502	-2.535881
C	1.280799	0.187383	2.724344	H	-1.778942	-1.310363	-2.93444
H	1.336375	-0.899892	2.863279	H	-1.249985	0.114079	-3.848848
H	1.499583	0.651614	3.693678	C	-3.450335	0.799292	-2.400767
H	0.245909	0.445465	2.467576	H	-3.402618	1.17896	-3.429212
O	3.704849	-2.930629	-0.035239	H	-4.018142	-0.13965	-2.414266
C	4.017859	-4.313882	-0.28568	H	-4.017153	1.529266	-1.814468

Table 7 (Continued).



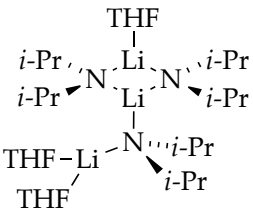


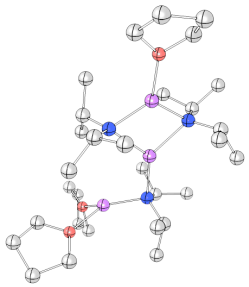
R-2$_b$
G = -1362.337705
G_{MP2} = -1358.220942

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	-3.9043	2.408759	-2.000251
Li	-1.855196	2.023135	-0.085893	H	-3.365144	3.371629	-2.140417
N	0.076333	2.039418	0.280808	C	-3.259375	1.413734	-2.971587
C	0.793414	2.829097	-0.732567	H	-2.235332	1.171655	-2.673482
H	1.890334	2.739316	-0.57738	H	-3.829385	0.473893	-3.002471
C	0.508834	2.30599	-2.146518	H	-3.222555	1.812954	-3.992752
H	1.124071	2.827229	-2.890226	C	-5.344179	2.6801	-2.492952
H	0.712444	1.232414	-2.235339	H	-5.326749	2.994517	-3.544046
H	-0.539031	2.471906	-2.428022	H	-5.958064	1.772993	-2.424192
C	0.50186	4.348843	-0.710288	H	-5.846409	3.471181	-1.927489
H	0.755014	4.795484	0.25653	N	-1.708027	-1.209978	-0.142575
H	1.083471	4.876954	-1.478564	C	-1.519533	-2.15048	-1.267846
H	-0.563768	4.541611	-0.900448	H	-0.90153	-3.013511	-0.950877
C	0.529652	2.410453	1.638328	C	-0.76653	-1.505206	-2.441581
H	1.4531	3.012338	1.559941	H	-0.635293	-2.220345	-3.264098
C	0.902033	1.18281	2.49337	H	-1.316736	-0.647355	-2.839842
H	1.266837	1.477384	3.48629	H	0.230304	-1.159753	-2.144274
H	0.03083	0.535356	2.652463	C	-2.831578	-2.765994	-1.812766
H	1.682124	0.582937	2.011384	H	-3.466972	-1.992172	-2.265313
C	-0.484209	3.268262	2.427094	H	-2.631103	-3.522812	-2.583747
H	-1.401728	2.696617	2.625569	H	-3.406926	-3.253438	-1.018889
H	-0.084707	3.585672	3.400782	C	-1.913953	-1.966961	1.109672
H	-0.765284	4.165719	1.86677	H	-2.633078	-2.797004	0.954093
N	-3.768139	1.908628	-0.617512	C	-2.522211	-1.071887	2.197845
Li	-3.528159	-0.112575	-0.366463	H	-3.521591	-0.716611	1.928074
O	-5.334494	-1.064892	-0.021417	H	-2.612704	-1.605871	3.152144
C	-6.543447	-0.460239	-0.548982	H	-1.896309	-0.188908	2.372184
C	-7.705774	-1.166795	0.151698	C	-0.640454	-2.635336	1.684278
C	-7.1212	-2.562003	0.41613	H	0.096034	-1.879516	1.988701
C	-5.671615	-2.229576	0.766884	H	-0.875881	-3.244532	2.567775
H	-4.964255	-3.024575	0.522738	H	-0.164725	-3.296338	0.952973
H	-5.565249	-1.980044	1.83073	O	1.890809	-0.808571	-0.291674
H	-7.164898	-3.175054	-0.49196	C	2.273595	-2.203497	-0.357361
H	-7.630587	-3.10388	1.218652	C	3.646645	-2.223725	-1.027738

Table 7 (Continued).

H	-8.611657	-1.182636	-0.461476	C	4.255825	-0.903792	-0.532809
H	-7.945056	-0.667626	1.098188	C	3.045319	0.031569	-0.547774
H	-6.494692	0.613191	-0.360341	H	2.91524	0.509294	-1.525614
H	-6.566388	-0.627231	-1.633153	H	3.078479	0.810072	0.21713
C	-4.568843	2.689632	0.338214	H	5.070984	-0.536421	-1.163231
C	-4.545362	2.03694	1.726153	H	4.641144	-1.020284	0.487145
H	-4.958989	1.023102	1.690391	H	3.54144	-2.211874	-2.119134
H	-3.523698	1.968179	2.123071	H	4.232519	-3.105412	-0.751208
H	-5.135343	2.618113	2.445642	H	2.317568	-2.605381	0.662187
H	-5.635787	2.707308	0.040823	H	1.501431	-2.74046	-0.912953
C	-4.147689	4.173297	0.466071	H	-4.179108	4.689259	-0.499711
H	-3.122733	4.257943	0.854119	H	-4.808668	4.718334	1.153257





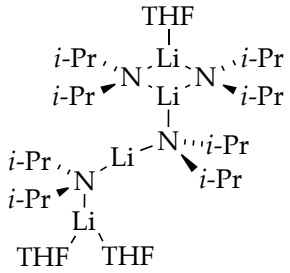
R-3
G = -1362.337705
G_{MP2} = -1358.220942

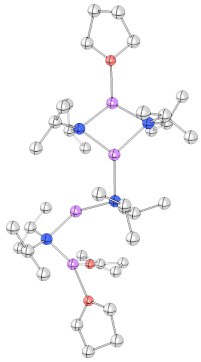
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	-4.694872	-2.07748	-1.142442
Li	-2.215681	-0.899809	0.79248	H	-3.219149	-3.013107	-0.857054
N	-0.226963	-1.826001	0.725784	H	-4.754863	-3.849279	-1.120164
C	0.387552	-2.208656	2.001063	H	-5.657164	-3.097955	0.977188
H	1.407294	-2.614525	1.841639	C	-3.916162	-4.214322	1.469687
C	0.585241	-0.991113	2.912196	H	-2.824371	-4.162396	1.401296
H	1.097095	-1.27508	3.840642	H	-4.181491	-4.35819	2.522358
H	1.187086	-0.217041	2.420725	H	-4.252509	-5.107589	0.926898
H	-0.373649	-0.539615	3.191843	C	-4.20845	-1.662469	2.903098
C	-0.371965	-3.298735	2.791711	H	-3.608889	-2.485824	3.332614
H	-0.507477	-4.209428	2.197948	C	-3.602818	-0.374407	3.472091
H	0.170583	-3.580119	3.705435	H	-2.541269	-0.291051	3.216423
H	-1.367621	-2.94069	3.080672	H	-4.105505	0.51517	3.0743
C	-0.23111	-2.937369	-0.236212	H	-3.679402	-0.345007	4.566448
H	-1.003674	-3.696736	0.01487	C	-5.636984	-1.84849	3.473048
C	1.088283	-3.736752	-0.369925	H	-5.633372	-1.866201	4.571245
H	1.003845	-4.47399	-1.179	H	-6.296452	-1.026366	3.154636
H	1.924464	-3.065807	-0.611408	H	-6.090654	-2.785623	3.132245
H	1.349473	-4.285317	0.540434	N	-1.699095	1.105979	-0.157718
C	-0.581409	-2.415816	-1.637186	C	-1.581111	2.362457	0.588782

Table 7 (Continued).

H	0.237166	-1.798891	-2.034526	H	-1.049139	3.128518	-0.022197
H	-0.74843	-3.239541	-2.343216	C	-0.758133	2.20534	1.87308
H	-1.486458	-1.800316	-1.628284	H	-0.663622	3.164045	2.399269
N	-4.131111	-1.657844	1.434259	H	-1.233875	1.498034	2.561166
Li	-5.322796	-0.257581	0.699089	H	0.253855	1.840148	1.665302
O	-6.214851	1.460352	1.311934	C	-2.938279	3.009662	0.965373
C	-6.680901	2.370655	0.283005	H	-3.482178	2.350897	1.652456
C	-6.931425	3.704395	0.987108	H	-2.804294	3.988094	1.450566
C	-7.326668	3.250076	2.400231	H	-3.564399	3.164381	0.078607
C	-6.388176	2.064424	2.618585	C	-2.14901	1.412709	-1.52705
H	-6.782942	1.301387	3.293843	H	-2.489222	2.461619	-1.587065
H	-5.410179	2.392821	2.98754	C	-3.361185	0.574235	-1.967875
H	-8.373658	2.924356	2.422184	H	-4.209615	0.765509	-1.297208
H	-7.195503	4.027376	3.158582	H	-3.679258	0.815537	-2.992879
H	-7.70283	4.298567	0.488255	H	-3.142671	-0.498277	-1.932697
H	-6.009593	4.295312	1.021362	C	-1.025617	1.30043	-2.584401
H	-5.916432	2.427911	-0.496676	H	-0.643795	0.275122	-2.652111
H	-7.59914	1.958567	-0.151275	H	-1.369883	1.593092	-3.587218
O	-6.864359	-0.65038	-0.598883	H	-0.188389	1.954986	-2.31589
C	-6.986948	-0.670627	-2.036848	O	1.833371	0.726389	-0.316822
C	-7.8976	-1.856669	-2.338208	C	2.260824	2.065527	-0.608559
C	-8.887694	-1.795016	-1.163696	C	3.444233	2.337093	0.343747
C	-8.005441	-1.319088	0.000604	C	3.91347	0.918455	0.77344
H	-7.622013	-2.152016	0.598373	C	3.029526	-0.026346	-0.055993
H	-8.516715	-0.612866	0.663529	H	2.728224	-0.941846	0.453601
H	-9.364329	-2.756144	-0.951503	H	3.507422	-0.285692	-1.012439
H	-9.679285	-1.065736	-1.371495	H	3.737928	0.762708	1.841928
H	-7.321466	-2.787941	-2.311265	H	4.97733	0.749029	0.58249
H	-8.382431	-1.777578	-3.315714	H	3.121992	2.919096	1.211901
H	-7.433904	0.275289	-2.375935	H	4.233629	2.903794	-0.159182
H	-5.983119	-0.756691	-2.457082	H	2.574072	2.121614	-1.661071
C	-4.558582	-2.948756	0.859631	H	1.40205	2.722281	-0.45986
C	-4.294032	-2.969523	-0.651568				

Table 8. Optimized geometries of LDA tetramer intermediates at B3LYP level of theory with 6-31G(d) basis set 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)





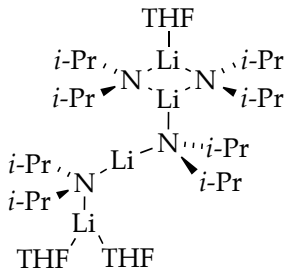
S_a
G = -1893.879194
G_{MP2} = -1888.176857

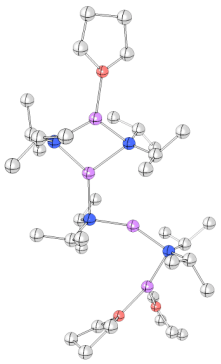
Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	H	-9.529513	0.018572	2.228396
Li	-1.646691	-1.202396	-0.044941	H	-9.070793	0.470815	0.5736
Li	-4.606241	-2.519729	0.555657	N	-2.497481	-2.979743	-0.077115
Li	-7.01109	-1.962917	0.995127	C	-1.909569	-3.972755	0.831058
N	-5.520134	-0.575957	1.031807	C	-1.787879	-3.389111	2.244689
C	-5.691837	0.463661	0.005311	H	-1.201468	-2.461387	2.253487
H	-6.275001	1.315467	0.413993	H	-2.772963	-3.159354	2.662697
C	-6.482507	-0.026831	-1.215115	H	-1.301645	-4.10127	2.92474
H	-6.607498	0.776691	-1.952486	H	-0.868664	-4.234291	0.522994
H	-5.967548	-0.852464	-1.717986	C	-2.660463	-5.320452	0.919819
H	-7.482732	-0.37907	-0.934313	H	-3.698429	-5.166118	1.233553
C	-4.359917	1.073651	-0.496276	H	-2.686067	-5.840129	-0.043295
H	-3.784682	0.31899	-1.047041	H	-2.174049	-5.991826	1.64112
H	-4.524809	1.925607	-1.172145	C	-2.643481	-3.499119	-1.449156
H	-3.743179	1.431807	0.335493	H	-3.425644	-4.281103	-1.499466
C	-5.258114	0.103471	2.314711	C	-3.102211	-2.371924	-2.383817
H	-4.674492	1.027899	2.141854	H	-3.976238	-1.848256	-1.983923
C	-4.41673	-0.72849	3.288803	H	-2.306409	-1.626761	-2.527167
H	-3.479586	-1.044501	2.821567	H	-3.366908	-2.756585	-3.376385
H	-4.16808	-0.14759	4.1873	C	-1.377047	-4.141951	-2.0627
H	-4.950744	-1.623683	3.618442	H	-1.561519	-4.443692	-3.101896
C	-6.547155	0.558909	3.041984	H	-0.542681	-3.426957	-2.062456
H	-7.138442	-0.314502	3.35262	H	-1.054601	-5.035229	-1.517346
H	-6.326511	1.15056	3.942569	Li	1.233581	-1.392872	0.7309
H	-7.172518	1.176895	2.387651	O	1.661564	-2.08719	2.586325
N	-6.37457	-3.847862	0.703611	C	1.844734	-3.522032	2.737488
C	-6.854834	-4.534447	-0.503406	C	1.730326	-3.802374	4.235696
H	-7.921723	-4.830949	-0.397773	C	2.249912	-2.494422	4.849805
C	-6.818895	-3.604186	-1.720827	C	1.678938	-1.451001	3.891583

Table 8 (Continued).

H	-7.223261	-4.104616	-2.610098	H	2.280934	-0.542043	3.81705
H	-7.410459	-2.697501	-1.553635	H	0.654108	-1.173836	4.162319
H	-5.792355	-3.298067	-1.955053	H	3.346177	-2.47078	4.838427
C	-6.115759	-5.844039	-0.8702	H	1.916555	-2.336271	5.879396
H	-6.191498	-6.599015	-0.080801	H	2.305468	-4.682932	4.536554
H	-6.538896	-6.284859	-1.783095	H	0.683796	-3.966014	4.514993
H	-5.050982	-5.6505	-1.044888	H	1.082671	-4.029493	2.140431
C	-6.478463	-4.72978	1.874629	H	2.835881	-3.784497	2.349887
H	-5.858546	-5.641064	1.749952	O	2.625595	-2.550042	-0.126762
C	-7.904064	-5.244653	2.19812	C	2.463645	-3.679451	-1.023319
H	-7.889498	-5.905636	3.075245	C	3.86147	-4.276469	-1.171813
H	-8.573644	-4.402515	2.421356	C	4.751735	-3.026904	-1.079707
H	-8.343245	-5.813354	1.372065	C	4.024616	-2.186354	-0.026421
C	-5.941018	-4.040619	3.131094	H	4.114572	-1.107923	-0.19165
H	-6.536408	-3.151351	3.381324	H	4.368257	-2.416727	0.989983
H	-5.976095	-4.712964	3.997799	H	4.771837	-2.501774	-2.041209
H	-4.901335	-3.724925	2.998887	H	5.783513	-3.248551	-0.792344
O	-8.980292	-1.550477	0.97882	H	3.981277	-4.82333	-2.111243
C	-9.616956	-0.262695	1.175183	H	4.077167	-4.965106	-0.346339
C	-11.075876	-0.426167	0.716456	H	1.729497	-4.357368	-0.580384
C	-11.011188	-1.657925	-0.201461	H	2.072933	-3.314515	-1.979715
C	-9.952735	-2.504567	0.498967	C	0.361387	0.559399	-1.321739
H	-9.430351	-3.212346	-0.146228	C	0.975793	-0.505332	-2.238679
H	-10.378488	-3.052762	1.350436	H	1.910657	-0.898542	-1.825028
H	-10.669306	-1.377197	-1.2046	H	0.285518	-1.348107	-2.374852
H	-11.970282	-2.1759	-0.297545	H	1.191632	-0.093144	-3.232082
H	-11.452477	0.46913	0.21305	H	1.134452	1.343179	-1.203888
H	-11.728565	-0.627995	1.57368	C	-0.815348	1.232776	-2.064103
H	-0.658159	-0.227774	2.631707	H	-0.468401	1.756799	-2.965173
H	-1.096327	1.463712	2.915206	H	-1.556354	0.487491	-2.379863
H	-0.645165	1.966907	0.50878	H	-1.331238	1.964975	-1.435074
C	1.206329	1.63209	1.509714	C	-0.145407	1.100035	0.975884
H	1.872623	1.923417	0.689695	C	-1.039003	0.681195	2.148464
H	1.073662	2.511729	2.154285	H	-2.06394	0.478101	1.817546
H	1.722315	0.863624	2.103335				

Table 8 (Continued).





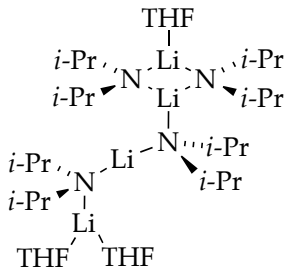
S_b
G = -1893.879904
G_{MP2} = -1888.178118

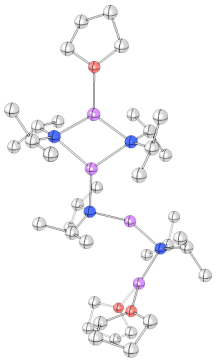
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	2.491297	0.703447	-2.426719
N	2.136146	0.49095	0.253539	H	0.973212	1.52789	-2.039328
Li	2.901182	-1.169983	-0.561624	H	2.386394	2.466629	-2.535457
N	4.447644	-2.291539	-1.237319	H	3.591073	1.875154	-0.499771
Li	5.90121	-0.988896	-0.787894	C	1.890627	3.026839	0.081937
O	6.417709	0.843787	-1.306811	H	0.800472	2.945324	0.154007
C	7.028784	1.720877	-0.323757	H	2.280739	3.270152	1.076106
C	6.776925	3.141869	-0.826207	H	2.12747	3.874912	-0.574648
C	6.778773	2.948232	-2.349874	C	2.452644	0.625868	1.684154
C	6.070623	1.601995	-2.498509	H	1.914226	1.482165	2.131205
H	6.395022	1.027403	-3.370271	C	1.98941	-0.60422	2.470063
H	4.98295	1.718948	-2.527608	H	0.926842	-0.801185	2.305902
H	7.805585	2.890032	-2.730204	H	2.540635	-1.502998	2.17278
H	6.260614	3.747193	-2.887546	H	2.144129	-0.464372	3.547586
H	7.537484	3.846159	-0.476486	C	3.948176	0.883127	2.001312
H	5.796904	3.495933	-0.488321	H	4.116522	0.969357	3.083197
H	6.573526	1.515216	0.647905	H	4.567895	0.05253	1.62938
H	8.100742	1.492245	-0.272752	H	4.309322	1.807772	1.537414
O	7.596432	-1.443928	0.174087	Li	-2.296363	-0.84021	-0.503682
C	7.806281	-1.88397	1.539993	N	-0.745445	-2.089665	-0.329662
C	9.321308	-1.990402	1.700945	C	-1.015678	-3.090896	0.709647
C	9.754657	-2.438075	0.296485	H	-1.716989	-3.86799	0.338171
C	8.805164	-1.643684	-0.603513	C	-1.719718	-2.466356	1.922512
H	8.538354	-2.166004	-1.526394	H	-2.035464	-3.242965	2.631149
H	9.215237	-0.658925	-0.859969	H	-1.056237	-1.781412	2.460799
H	9.590127	-3.514301	0.171927	H	-2.616543	-1.901774	1.63552
H	10.805433	-2.22732	0.077972	C	0.216519	-3.875436	1.220874
H	9.607144	-2.694787	2.487229	H	0.943553	-3.194758	1.678265
H	9.752935	-1.012373	1.944099	H	-0.076604	-4.617096	1.976682
H	7.337822	-1.152783	2.204522	H	0.72299	-4.416222	0.41435
H	7.315681	-2.853938	1.676568	C	-0.127122	-2.700293	-1.50966
C	4.794716	-3.482786	-0.432718	H	0.907314	-3.057818	-1.292769
C	4.48116	-3.219513	1.045389	C	0.008202	-1.671551	-2.637684

Table 8 (Continued).

H	4.87684	-2.25439	1.38646	H	0.527034	-0.765272	-2.305329
H	3.397944	-3.212969	1.214253	H	0.568929	-2.083444	-3.486315
H	4.904172	-4.001107	1.689238	H	-0.978397	-1.36987	-3.007481
H	5.885525	-3.701831	-0.486159	C	-0.856471	-3.93218	-2.104497
C	4.089714	-4.796042	-0.838774	H	-1.877228	-3.65907	-2.407066
H	4.297502	-5.582116	-0.101823	H	-0.328687	-4.299176	-2.994749
H	3.003173	-4.648707	-0.884679	H	-0.92562	-4.767743	-1.400838
H	4.420946	-5.172183	-1.812037	N	-1.846608	1.107456	-0.170982
C	4.532541	-2.568637	-2.683274	C	-2.26024	1.720446	1.102229
C	3.907769	-1.434895	-3.500292	H	-2.237057	2.823478	1.028797
H	2.842711	-1.325713	-3.272869	C	-3.707073	1.365535	1.527315
H	4.398216	-0.475066	-3.29641	H	-4.012987	1.90703	2.434191
H	3.994643	-1.628224	-4.576821	H	-4.424382	1.622942	0.738771
H	3.953904	-3.471079	-2.940772	H	-3.796617	0.289806	1.732154
C	5.97241	-2.825197	-3.194745	C	-1.30179	1.371501	2.247576
H	6.467231	-3.626751	-2.634059	H	-0.285596	1.712058	2.022305
H	5.978968	-3.11192	-4.254461	H	-1.61421	1.84265	3.189064
H	6.589445	-1.916559	-3.102349	H	-1.272708	0.290359	2.423526
C	2.487755	1.717618	-0.484631	C	-2.366433	1.914102	-1.28459
C	2.063497	1.593123	-1.953332	H	-3.440954	2.153349	-1.123321
C	-6.497041	-1.5911	-0.891755	C	-2.304953	1.156239	-2.619061
C	-5.28191	-0.772084	-1.323584	H	-2.737739	1.754383	-3.431226
H	-5.208126	0.20609	-0.84524	H	-1.268467	0.930045	-2.892639
H	-5.257201	-0.636946	-2.413328	H	-2.856014	0.207254	-2.584708
H	-6.727057	-1.404868	0.164057	C	-1.671769	3.283473	-1.492737
H	-7.388964	-1.360063	-1.482066	H	-0.636771	3.145532	-1.824702
H	-6.544568	-3.768648	-0.502704	H	-2.196149	3.880071	-2.253131
H	-6.052594	-3.313911	-2.143635	H	-1.648671	3.876475	-0.572558
H	-3.85117	-3.588065	-1.177585	O	-4.131637	-1.551175	-0.923008
H	-4.416698	-3.093453	0.432538	C	-4.52793	-2.917293	-0.64389
C	-5.989801	-3.028228	-1.086748				

Table 8 (Continued).





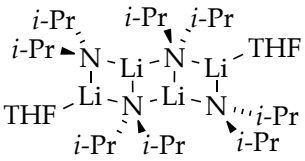
S$_c$
G = -1893.877324
G_{MP2} = -1888.176843

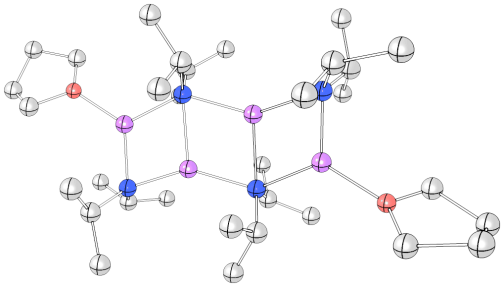
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	2.817179	-0.862614	1.694185
Li	-2.404951	0.559818	0.434599	H	3.403213	0.065378	1.699081
N	-0.913285	1.946068	0.467474	H	1.831958	-0.631333	2.11106
C	-1.084211	2.981893	-0.562941	H	3.303431	-1.57174	2.377393
H	-1.667114	3.835477	-0.157618	H	3.73678	-1.71549	-0.023572
C	-1.874819	2.487145	-1.781674	C	1.944694	-2.79961	0.377635
H	-1.999438	3.28794	-2.522078	H	0.906778	-2.643773	0.690827
H	-1.360098	1.659448	-2.281397	H	1.918923	-3.323429	-0.583231
H	-2.875211	2.136354	-1.499643	H	2.43106	-3.467934	1.101783
C	0.24815	3.589352	-1.066421	C	1.962618	-0.988938	-1.999477
H	0.823245	2.832247	-1.613976	H	1.180418	-1.771053	-2.046476
H	0.083921	4.438712	-1.745711	C	1.504367	0.134107	-2.939325
H	0.864732	3.950472	-0.235812	H	0.630452	0.659906	-2.542001
C	-0.651733	2.63013	1.74801	H	2.30047	0.878308	-3.086018
H	-0.068131	3.553987	1.572033	H	1.239728	-0.254969	-3.930181
C	0.189418	1.801705	2.725325	C	3.229213	-1.634455	-2.609833
H	1.127003	1.484638	2.259716	H	3.045	-1.941051	-3.647658
H	0.437182	2.38554	3.622165	H	4.063401	-0.919247	-2.61276
H	-0.344388	0.9073	3.05741	H	3.551773	-2.525137	-2.060315
C	-1.941063	3.08807	2.473152	N	4.606747	2.516764	-0.570802
H	-2.532438	2.215756	2.786686	Li	5.841682	1.127973	0.164795
H	-1.720818	3.682969	3.371695	O	6.274794	0.447599	2.023722
H	-2.566186	3.703667	1.816338	C	6.449539	-0.986898	2.186346
N	-1.769517	-1.326704	0.151319	C	6.334308	-1.253535	3.686739
C	-2.249176	-2.017979	-1.053261	C	6.869758	0.053679	4.288666
H	-3.316322	-2.313401	-0.947318	C	6.309435	1.09608	3.322717
C	-2.211618	-1.092797	-2.274495	H	6.925106	1.994867	3.23651
H	-2.615252	-1.596742	-3.162109	H	5.290485	1.391948	3.595614
H	-2.803023	-0.185197	-2.1117	H	7.966196	0.0643	4.275478
H	-1.184738	-0.788015	-2.508884	H	6.540111	0.224404	5.317436
C	-1.51065	-3.329577	-1.41403	H	6.900141	-2.137836	3.994211
H	-1.586888	-4.080977	-0.621279	H	5.286416	-1.40316	3.968806

Table 8 (Continued).

H	-1.933871	-3.774266	-2.32501	H	5.684046	-1.494241	1.593675
H	-0.445747	-3.137404	-1.589449	H	7.438917	-1.259043	1.800633
C	-1.875482	-2.203435	1.32601	O	7.230885	-0.036608	-0.687223
H	-1.256596	-3.116033	1.205855	C	7.067775	-1.16869	-1.580199
C	-3.302021	-2.71508	1.650581	C	8.46447	-1.769377	-1.724317
H	-3.28893	-3.372734	2.530229	C	9.357322	-0.521422	-1.635594
H	-3.970534	-1.871142	1.870202	C	8.630511	0.324651	-0.586516
H	-3.741512	-3.286271	0.826407	H	8.722922	1.40225	-0.75586
C	-1.338189	-1.509543	2.579936	H	8.972347	0.097562	0.431215
H	-1.93223	-0.618051	2.825403	H	9.379973	0.00004	-2.599036
H	-1.375488	-2.177856	3.44966	H	10.388201	-0.744221	-1.3459
H	-0.297756	-1.196403	2.447483	H	8.584507	-2.320057	-2.661482
O	-4.374197	0.972852	0.415955	H	8.677376	-2.455319	-0.895885
C	-5.010692	2.261246	0.608799	H	6.331328	-1.843337	-1.136122
C	-6.469701	2.096503	0.151041	H	6.679513	-0.806145	-2.538511
C	-6.404774	0.863367	-0.764965	C	4.967371	3.070862	-1.894935
C	-5.346294	0.017932	-0.063095	C	5.583183	2.002745	-2.807006
H	-4.823544	-0.690551	-0.707226	H	6.518178	1.61205	-2.391187
H	-5.772132	-0.529319	0.788914	H	4.893697	1.158793	-2.939948
H	-6.062855	1.142638	-1.768502	H	5.799246	2.410842	-3.802048
H	-7.363774	0.345087	-0.860351	H	5.739445	3.856128	-1.780622
H	-6.846907	2.990874	-0.35356	C	3.789861	3.739449	-2.640363
H	-7.121907	1.895663	1.00887	H	4.136181	4.259599	-3.543911
H	-4.922794	2.545531	1.661155	H	3.049616	2.991907	-2.952561
H	-4.46481	2.993055	0.004855	H	3.273217	4.474065	-2.014773
N	2.108288	-0.463397	-0.629725	C	4.459376	3.620552	0.400538
Li	2.960125	1.313824	-0.608934	C	3.569055	3.203529	1.576268
C	2.695826	-1.452431	0.283076	H	2.544299	2.995256	1.247969
C	5.810083	4.159142	0.930303	H	3.954106	2.298052	2.062782
H	6.474333	4.449478	0.108301	H	3.51	3.989191	2.339644
H	5.675316	5.040844	1.57161	H	3.956031	4.483823	-0.069399
H	6.329277	3.394636	1.526148				

Table 8 (Continued).



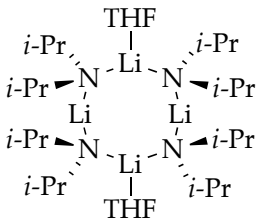


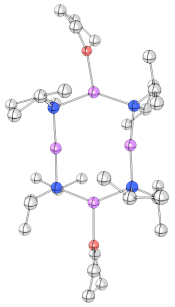
T
G = -1661.533838
G_{MP2} = -1656.500785

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	-1.754553	-1.586992	1.965124
N	-2.156026	-0.271004	0.33449	C	-1.797294	0.389756	2.704235
Li	-1.77685	1.950746	0.035036	H	-0.733973	0.566034	2.530905
N	-3.705226	2.807429	-0.303196	H	-2.324546	1.340584	2.589766
Li	-3.964163	0.834629	-0.135468	H	-1.911417	0.076846	3.74948
O	-5.770511	0.042599	-0.463549	C	-3.792257	-1.020216	2.159044
C	-6.914841	0.58265	0.247996	H	-3.823833	-1.399838	3.188609
C	-8.150268	-0.066453	-0.386141	H	-4.440816	-0.133809	2.124519
C	-7.664227	-0.387406	-1.80835	H	-4.235395	-1.784016	1.511632
C	-6.212675	-0.790856	-1.558418	N	1.849696	-0.90347	-0.259117
H	-5.549401	-0.609665	-2.408541	Li	2.178555	1.090211	-0.463263
H	-6.12944	-1.845373	-1.264739	N	0.470916	2.272267	-0.200046
H	-7.706673	0.506837	-2.440633	C	0.901326	3.185781	0.883827
H	-8.240849	-1.179909	-2.294437	H	1.706419	3.847921	0.51996
H	-9.020184	0.596253	-0.366198	C	1.514067	2.435492	2.073493
H	-8.415319	-0.989271	0.142785	H	1.910471	3.146237	2.809552
H	-6.802765	0.346871	1.310699	H	0.773825	1.816121	2.586991
H	-6.904385	1.670077	0.122218	H	2.344	1.781672	1.776868
C	-4.344949	3.688258	0.690573	C	-0.198568	4.129693	1.411007
C	-4.20114	3.154871	2.11942	H	-0.990041	3.564999	1.920743
H	-4.533974	2.112815	2.201839	H	0.203469	4.8522	2.134443
H	-3.163533	3.207988	2.468571	H	-0.664464	4.698416	0.600397
H	-4.806128	3.749033	2.815697	C	0.168209	3.032594	-1.444498
H	-5.438646	3.732761	0.514763	H	-0.834241	3.512127	-1.392905
C	-3.866996	5.159619	0.675938	C	0.14361	2.077982	-2.644643
H	-4.417265	5.754493	1.417363	H	-0.431748	1.170096	-2.439993
H	-2.799765	5.223471	0.91515	H	-0.295377	2.558898	-3.526975
H	-4.017276	5.634979	-0.298722	H	1.161035	1.770112	-2.909916
C	-3.949604	3.323096	-1.665099	C	1.1315	4.185724	-1.813998
C	-3.487402	2.315466	-2.721406	H	2.166053	3.821278	-1.870425
H	-2.451991	2.008192	-2.563273	H	0.8632	4.583906	-2.800154
H	-4.119634	1.41551	-2.710381	H	1.098586	5.022701	-1.109753
H	-3.549677	2.741642	-3.7304	O	3.994149	1.915822	-0.768553
H	-3.36703	4.248115	-1.854223	C	4.539676	3.075456	-0.08641
C	-5.419565	3.682244	-1.999824	C	6.0145	3.151119	-0.492801

Table 8 (Continued).

H	-5.807796	4.511967	-1.402113	C	6.349462	1.681056	-0.78578
H	-5.507369	3.9749	-3.054064	C	5.058113	1.192122	-1.43578
H	-6.072957	2.814145	-1.835134	H	4.868887	0.125467	-1.30566
C	-2.515741	-1.396238	-0.571287	H	5.031205	1.43336	-2.506793
C	-2.089655	-1.088401	-2.011957	H	6.536643	1.134667	0.145933
H	-2.472517	-0.125475	-2.357223	H	7.218751	1.555908	-1.438107
H	-0.996499	-1.069312	-2.101804	H	6.636513	3.590304	0.292564
H	-2.455767	-1.859876	-2.701064	H	6.134192	3.757322	-1.398361
H	-3.617182	-1.542986	-0.603321	H	3.96065	3.954147	-0.380701
C	-1.943928	-2.781597	-0.190283	H	4.423057	2.922035	0.992579
H	-0.855955	-2.733184	-0.065486	C	2.372721	-1.565945	0.953604
H	-2.375515	-3.180912	0.732752	H	2.432477	-2.656511	0.792968
H	-2.158904	-3.506041	-0.985743	C	3.807492	-1.127533	1.335672
C	-2.338869	-0.676449	1.75058	H	4.198336	-1.708207	2.183132
H	3.410338	-1.886892	-1.318764	H	4.500107	-1.26874	0.497683
C	2.221313	-0.837698	-2.733172	H	3.829362	-0.066567	1.619939
H	2.625019	-1.402345	-3.582871	C	1.452328	-1.387139	2.166571
H	1.177086	-0.601741	-2.964571	H	0.455779	-1.79569	1.9652
H	2.774733	0.108755	-2.681345	H	1.852012	-1.903163	3.049168
C	1.632286	-3.010514	-1.675419	H	1.345599	-0.33087	2.436094
H	0.589711	-2.860673	-1.97765	C	2.331121	-1.649811	-1.436141
H	2.136216	-3.580008	-2.468997	H	1.630694	-3.634552	-0.77579





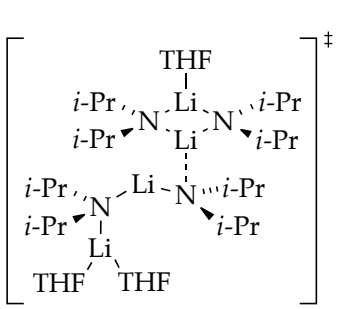
U
G = -1661.537728
G_{MP2} = -1656.49475

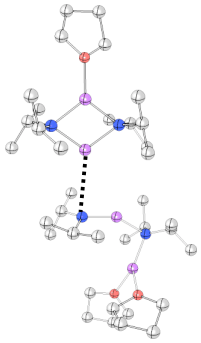
Atom	X	Y	Z	Atom	X	Y	Z
C	0	0	0	H	3.445614	-7.280682	-1.011027
Li	1.65886	-1.485071	-1.615402	C	5.505144	-6.885702	-1.37996
N	-0.28003	-1.285513	-2.12282	H	5.849863	-7.584127	-0.606884
Li	-1.046697	-3.16368	-1.711183	H	5.545618	-7.4172	-2.335896
N	-0.350376	-5.05736	-1.097101	H	6.209394	-6.047812	-1.42736
C	-1.106719	-6.019421	-1.921357	C	4.117676	-5.833686	0.39514
H	-2.188859	-5.922807	-1.696899	H	3.139814	-5.457744	0.711391
C	-0.948043	-5.686314	-3.411429	H	4.412902	-6.615841	1.105234
H	-1.307328	-4.676484	-3.639887	H	4.836097	-5.007917	0.491287
H	0.100647	-5.742152	-3.72889	C	3.684939	-5.751863	-3.369989
N	3.526754	-5.355326	-1.958677	C	4.086396	-6.372957	-1.039928

Table 8 (Continued).

H	-1.515364	-6.385908	-4.037295	H	4.75547	-5.870586	-3.628189
C	-0.780861	-7.518638	-1.710921	C	3.153637	-4.649556	-4.293229
H	0.286601	-7.722905	-1.873074	H	3.311976	-4.902786	-5.348703
H	-1.036009	-7.851225	-0.700451	H	2.077104	-4.493928	-4.151635
H	-1.352048	-8.143671	-2.411023	H	3.649842	-3.687812	-4.108935
C	-0.704644	-5.189326	0.329592	C	3.017848	-7.092229	-3.758333
H	-1.735107	-5.59118	0.411814	H	1.930894	-7.051507	-3.6094
C	0.19448	-6.132701	1.167144	H	3.199859	-7.330554	-4.814654
H	0.328327	-7.107451	0.692721	H	3.398642	-7.928302	-3.162748
H	1.188739	-5.689618	1.306472	O	6.390515	-3.573922	-1.951305
H	-0.225259	-6.298584	2.169315	C	7.381971	-3.372015	-0.91743
C	-0.700552	-3.818436	1.028196	C	8.709001	-3.840714	-1.517427
H	-0.911693	-3.906979	2.101591	C	8.516622	-3.518364	-3.007373
H	0.282994	-3.343852	0.9255	C	7.037756	-3.850141	-3.215857
H	-1.448043	-3.13288	0.609221	H	6.887291	-4.907986	-3.459829
O	-3.177549	-3.464438	-1.894409	H	6.558387	-3.238812	-3.986712
C	-4.075907	-3.682129	-0.795251	H	9.16956	-4.099561	-3.665148
C	-5.191807	-4.579748	-1.355444	H	8.700819	-2.454251	-3.194353
C	-5.172762	-4.283734	-2.880104	H	8.836402	-4.919718	-1.372318
C	-4.01407	-3.281884	-3.046652	H	9.568996	-3.332325	-1.071573
H	-4.381091	-2.245969	-3.069794	H	7.406553	-2.306697	-0.66087
H	-3.399863	-3.456684	-3.931907	H	7.075384	-3.942811	-0.03589
H	-6.116117	-3.860955	-3.238155	C	4.041225	-1.371624	0.104989
H	-4.981875	-5.197733	-3.449256	H	5.084924	-1.736569	0.240714
H	-6.15765	-4.355403	-0.893256	C	3.148599	-2.287616	0.955127
H	-4.965939	-5.632702	-1.165184	H	3.554616	-2.42735	1.964803
H	-3.503783	-4.139401	0.012808	H	2.144715	-1.857547	1.061285
H	-4.472654	-2.714575	-0.454341	H	3.042283	-3.278296	0.501323
C	-0.809788	-0.178282	-1.296288	C	4.024899	0.034717	0.74756
C	-2.303915	-0.301561	-0.917081	H	3.0297	0.490317	0.673876
H	-2.932666	-0.457713	-1.797424	H	4.281544	-0.036876	1.812184
H	-2.459791	-1.152725	-0.241316	H	4.739977	0.721869	0.285633
H	-2.658986	0.599423	-0.397061	C	4.202331	-0.381109	-2.135897
H	-0.704654	0.773659	-1.850842	H	3.874337	0.609681	-1.764078
C	-0.254151	-0.8979	-3.546549	C	3.688458	-0.474318	-3.578035
C	0.351924	-2.021281	-4.394848	H	2.59692	-0.392411	-3.633974
H	1.322199	-2.350161	-4.008179	H	4.101638	0.333589	-4.194374
H	-0.308443	-2.897132	-4.416212	H	3.977452	-1.427544	-4.040142
H	0.50398	-1.699058	-5.432085	C	5.745984	-0.317149	-2.17627
H	0.399518	-0.005271	-3.681754	H	6.156025	-1.211135	-2.657229
C	-1.601673	-0.486488	-4.182825	H	6.081649	0.56276	-2.740867
H	-2.047514	0.376721	-3.679763	H	6.181485	-0.247237	-1.17373
H	-1.458295	-0.211171	-5.236383	H	-0.414063	0.796131	0.631981
H	-2.32312	-1.311544	-4.144129	H	-0.002215	-0.923052	0.593726
N	3.623594	-1.459738	-1.309647	H	1.042645	0.270963	-0.210687
Li	4.313422	-3.431602	-1.731915	Li	1.593528	-5.155649	-1.497991

Table 9. Optimized geometries of LDA aggregation transition structures at B3LYP level of theory with 6-31G(d) basis set 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)





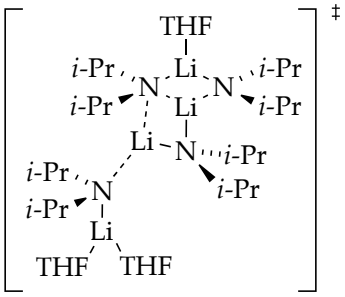
V
G = -1893.880012
G_{MP2} = -1888.161058

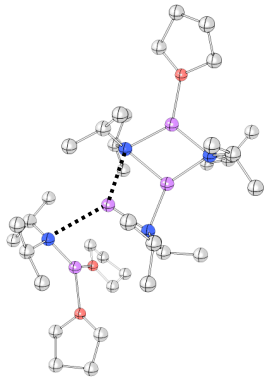
Atom	X	Y	Z	Atom	X	Y	Z
N	0	0	0	C	-1.13489	1.260205	-1.879603
Li	-1.464073	-1.397256	-0.142253	H	-0.945244	1.887159	-2.761813
N	-2.074315	-3.180441	-0.317334	H	-1.788694	0.435811	-2.19433
C	-1.804487	-4.203705	0.680899	H	-1.690993	1.867261	-1.157741
C	-1.75191	-3.557368	2.072808	C	-0.212536	0.96659	1.093929
H	-1.004723	-2.754347	2.109943	C	-0.977097	0.325611	2.258243
H	-2.722945	-3.115077	2.330078	H	-1.978737	0.004542	1.947548
H	-1.496075	-4.289999	2.850437	H	-0.448578	-0.556936	2.639299
H	-0.804857	-4.686558	0.531036	H	-1.102147	1.025737	3.093805
C	-2.801189	-5.385237	0.723255	H	-0.836595	1.809925	0.747841
H	-3.829437	-5.019372	0.835698	C	1.100778	1.597601	1.614698
H	-2.769575	-5.988373	-0.190037	H	1.678058	2.041861	0.795561
H	-2.577654	-6.05434	1.564956	H	0.912722	2.388665	2.353786
C	-2.292427	-3.713251	-1.657308	H	1.732796	0.83691	2.095656
H	-3.106134	-4.464236	-1.669462	Li	-5.530291	-2.588074	0.598535
C	-2.747725	-2.595083	-2.603757	Li	-7.835154	-2.010928	0.61328
H	-3.643084	-2.096861	-2.213156	N	-6.287801	-0.771632	1.042997
H	-1.963965	-1.83331	-2.725505	C	-6.018093	0.34642	0.135665
H	-2.980422	-2.981295	-3.604048	H	-6.718632	1.186836	0.342547
C	-1.060823	-4.420687	-2.274852	C	-6.250634	-0.056235	-1.325388
H	-1.289074	-4.850372	-3.260188	H	-6.083585	0.790947	-2.002043
H	-0.237256	-3.703337	-2.39818	H	-5.559171	-0.85426	-1.62854
H	-0.703057	-5.236901	-1.635669	H	-7.271866	-0.42039	-1.488034
Li	1.332345	-1.399458	0.4531	C	-4.599794	0.950615	0.257951
O	1.856329	-2.254662	2.198878	H	-3.84665	0.195195	-0.005921
C	1.959325	-3.704493	2.203399	H	-4.467883	1.812904	-0.410747
C	1.948075	-4.111376	3.675622	H	-4.391783	1.288624	1.278616
C	2.638757	-2.913136	4.343629	C	-6.312533	-0.305968	2.442829
C	2.087991	-1.738177	3.534785	H	-6.266759	0.797748	2.465049
H	2.778059	-0.893078	3.459578	C	-5.115641	-0.800247	3.283682

Table 9 (Continued).

H	1.136208	-1.378743	3.940659	H	-4.170168	-0.496254	2.82334
H	3.72713	-2.984192	4.229742	H	-5.139838	-0.403793	4.309204
H	2.41419	-2.821423	5.410161	H	-5.11243	-1.895432	3.356178
H	2.462752	-5.061168	3.847794	C	-7.632559	-0.670628	3.157109
H	0.917482	-4.209794	4.033709	H	-7.790011	-1.757435	3.180348
H	1.120011	-4.108704	1.631393	H	-7.645869	-0.322591	4.199021
H	2.898278	-3.986235	1.711038	H	-8.488528	-0.219414	2.640548
O	2.809243	-2.314709	-0.5501	N	-7.044127	-3.878132	0.366664
C	2.763101	-3.253168	-1.655776	C	-7.363334	-4.501117	-0.927135
C	4.212933	-3.679301	-1.883093	H	-8.287815	-5.109824	-0.845756
C	4.981673	-2.402791	-1.507051	C	-7.645008	-3.44728	-2.007592
C	4.170367	-1.878008	-0.320473	H	-7.898635	-3.919534	-2.965115
H	4.173656	-0.786354	-0.237694	H	-8.479219	-2.791375	-1.72709
H	4.516134	-2.303855	0.63011	H	-6.764066	-2.816583	-2.179017
H	4.956458	-1.685178	-2.334854	C	-6.265747	-5.456081	-1.45061
H	6.028189	-2.585064	-1.246234	H	-6.003885	-6.21719	-0.707869
H	4.393152	-4.005366	-2.911309	H	-6.587665	-5.980233	-2.361888
H	4.483127	-4.50296	-1.211672	H	-5.352695	-4.894057	-1.68522
H	2.092892	-4.069766	-1.377463	C	-7.245074	-4.855789	1.447938
H	2.348429	-2.740788	-2.531109	H	-6.93639	-5.865166	1.118815
C	0.182443	0.719444	-1.277454	C	-8.723588	-4.983972	1.888063
C	0.883858	-0.161866	-2.319108	H	-8.871691	-5.804028	2.605224
H	1.897805	-0.42439	-1.996668	H	-9.062456	-4.054624	2.368476
H	0.327703	-1.095949	-2.478358	H	-9.375378	-5.175962	1.027872
H	0.956683	0.347889	-3.287742	C	-6.385648	-4.537615	2.679173
H	0.836283	1.600761	-1.131017	H	-6.636711	-3.554647	3.094291
H	-11.134582	-2.579438	1.157889	H	-6.540947	-5.27499	3.477358
H	-11.831625	-1.51119	-1.627012	H	-5.317311	-4.541644	2.430278
H	-12.929745	-1.755251	-0.256195	O	-9.679761	-1.416404	0.242205
H	-11.975747	0.765035	-0.708073	C	-10.041365	-0.051249	-0.075998
H	-11.943067	0.147176	0.95414	C	-11.570131	-0.02022	-0.063321
H	-9.574081	0.604365	0.662792	C	-11.920372	-1.439909	-0.536509
H	-9.640457	0.195448	-1.067039	C	-10.838813	-2.280022	0.145214
H	-10.550006	-3.17339	-0.414				

Table 9 (Continued).





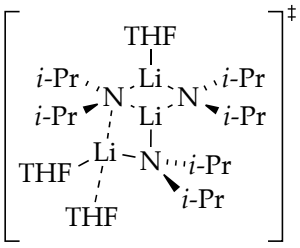
W
G = -1893.865927
G_{MP2} = -1888.166029

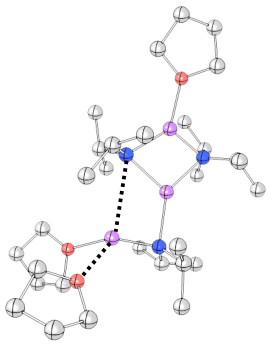
Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	-6.135808	4.092197	-0.260542
Li	-2.077429	1.150198	0.588834	H	-6.566688	3.297665	1.258704
N	-0.244757	2.249699	0.284575	H	-4.303991	3.603858	1.869617
C	-0.66182	3.293797	-0.689882	H	-3.789281	3.855032	0.186679
H	-1.195573	4.105595	-0.159647	N	1.925404	-0.394507	-0.678198
C	-1.645738	2.782303	-1.751921	Li	1.98306	1.583058	-0.431058
H	-1.88902	3.578781	-2.466922	C	2.605965	-1.392978	0.152695
H	-1.225713	1.949813	-2.323793	C	2.875943	-0.850019	1.559901
H	-2.590508	2.443004	-1.312145	H	3.472675	0.069844	1.532305
C	0.522601	3.969164	-1.409266	H	1.943624	-0.623396	2.087348
H	1.000567	3.268482	-2.104744	H	3.41872	-1.588839	2.164466
H	0.203157	4.83865	-2.001003	H	3.604402	-1.637937	-0.264489
H	1.283363	4.31754	-0.702968	C	1.860957	-2.74274	0.284188
C	0.101694	2.945169	1.549251	H	0.881367	-2.599603	0.756901
H	0.617722	3.896495	1.323519	H	1.68705	-3.208035	-0.691592
C	1.068535	2.142431	2.424122	H	2.435261	-3.456348	0.891673
H	2.00897	1.9281	1.90506	C	1.774938	-0.851277	-2.073408
H	1.326073	2.701919	3.332603	H	0.977052	-1.619569	-2.162806
H	0.629854	1.190836	2.735806	C	1.336739	0.326211	-2.954468
C	-1.122077	3.34073	2.411659	H	0.466485	0.839238	-2.531942
H	-1.644344	2.450434	2.790151	H	2.147715	1.06066	-3.054206
H	-0.823699	3.939262	3.283374	H	1.06379	-0.003786	-3.964479
H	-1.838047	3.938013	1.838077	C	3.023213	-1.489782	-2.724742
N	-1.843598	-0.836457	0.440545	H	2.826765	-1.705008	-3.78276
C	-2.494074	-1.559406	-0.66335	H	3.88027	-0.806941	-2.672278
H	-3.566237	-1.747937	-0.441454	H	3.311043	-2.433417	-2.250206
C	-2.486718	-0.724449	-1.949501	N	4.681424	3.029085	-0.548121
H	-3.003221	-1.25069	-2.76176	Li	5.502983	1.526575	0.36703
H	-2.98626	0.240566	-1.809922	O	5.830263	1.056991	2.35133
H	-1.46221	-0.527524	-2.290047	C	6.321075	-0.25865	2.715699
C	-1.896016	-2.94883	-0.988091	C	6.02993	-0.414933	4.208324
H	-1.935485	-3.63014	-0.132106	C	6.135668	1.033088	4.706405
H	-2.447358	-3.426972	-1.80889	C	5.50271	1.805541	3.550194

Table 9 (Continued).

H	-0.846191	-2.853531	-1.290974	H	5.88737	2.820817	3.431616
C	-1.960449	-1.585147	1.701887	H	4.411623	1.850106	3.648648
H	-1.525944	-2.599452	1.604917	H	7.185946	1.321376	4.834004
C	-3.405807	-1.794818	2.214995	H	5.617326	1.206789	5.653888
H	-3.411419	-2.403525	3.129079	H	6.729932	-1.098147	4.698504
H	-3.871588	-0.828379	2.450927	H	5.014232	-0.797211	4.361207
H	-4.040401	-2.305292	1.483208	H	5.813692	-0.998977	2.093735
C	-1.162484	-0.906125	2.819078	H	7.39683	-0.298949	2.507725
H	-1.539068	0.106258	3.022089	O	6.940416	0.215232	-0.224535
H	-1.231315	-1.472959	3.755873	C	6.817204	-1.02799	-0.95922
H	-0.102017	-0.829981	2.558799	C	8.250116	-1.467488	-1.264179
O	-3.959362	1.881648	0.75105	C	8.977187	-0.119913	-1.396638
C	-4.426322	3.251874	0.840404	C	8.294197	0.720842	-0.316738
C	-5.90077	3.245153	0.390262	H	8.243625	1.78764	-0.55352
C	-6.050043	1.884845	-0.313223	H	8.779731	0.598846	0.660779
C	-5.08753	1.016458	0.489158	H	8.798428	0.314241	-2.386655
H	-4.710133	0.136864	-0.032275	H	10.058189	-0.192535	-1.24554
H	-5.534077	0.6989	1.441436	H	8.31143	-2.081865	-2.166944
H	-5.721822	1.946713	-1.357139	H	8.663188	-2.04627	-0.429484
H	-7.075638	1.504055	-0.297552	H	6.258564	-1.734947	-0.339034
H	3.499553	4.82031	-2.282194	H	6.245153	-0.836898	-1.873451
C	4.76309	4.297377	0.188604	C	5.02719	3.269295	-1.954981
C	3.815316	4.322437	1.391748	C	5.442852	1.976932	-2.667207
H	2.771962	4.292777	1.063632	H	6.363725	1.56503	-2.242072
H	3.979002	3.452901	2.038023	H	4.65455	1.220597	-2.565813
H	3.953674	5.224724	2.002907	H	5.609779	2.144175	-3.738914
H	4.455079	5.14513	-0.451584	H	5.900594	3.952991	-2.027056
C	6.205092	4.630414	0.653583	C	3.907371	3.937578	-2.785209
H	6.903015	4.594458	-0.191656	H	4.273455	4.254933	-3.772286
H	6.281375	5.630526	1.104971	H	3.081468	3.234019	-2.944789
H	6.548515	3.89942	1.401231				

Table 9 (Continued).



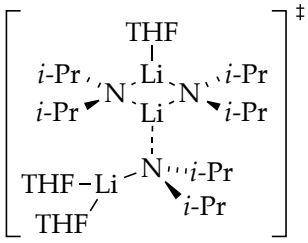


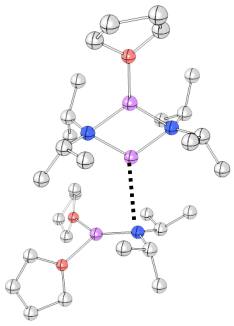
X
G = -1594.669023
G_{MP2} = -1589.893992

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	C	-1.45471	-1.767731	-1.858058
Li	-2.024694	1.474731	-0.067723	H	-1.698854	-2.624505	-2.499796
N	0.061697	1.977493	-0.139925	H	-1.769609	-0.861855	-2.386773
C	0.536344	2.543577	-1.407042	H	-0.364748	-1.731872	-1.750534
H	1.650669	2.511854	-1.442528	C	-3.65841	-2.134228	-0.725595
C	0.054047	1.716234	-2.605621	H	-4.085904	-1.344295	-1.356647
H	0.478562	2.095736	-3.543682	H	-3.845664	-3.092351	-1.233114
H	0.340068	0.661398	-2.512318	H	-4.205086	-2.159994	0.22513
H	-1.036716	1.762908	-2.703144	C	-2.069117	-1.135613	1.781315
C	0.164533	4.024492	-1.652769	H	-2.968324	-1.779222	1.882262
H	0.541107	4.670248	-0.852442	C	-2.317822	0.078143	2.682697
H	0.588697	4.392044	-2.598461	H	-3.224738	0.611208	2.384448
H	-0.925287	4.142972	-1.695039	H	-2.424671	-0.214966	3.735723
C	0.782707	2.597103	0.988278	H	-1.486335	0.789871	2.627241
H	1.645595	3.169101	0.598025	C	-0.904656	-1.968795	2.375052
C	1.393483	1.551446	1.948466	H	0.004428	-1.358046	2.458155
H	1.952613	2.027715	2.765387	H	-1.144829	-2.344066	3.380161
H	0.614243	0.934161	2.413709	H	-0.672742	-2.837462	1.748644
H	2.080008	0.880907	1.417851	O	1.651436	-1.082744	-0.409917
C	-0.048553	3.597641	1.819632	C	1.975841	-2.430267	0.008605
H	-0.893567	3.092148	2.304593	C	3.34079	-2.74713	-0.612169
H	0.553065	4.067466	2.611682	C	3.977224	-1.353433	-0.732564
H	-0.457692	4.391208	1.188558	C	2.772777	-0.494194	-1.110986
N	-3.976788	2.321603	-0.490666	H	2.576281	-0.531197	-2.190569
Li	-4.771122	0.603956	-0.011167	H	2.844287	0.550908	-0.80384
O	-6.020936	0.128996	1.464475	H	4.776553	-1.304687	-1.478007
C	-7.251435	0.899455	1.516103	H	4.388359	-1.032993	0.232102
C	-7.81826	0.675225	2.918946	H	3.217147	-3.19459	-1.605388
C	-7.316126	-0.738853	3.24894	H	3.923762	-3.440615	0.001115
C	-5.920288	-0.730376	2.626344	H	2.010677	-2.45034	1.103765
H	-5.57521	-1.71279	2.293233	H	1.177766	-3.09903	-0.32719
H	-5.175022	-0.31059	3.310725	C	-7.564988	0.039435	-2.550613
H	-7.949742	-1.493518	2.767393	O	-6.786987	-0.457183	-1.439682
H	-7.290365	-0.951277	4.321688	C	-7.18509	-1.8072	-1.129793

Table 9 (Continued).

H	-8.908127	0.766504	2.945391	C	-8.503904	-2.041614	-1.870755
H	-7.398181	1.402473	3.623008	C	-8.316049	-1.167989	-3.119465
H	-7.006443	1.942986	1.300289	H	-7.698014	-1.689866	-3.859433
H	-7.917157	0.522556	0.732601	H	-9.257019	-0.886665	-3.601697
C	-4.331349	3.492052	0.331504	H	-8.675345	-3.098018	-2.098659
C	-4.202653	3.173807	1.827031	H	-9.351361	-1.680427	-1.275158
H	-4.785427	2.287935	2.104377	H	-6.404997	-2.499068	-1.472047
H	-3.158727	2.987315	2.103036	H	-7.269374	-1.895228	-0.042279
H	-4.558384	4.014976	2.435688	H	-8.259265	0.806531	-2.180757
H	-5.39493	3.772976	0.176052	H	-6.887137	0.508387	-3.268164
C	-3.513708	4.770208	0.038921	H	-4.698669	0.627455	-2.588266
H	-2.446555	4.585868	0.20135	H	-3.837143	1.559821	-3.824716
H	-3.636948	5.116086	-0.992645	C	-5.431292	3.257948	-2.367642
H	-3.825671	5.591573	0.698132	H	-5.477101	3.352494	-3.460826
C	-4.090304	2.621425	-1.929145	H	-6.2769	2.636995	-2.041748
H	-3.301812	3.32921	-2.256785	H	-5.578419	4.259049	-1.950772
C	-3.880743	1.342216	-2.75006	N	-1.870759	-0.734119	0.379587
H	-2.947847	0.841166	-2.47694	C	-2.149155	-1.883677	-0.492918
H	-1.762841	-2.819465	-0.040099				





Y
G = -1594.667347
G_{MP2} = -1589.877074

Atom	X	Y	Z	Atom	X	Y	Z
Li	0	0	0	H	3.556206	0.133741	0.858635
Li	-2.228386	0.72715	-0.431385	H	3.824858	-0.556578	-2.086223
N	-0.591668	1.8635	-0.553922	H	4.964998	-0.870567	-0.775107
C	-0.006441	2.332485	-1.818591	H	2.844422	-2.650543	-1.826728
H	0.940358	2.879556	-1.62734	H	4.012566	-3.059837	-0.566343
C	0.35952	1.160773	-2.740147	H	2.561458	-2.313213	1.188025
H	0.818702	1.51829	-3.670357	H	1.276475	-2.687226	0.008305
H	1.067105	0.470732	-2.263102	N	-5.472771	1.873344	-1.487137
H	-0.533505	0.587198	-3.01691	Li	-6.453414	0.499521	-0.620606
C	-0.911443	3.303605	-2.610574	O	-7.512539	-1.043663	-1.396178
H	-1.224994	4.15726	-2.001354	C	-7.334756	-2.410008	-0.950824
H	-0.395801	3.70067	-3.496606	C	-7.885316	-3.285857	-2.077483

Table 9 (Continued).

H	-1.820089	2.787315	-2.946133	C	-8.99293	-2.396372	-2.663021
C	-0.523655	2.931392	0.456476	C	-8.366208	-1.004361	-2.565676
H	-0.691029	3.918834	-0.010717	H	-9.094311	-0.199652	-2.428737
C	0.850677	3.019918	1.161998	H	-7.749325	-0.772121	-3.440911
H	0.912425	3.884028	1.838886	H	-9.898104	-2.456243	-2.046789
H	1.036378	2.113631	1.756206	H	-9.263225	-2.659164	-3.689854
H	1.662826	3.116282	0.431692	H	-8.249123	-4.251559	-1.714347
C	-1.62364	2.782257	1.51759	H	-7.109352	-3.474155	-2.82811
H	-1.523052	1.835814	2.062765	H	-6.27233	-2.570881	-0.749768
H	-1.576408	3.588262	2.260986	H	-7.895293	-2.549022	-0.017177
H	-2.621212	2.813833	1.06053	O	-7.24418	0.20329	1.223702
N	-1.677958	-1.120189	0.250652	C	-6.622395	0.478235	2.505069
C	-1.806919	-2.318387	-0.581661	C	-7.718617	1.101883	3.367301
H	-1.213255	-3.153259	-0.143249	C	-8.976588	0.394026	2.840992
C	-1.242567	-2.088215	-1.98904	C	-8.683838	0.296598	1.342007
H	-1.308837	-2.999867	-2.59582	H	-9.019343	1.195892	0.808408
H	-1.799682	-1.30366	-2.516086	H	-9.125935	-0.57993	0.860961
H	-0.189741	-1.783644	-1.955401	H	-9.901962	0.93946	3.048221
C	-3.249331	-2.869058	-0.710101	H	-9.065104	-0.606405	3.280966
H	-3.891071	-2.128328	-1.204771	H	-7.78023	2.180511	3.184176
H	-3.275077	-3.797306	-1.298934	H	-7.547689	0.94469	4.436312
H	-3.679663	-3.090449	0.273195	H	-6.262404	-0.467855	2.926781
C	-1.956442	-1.448916	1.661081	H	-5.767879	1.133856	2.329606
H	-2.070244	-2.542408	1.771314	C	-5.692487	3.272527	-1.133791
C	-3.268659	-0.830225	2.187322	C	-6.178774	3.380835	0.317633
H	-4.110964	-1.134737	1.556858	H	-7.094734	2.795952	0.473137
H	-3.482698	-1.133439	3.223061	H	-5.410571	3.002931	1.006082
H	-3.219915	0.266481	2.169668	H	-6.396259	4.420736	0.591528
C	-0.788716	-1.066638	2.595651	H	-6.49821	3.728844	-1.751105
H	-0.571876	0.00853	2.54767	C	-4.470153	4.204544	-1.305412
H	-1.006556	-1.305227	3.645794	H	-3.62164	3.838688	-0.714163
H	0.122755	-1.604865	2.310461	H	-4.140788	4.26649	-2.347449
O	1.832452	-0.717361	0.079354	H	-4.70706	5.22631	-0.978217
C	2.185442	-2.106975	0.175259	C	-5.041512	1.69876	-2.868656
C	3.281887	-2.310145	-0.88373	H	-4.13742	2.299171	-3.09606
C	3.906398	-0.895606	-1.04975	C	-4.633255	0.2404	-3.113557
C	3.06599	-0.003859	-0.115493	H	-3.833478	-0.057508	-2.424477
H	2.813743	0.974571	-0.526409	H	-5.476926	-0.442341	-2.943674
H	-7.009311	1.523467	-3.814542	H	-4.27553	0.082981	-4.139098
H	-6.367554	3.170802	-3.828909	C	-6.090691	2.115706	-3.930164
				H	-5.713372	1.972421	-4.952401