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

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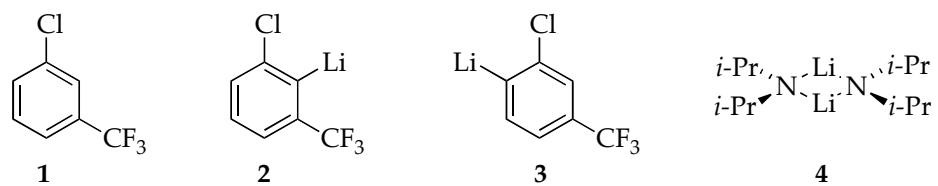
Part 1: Experimental Procedures	S6
<hr/>	
Part 2: NMR Spectroscopic Studies	S7
Figure 1. ^{19}F NMR spectrum of LDA (0.10 M) with 1 (0.050 M) in 12.2 M THF after aging for 10 minutes at -90 °C.	S7
Figure 2. ^6Li NMR spectrum of $[^6\text{Li}, ^{15}\text{N}]$ LDA (0.10 M) and 1 (0.050 M) in neat THF recorded at -90 °C.	S7
Figure 3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 2 generated from 1 (0.20 M) with $[^6\text{Li}]$ LDA (0.30 M) in 12.2 M THF- d_8 at -105 °C.	S8
Figure 4. $^{13}\text{C}\{^{19}\text{F}\}$ NMR spectrum of 2 generated from 1 (0.20 M) with $[^6\text{Li}]$ LDA (0.30 M) in 12.2 M THF- d_8 at -105 °C.	S9
Figure 5. $^{13}\text{C}\{^{19}\text{F}\}$ NMR spectrum of 3 generated from 1 (0.15 M) with $[^6\text{Li}, ^{15}\text{N}]$ LiTMP (0.20 M) in 12.2 M THF- d_8 at -90 °C.	S10
Figure 6. ^1H and ^{13}C NMR spectra of 1 in CDCl_3 and THF- d_8 .	S11
Figure 7. ^1H and ^{13}C NMR spectra of 1-2-d₁ in CDCl_3 prepared using the Grignard method.	S12
Figure 8. ^1H and ^{13}C NMR spectra of 1-2-d₁ in CDCl_3 prepared using an LDA-mediated ortholithiation.	S13
Figure 9. ^1H and ^{13}C NMR spectra of 1-6-d₁ in CDCl_3 prepared using the Grignard method.	S14

Figure 10. ^1H and ^{13}C NMR spectra of 1 - <i>d</i> ₁ in CDCl_3 prepared using LiTMP.	S15
Figure 11. ^1H NMR spectra of 1 - <i>d</i> ₁ in CDCl_3 prepared using the Grignard method.	S16
Figure 12. ^1H and ^{13}C NMR spectra of 1 -2,6- <i>d</i> ₂ in CDCl_3 .	S17
Part 3: Rate Studies	S18
<hr/>	
Figure 13. Representative in situ IR trace for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) in THF at -78 °C with listed IR absorbances.	S18
Figure 14. Representative plots of concentration versus time monitored by ^{19}F NMR spectroscopy for the ortholithiation of 1 by LDA (0.10 M) in THF (12.2 M) at -60 °C.	S19
Figure 15. Representative plot showing absorbance of arene 1 vs time for the ortholithiation of 1 (0.010 M) with LDA (0.10 M) in THF (12.20 M) at -78 °C.	S24
Figure 16. Ortholithiation of 1 (0.010 M) with LDA (0.10 M) in THF (12.2 M) at -78 °C monitored by IR spectroscopy (1325 cm^{-1}) with injection of 1.0 mol % LiCl.	S24
Figure 17. Competitive ortholithiation of 1 (0.050 M) and 1 -2,6- <i>d</i> ₂ (0.050 M) with LDA (0.10 M) in THF (12.2 M) at -78 °C.	S25
Figure 18. Plot of initial rate versus [1-2,6- <i>d</i> ₂] for the ortholithiation of 1 -2,6- <i>d</i> ₂ by 0.10 M LDA in 12.2 M THF at -78 °C.	S26
Figure 19. Plot of 2/3 versus time for the ortholithiation of 1 by LDA in THF (12.2 M) at -65 °C.	S27
Table 1. Relative initial rates of 2 and 3 for the ortholithiation of 1 , 1 -2- <i>d</i> , 1 -6- <i>d</i> and 1 -2,6- <i>d</i> ₂ (0.050 M each) by LDA (0.10 M) in THF (12.2 M) at -78 °C.	S28
Table 2. Table showing the relative initial rates of 2 and 3 with various lithium salts (0.020 M) for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) in 12.2 M THF at -90 °C.	S29
Table 3. Table showing regioselectivity at equilibrium for the ortholithiation of 1 by <i>sec</i> -BuLi (0.11 M) and <i>n</i> -BuLi (0.11 M) in 12.2 M THF at -90 °C.	S30
Figure 20. Representative IR plot for the equilibration of 3 (1151 cm^{-1}) to 2 (1306 cm^{-1}).	S31
Figure 21. Plot of initial rate vs [1] (initial arene concentration) for the ortholithiation of 1 with LDA (0.10 M) in THF (12.2 M) at -78 °C.	S32

Figure 22. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of 1 (0.050 M) at -78 °C.	S33
Figure 23. Plot of initial rate versus [THF] for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) at -78 °C.	S34
Figure 24. Ratio of relative initial rates of formation 2 and 3 , $(\Delta 2 / \Delta t) / (\Delta 3 / \Delta t)$, versus [THF] for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) at -65 °C.	S35
Table 4. Table of relative initial rate versus [LDA] for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) at -65 °C.	S36
Figure 25. Plot of k_{obsd} versus [LDA] in THF (12.2 M) for the ortholithiation of 1-2,6-d₂ (0.002 M) -65 °C.	S37
Figure 26. Plot of k_{obsd} versus [THF] in hexanes for the ortholithiation of 1-2,6-d₂ (0.002 M) by LDA (0.050 M) -65 °C.	S38
Figure 27. Representative plot of 1 (0.005 M) versus time for the ortholithiation by LDA (0.10 M) in 12.2 M THF in the presence of 5 mol% LiCl at -90 °C.	S39
Figure 28. Plot of initial rate versus [LiCl] for the ortholithiation of 1 (0.074 M) by 0.10 M LDA in 12.2 M THF at -78 °C.	S40
Figure 29. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of 1 (0.075 M) in the presence of 5 mol% LiCl at -78 °C.	S41
Figure 30. Plot of initial rate versus [THF] in hexanes and 2,5-dimethyltetrahydrofuran as a cosolvent for the ortholithiation of 1 (0.075 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at -78 °C.	S42
Figure 31. Plot of relative initial rate versus [THF] in 2,5-dimethyltetrahydrofuran cosolvent for the ortholithiation of 1 (0.050 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at -78 °C.	S43
Figure 32. Plot of k_{obsd} versus [<i>i</i> -Pr ₂ NH] for the isomerization of 3 (0.050 M) to 2 in 12.2 M THF at -78 °C.	S44
Figure 33. Plot of k_{obsd} versus [THF] for the isomerization of 3 (0.050 M) to 2 in 12.2 M THF at -78 °C.	S45
Figure 34. Plot of initial rate versus [2-6- <i>d</i>] ($=[\text{ArLi}]$) for the ortholithiation of 1 (0.075 M) by 0.10 M LDA in 12.2 M THF at -78 °C.	S46
Figure 35. Plot of the equilibrium constant (K_{eq}) versus total concentration of lithium titer.	S48

Part 4: Computational Studies	S50
Figure 36. Relative free energies for the solvation (ΔG , kcal / mol) of 2 , 3 and 4-lithio-3-chlorobenzotrifluoride at -78 °C.	S51
Figure 37. DFT computations [MP2/6–31G(d) // B3LYP/6–31G(d)] of monomer-based transition structures for the metalation of 1 .	S52
Figure 38. DFT computations [MP2/6–31G(d) // B3LYP/6–31G(d)] of dimer-based transition structures for the metalation of 1 .	S53
Figure 39. Relative free energies (ΔG , kcal / mol) at -78 °C for the solvation of (A) THF-tetrasolvated lithium ion and (B) THF-hexasolvated lithium chloride triple ion.	S54
Figure 40. Relative free energies (ΔG , kcal / mol) at -78 °C of (A) dimeric lithium chloride and (B) monomeric lithium chloride.	S55
Figure 41. Reaction scheme showing lithium chloride deaggregating THF-disolvated closed dimer.	S56
Table 5. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of 2 , 3 and 3-chloro-4-lithiobenzotrifluoride at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z).	S57
Table 6. Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the ortholithiation of 1 at -78 °C with free energies (Hartrees), and cartesian coordinates (X, Y, Z).	S64
Table 7. Optimized geometries of reactants and dimer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the ortholithiation of 1 at -78 °C with free energies (Hartrees), and cartesian coordinates (X, Y, Z).	S74
Table 8. Optimized geometries at the B3LYP level of theory with 6-31G(d) basis set of lithium ions, lithium chloride aggregates, lithium chloride triple ions, lithium chloride-LDA mixed aggregates and lithium chloride-LDA triple ions at -78 °C with free energies (Hartrees), and cartesian coordinates (X, Y, Z).	S87
References	S110

Chart 1



Part 1: Experimental Procedures:

Synthesis of deuterated 3-chlorobenzotrifluoride derivatives:

2-Deutero-1-chloro-3-(trifluoromethyl)benzene (1-2-d).

Using a method published by Knochel,^{ref 14} commercially available 2-bromo-1-chloro-3-(trifluoromethyl)benzene (4.86 g, 18.7 mmol, 1.0 equiv) was added via syringe to a 1.3 M THF solution of isopropylmagnesium chloride–LiCl complex (29.0 mL, 22.3 mmol, 1.2 equiv) in dry THF at 0 °C under argon. After the solution was stirred for 20 minutes, 10 equiv of deuterium oxide (3.7 mL) was added to the solution. The mixture was allowed to warm to room temperature, and the pH was adjusted to 1.0 with 2.0 M aqueous HCl solution to dissolve all salts. Organic and aqueous layers were separated, and the aqueous layer was washed with 3 x 20 mL Et₂O. The organic layers were combined, dried over granular Na₂SO₄ and distilled, and **1-2-d** was collected at 135 °C as a colorless liquid (3.69g, 14.2 mmol) in 76% yield. ¹H NMR δ 7.52 (m, 2H), 7.43 (m, 1H); ¹³C NMR δ 135.2 (s), 132.6 (q, ²J_{C-F} = 33 Hz), 132.1 (s), 130.2 (s), 125.5 (tq, ²J_{C-D} = 26 Hz, ²J_{C-F} = 4.0 Hz), 123.8 (q, ²J_{C-F} = 272 Hz), 123.4 (q, ²J_{C-F} = 4.0 Hz).

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

2,6-Dideutero-1-chloro-3-(trifluoromethyl)benzene (1-2,6-d₂). A 2.5 M solution of *n*-BuLi in hexane (14.8 mL, 37.0 mmol) was added via syringe pump to a solution of dry diisopropylamine (5.7 mL, 40.7 mmol) and Et₃N·HCl (0.25 g, 1.85 mmol, 0.050 equiv) in 100 mL of dry THF at -78 °C under argon. After the solution was stirred for 20 minutes, **1** (5.0 mL, 37.0 mmol, 1 equiv) was added to the in situ generated LDA solution. After stirring at -78 °C for 30 min, *d*-MeOH (1.51 mL, 37.0 mmol, 1 equiv) was added. The process of sequential *n*-BuLi and *d*-MeOH addition of 1.0 equiv was repeated three more times. A final amount of *d*-MeOH (15 mL, 10 equiv) was added to fully quench the reaction. After the mixture was allowed to warm to room temperature, the pH was adjusted to 1.0 with 2.0 M HCl solution to dissolve all salts. Organic and aqueous layer were separated, and the aqueous layer was washed with 3 x 20 mL Et₂O. The organic layers were combined and dried over granular Na₂SO₄ and distilled, and **1-2,6-d₂** was collected at 135 °C as a colorless liquid (3.74 g, 18.2 mmol) in 49% yield. ¹H NMR δ 7.52 (m, 1H), 7.43 (m, 1H); ¹³C NMR δ 135.3 (s), 132.6 (q, ²J_{C-F} = 33 Hz), 131.9 (t, ²J_{C-D} = 26 Hz), 130.2 (s), 125.8 (tq, ²J_{C-D} = 26 Hz, ²J_{C-F} = 4.0 Hz), 123.8 (q, ²J_{C-F} = 272 Hz), 123.5 (q, ²J_{C-F} = 4.0 Hz).

Part 2: NMR Spectroscopic Studies

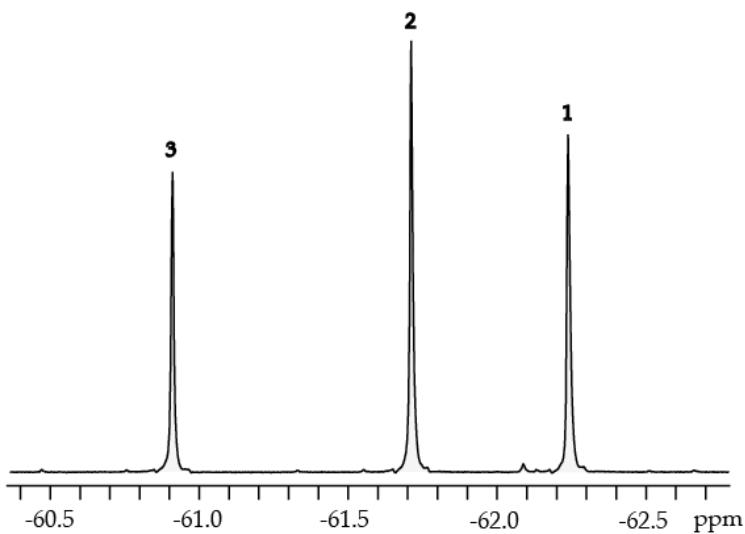


Figure 1. ¹⁹F NMR spectrum of LDA (0.10 M) with **1** (0.050 M) in 12.2 M THF after aging for 10 minutes at -90 °C: δ -60.90 (s), -61.70 (s), -62.23 (s).

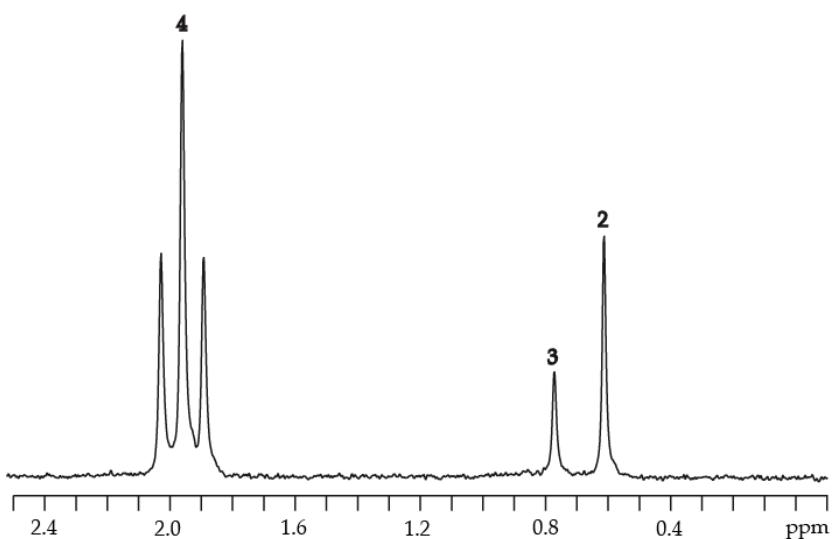


Figure 2. ⁶Li NMR spectrum of $[{}^6\text{Li}, {}^{15}\text{N}]$ LDA (0.10 M) and **1** (0.050 M) in neat THF recorded at -90 °C: δ 1.96 (t, $^2J_{\text{Li-N}} = 5.0$ Hz), 0.77 (s), 0.61 (s).

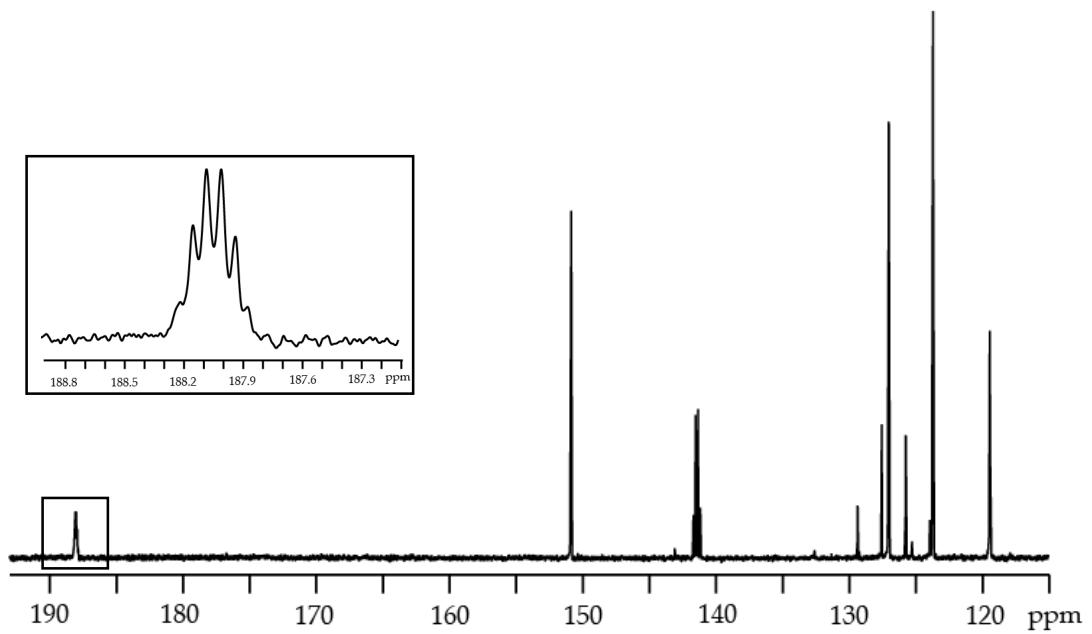


Figure 3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** generated from **1** (0.20 M) with $[^6\text{Li}]$ LDA (0.30 M) in 12.2 M THF- d_8 at -105 °C: δ 188.05 (m), 150.87 (s), 141.45 (q, $^2J_{\text{C}-\text{F}} = 26.6$ Hz), 127.04 (s), 126.67 (q, $^2J_{\text{C}-\text{F}} = 272.0$ Hz), 123.73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

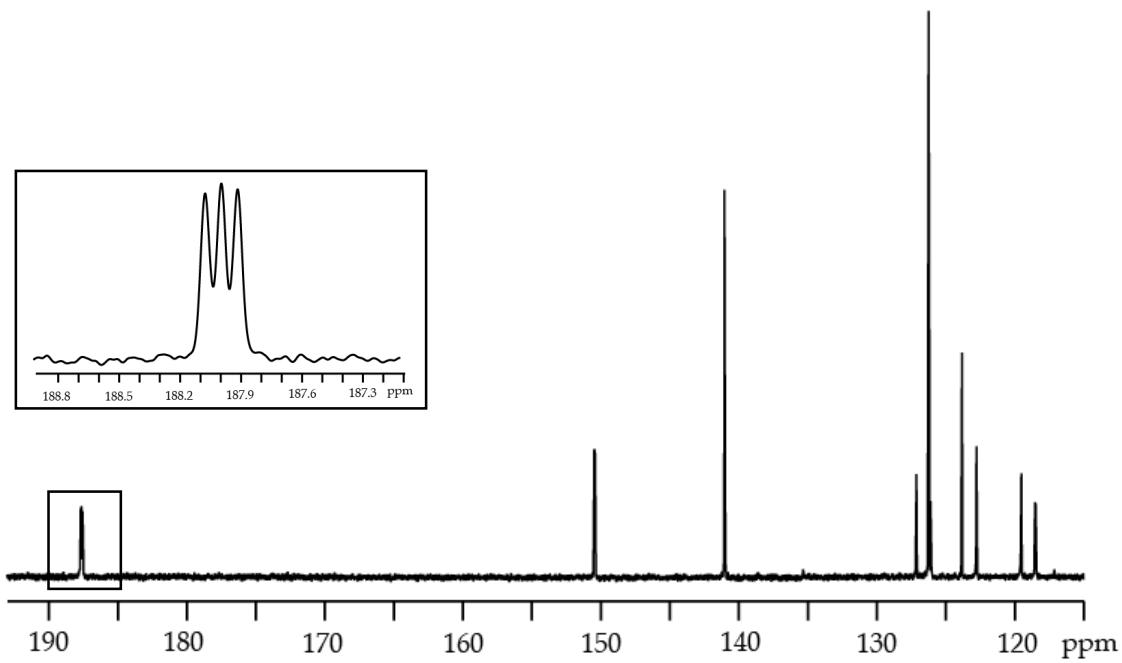


Figure 4. $^{13}\text{C}\{^{19}\text{F}\}$ NMR spectrum of **2** generated from **1** (0.20 M) with $[^6\text{Li}]\text{LDA}$ (0.30 M) in 12.2 M THF- d_8 at -105 °C: δ 188.05 (t, $^2J_{\text{C-Li}} = 11.4$ Hz), 150.87 (dm, $^2J_{\text{C-H}} = 10.8$ Hz), 141.45 (d, $^2J_{\text{C-H}} = 8.6$ Hz), 127.04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

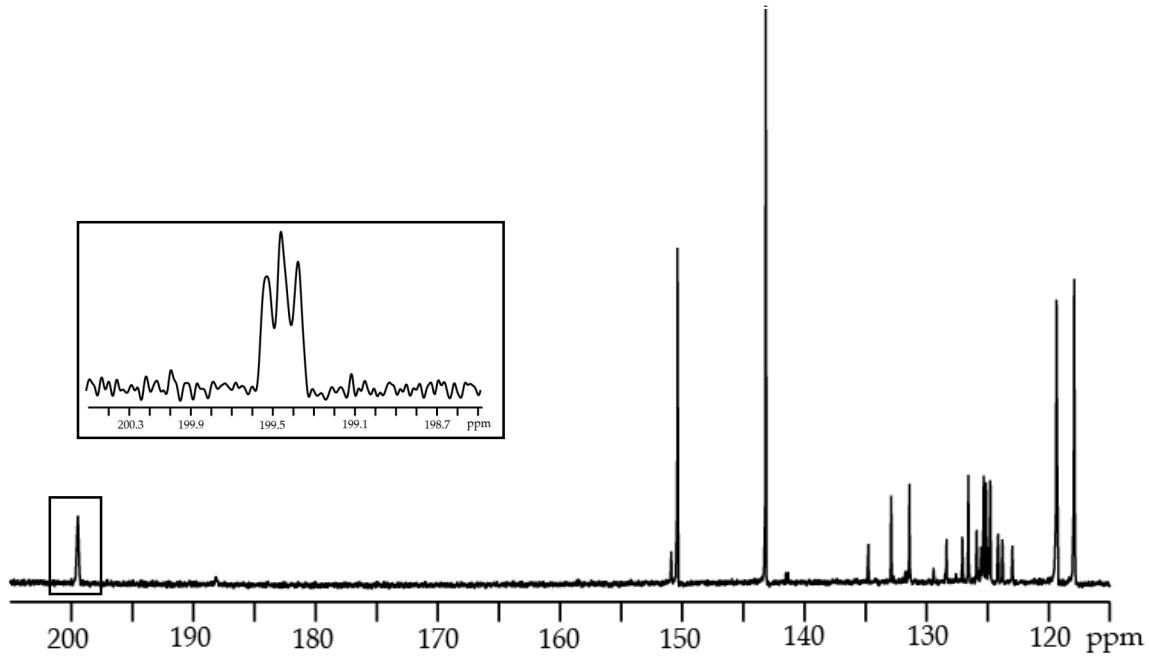


Figure 5. $^{13}\text{C}\{^{19}\text{F}\}$ NMR spectrum of **3** generated from **1** (0.15 M) with $[^{6}\text{Li}, ^{15}\text{N}]\text{LiTMP}$ (0.20 M) in 12.2 M THF- d_8 at -90 °C: δ 199.52 (t, $^2J_{\text{C-Li}} = 11.0$ Hz), 150.40 (s), 143.17 (s), 125.68 (q, $^2J_{\text{C-F}} = 270.5$ Hz), 125.23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

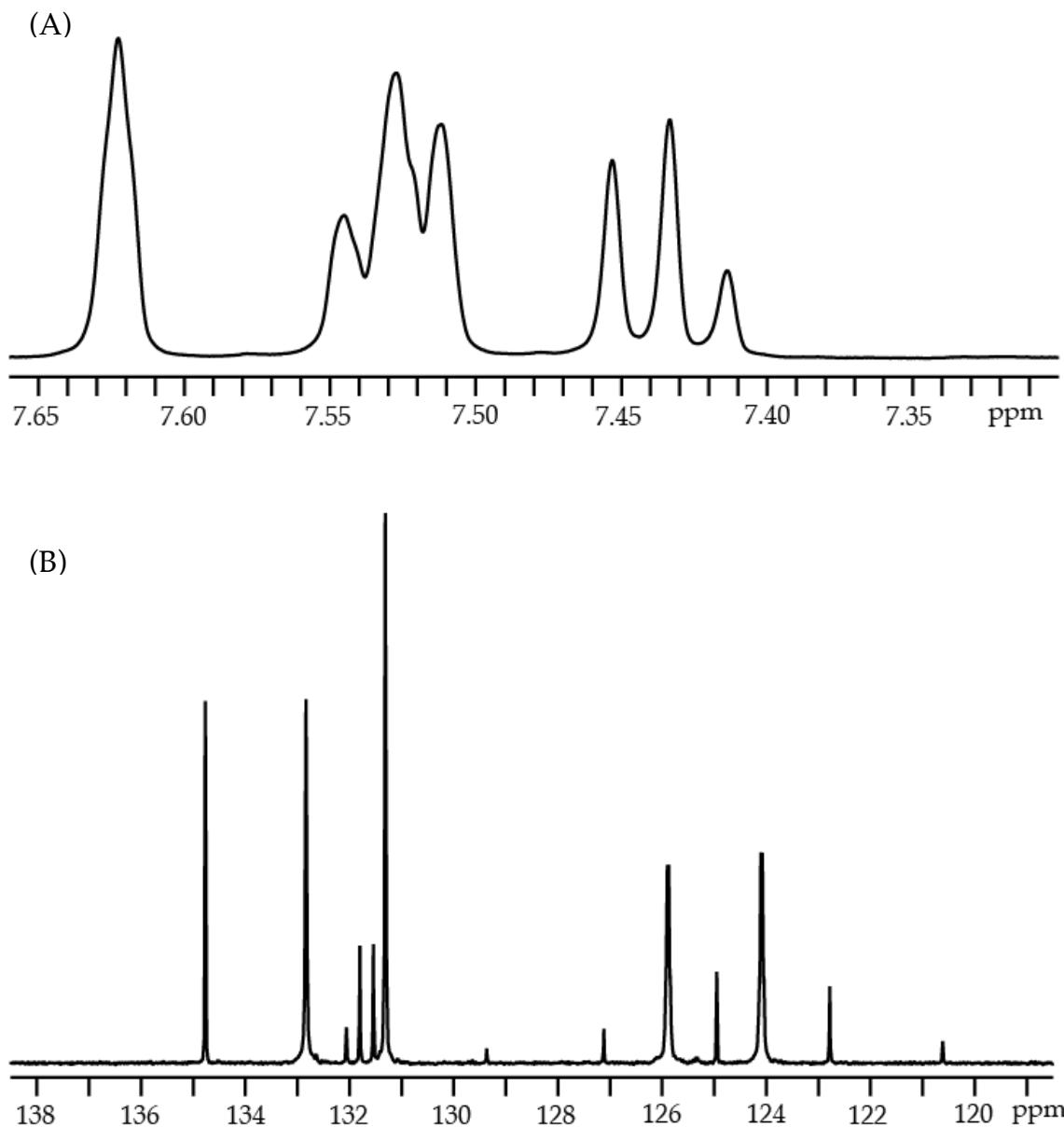


Figure 6. ^1H and ^{13}C NMR spectra of **1** in CDCl_3 and $\text{THF}-d_8$, respectively: (A) ^1H NMR δ 7.62 (s, 1H), 7.52 (m, 2H), 7.43 (m, 1H); (B) ^{13}C NMR δ 134.8 (s), 132.8 (s), 131.7 (q, $^2J_{\text{C-F}} = 33$ Hz), 131.3 (s), 125.9 (q, $^2J_{\text{C-F}} = 3.8$ Hz), 124.1 (q, $^2J_{\text{C-F}}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

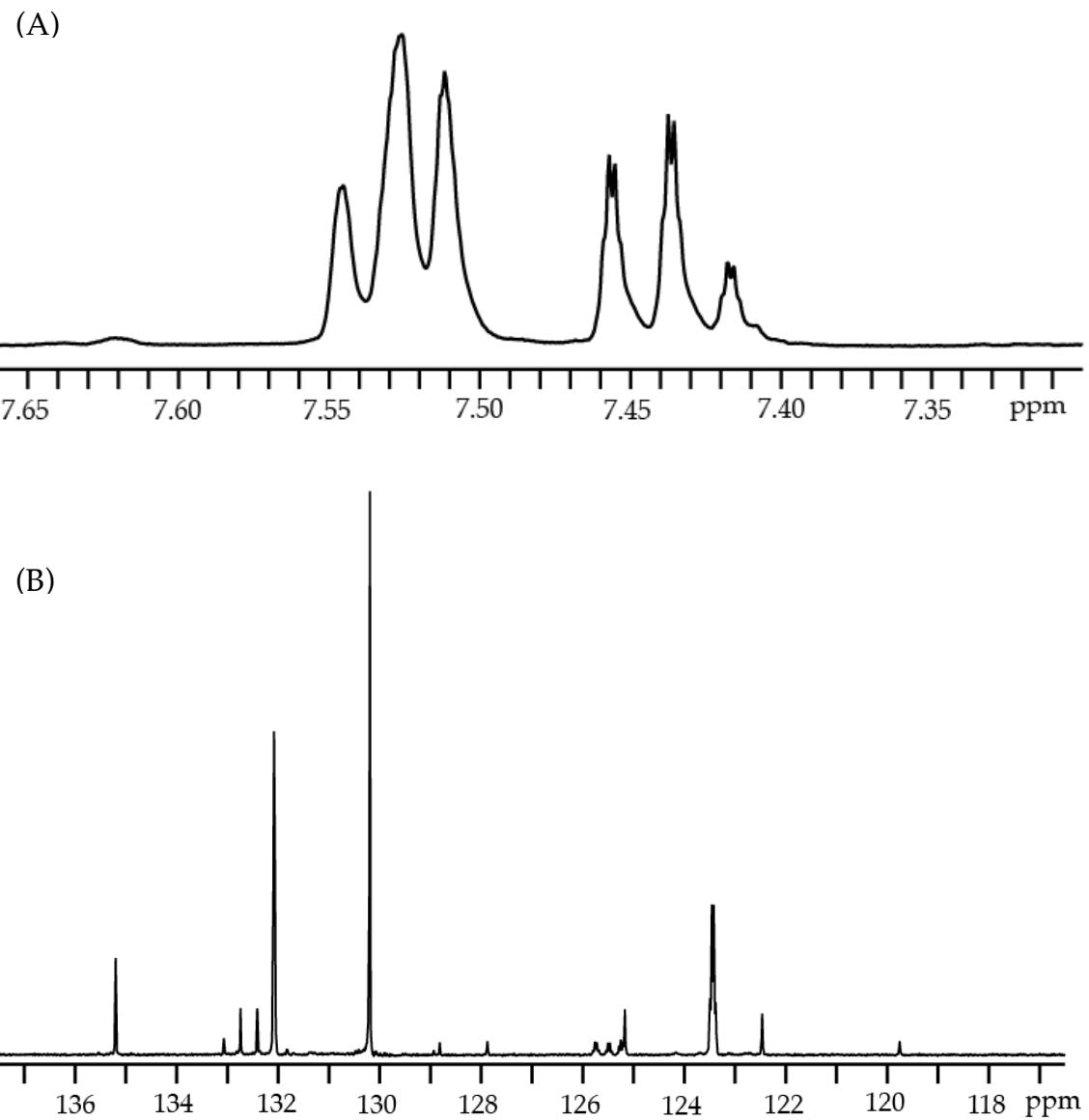


Figure 7. ^1H and ^{13}C NMR spectra of **1-2-*d*₁** in CDCl_3 . The compound was prepared as described in Part 1 using the Grignard method: (A) ^1H NMR δ 7.52 (m, 2H), 7.43 (m, 1H); (B) ^{13}C NMR δ 135.2 (s), 132.6 (q, $^2J_{\text{C-F}} = 33$ Hz), 132.1 (s), 130.2 (s), 125.5 (tq, $^2J_{\text{C-D}}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

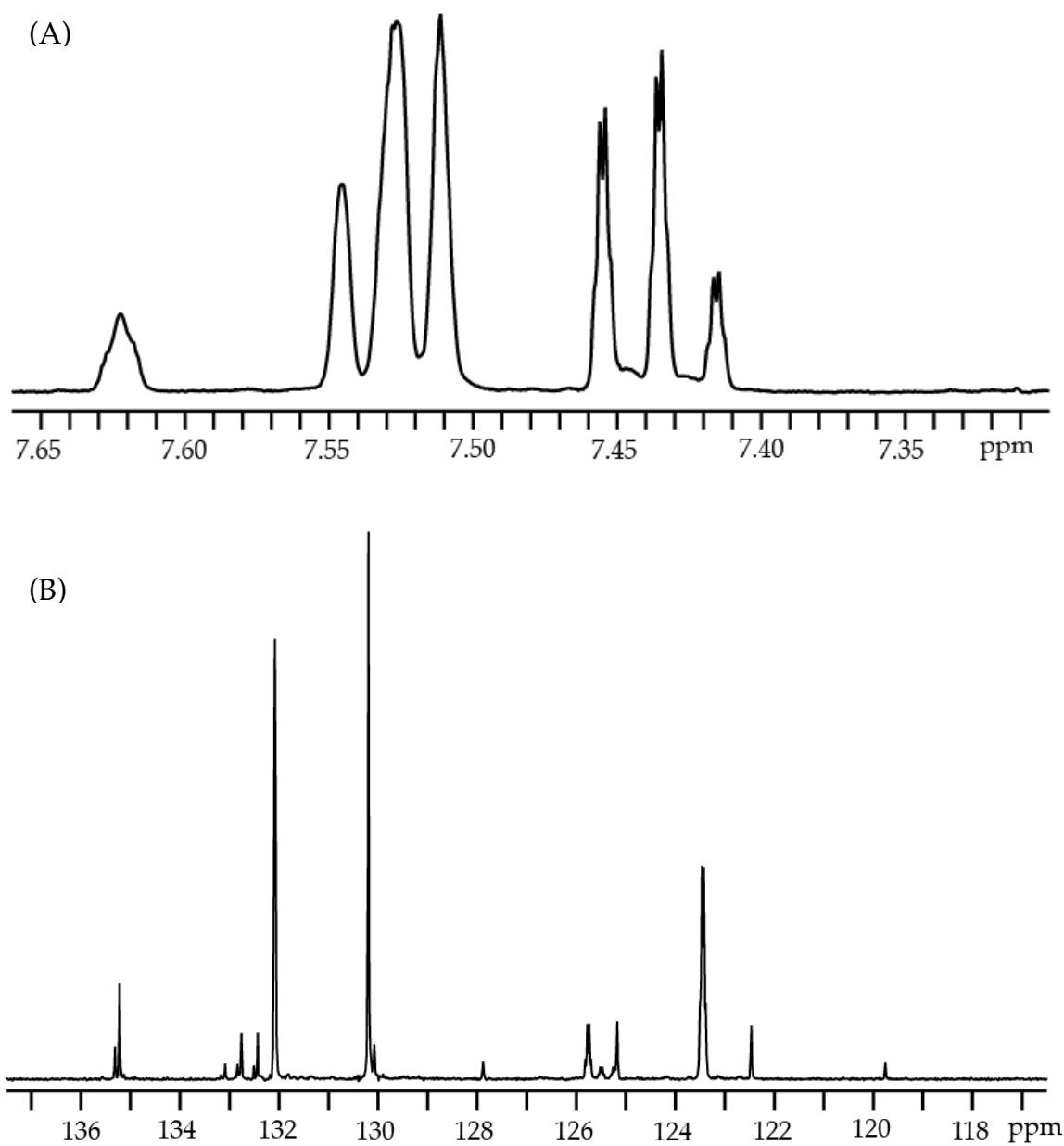


Figure 8. ^1H and ^{13}C NMR spectra of **1-2-*d*₁** in CDCl_3 . The compound was prepared as described in Part 1 using an LDA-mediated ortholithiation: (A) ^1H NMR δ 7.62 (s, 0.2 H*), 7.52 (m, 2H), 7.43 (m, 1H); (B) ^{13}C NMR δ 135.2 (s), 135.2 (s)*, 132.6 (q, $^{2}\text{J}_{\text{C}-\text{F}} = 33$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

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

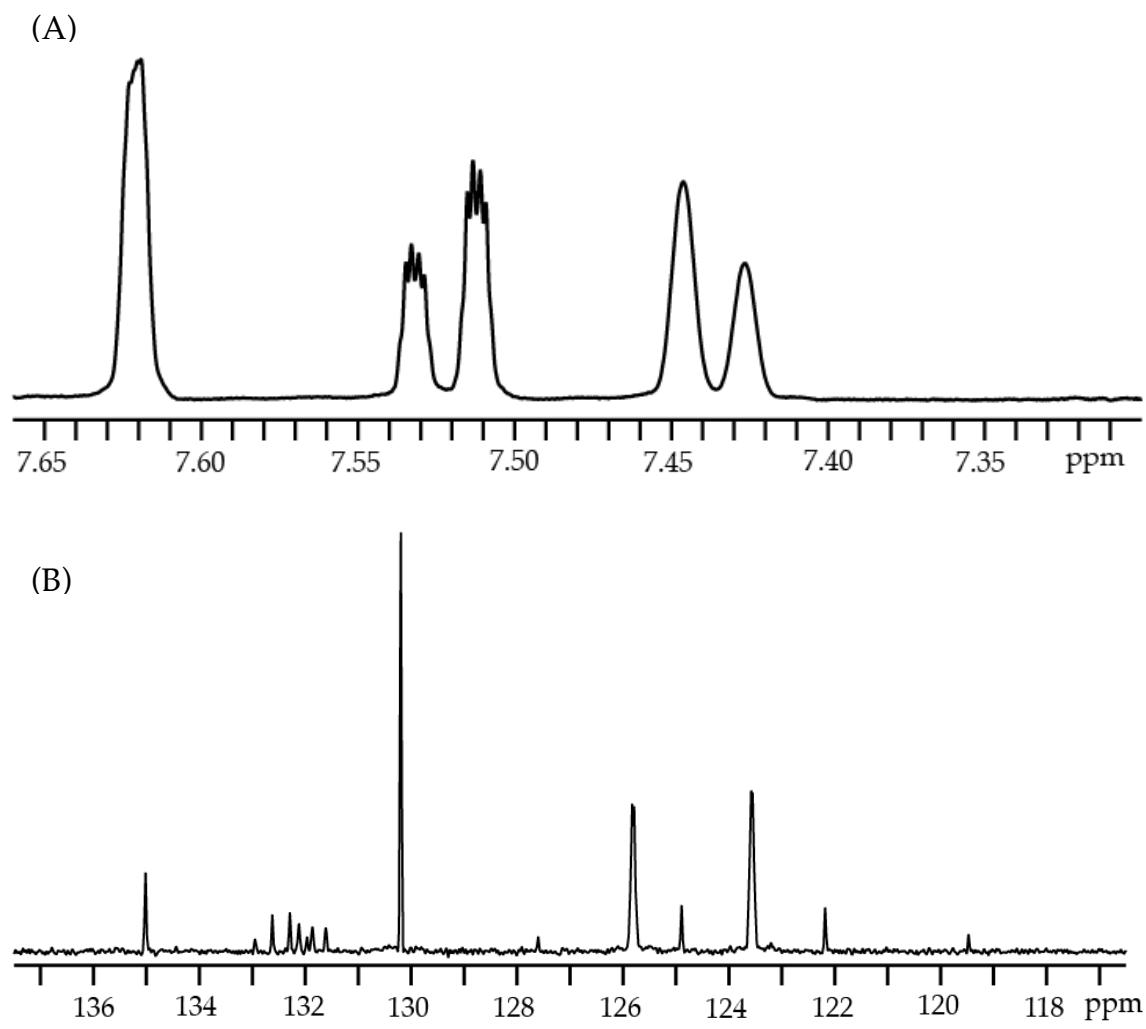


Figure 9. ^1H and ^{13}C NMR spectra of **1-6-*d*₁** in CDCl_3 . The compound was prepared as described in Part 1 using the Grignard method: (A) ^1H NMR δ 7.62 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H); (B) ^{13}C NMR δ 135.0 (s), 132.5 (q, $^2J_{\text{C-F}} = 33$ Hz), 131.9 (t, $^2J_{\text{C-D}} = 26$ Hz),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

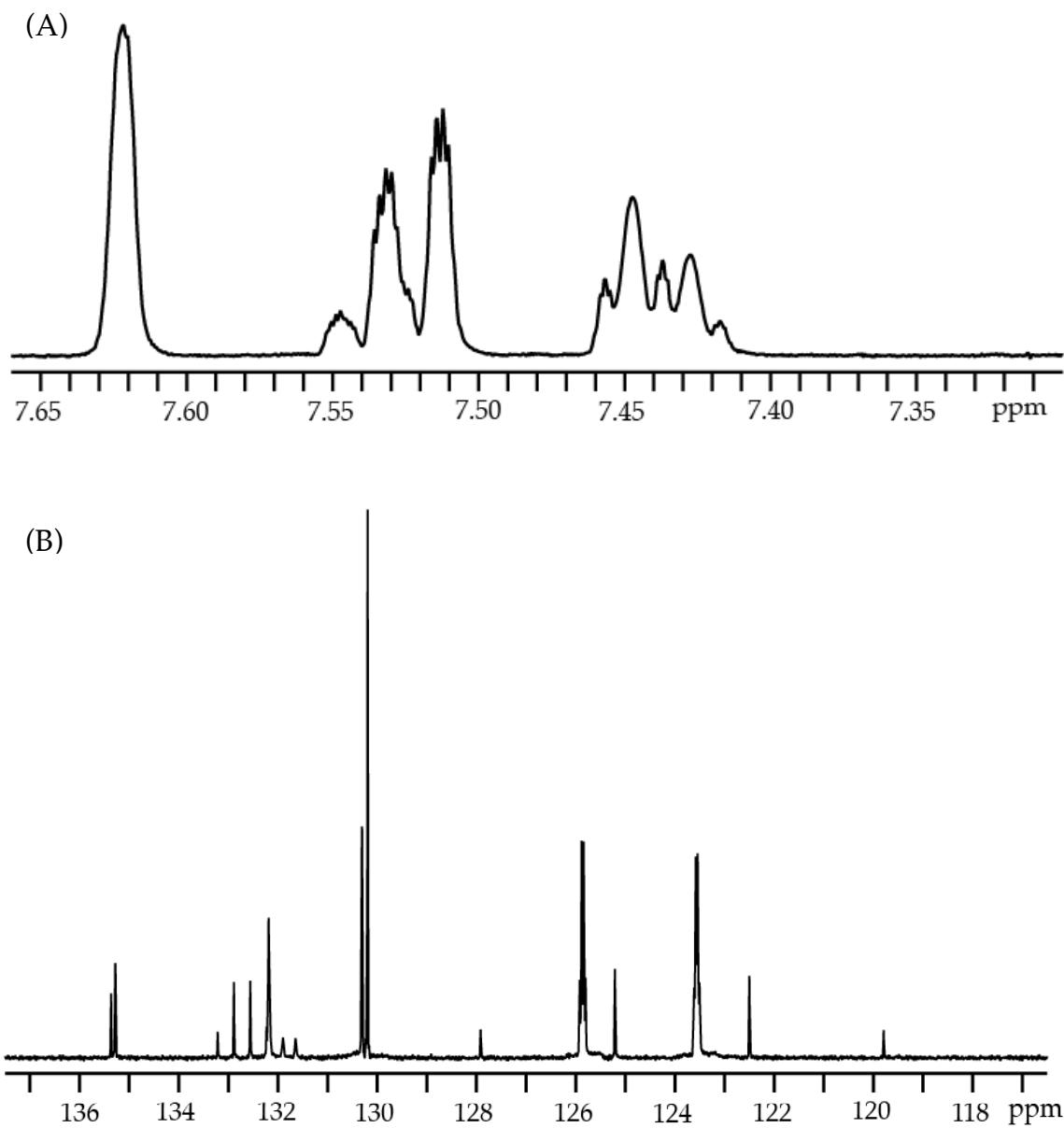


Figure 10. ¹H and ¹³C NMR spectra of **1-6-d₁** in CDCl₃. The compound was prepared as described in Part 1 using LiTMP: (A) ¹H NMR δ 7.62 (s, 1H), 7.52 (m, 2H), 7.43 (m, 1H)*; (B) ¹³C NMR δ 135.4 (s), 135.3 (s)*, 132.7 (q, ²J_{C-F} = 33 Hz), 132.1 (s)*, 131.9 (t, ²J_{C-D} = 26 Hz), 130.3 (s), 130.2 (s)*, 125.9 (q, ²J_{C-F} = 4.0 Hz), 123.9 (q, ²J_{C-F} = 272 Hz), 123.6 (q, ²J_{C-F} = 4.0 Hz).

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

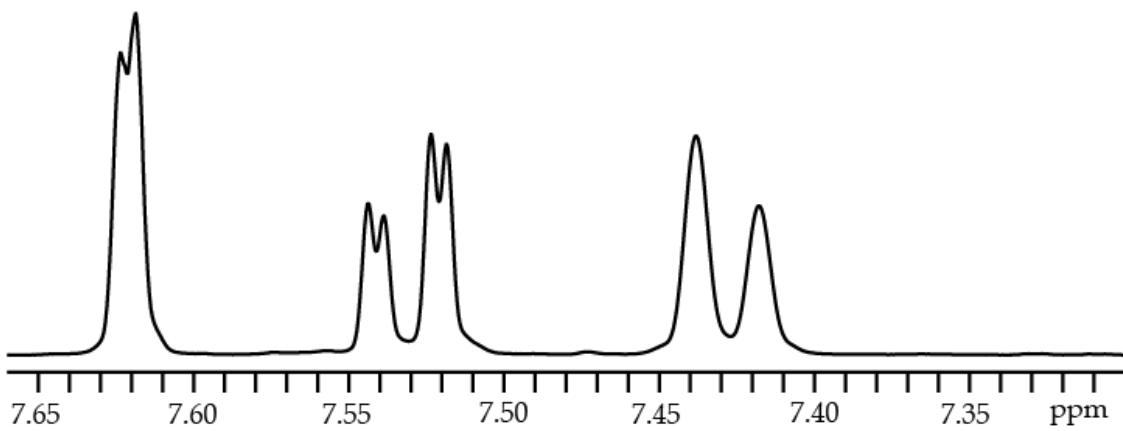


Figure 11. ^1H NMR spectra of **1-6-*d*₁** in CDCl_3 . The compound was prepared as described in Part 1 using the Grignard method: ^1H NMR δ 7.62 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H).

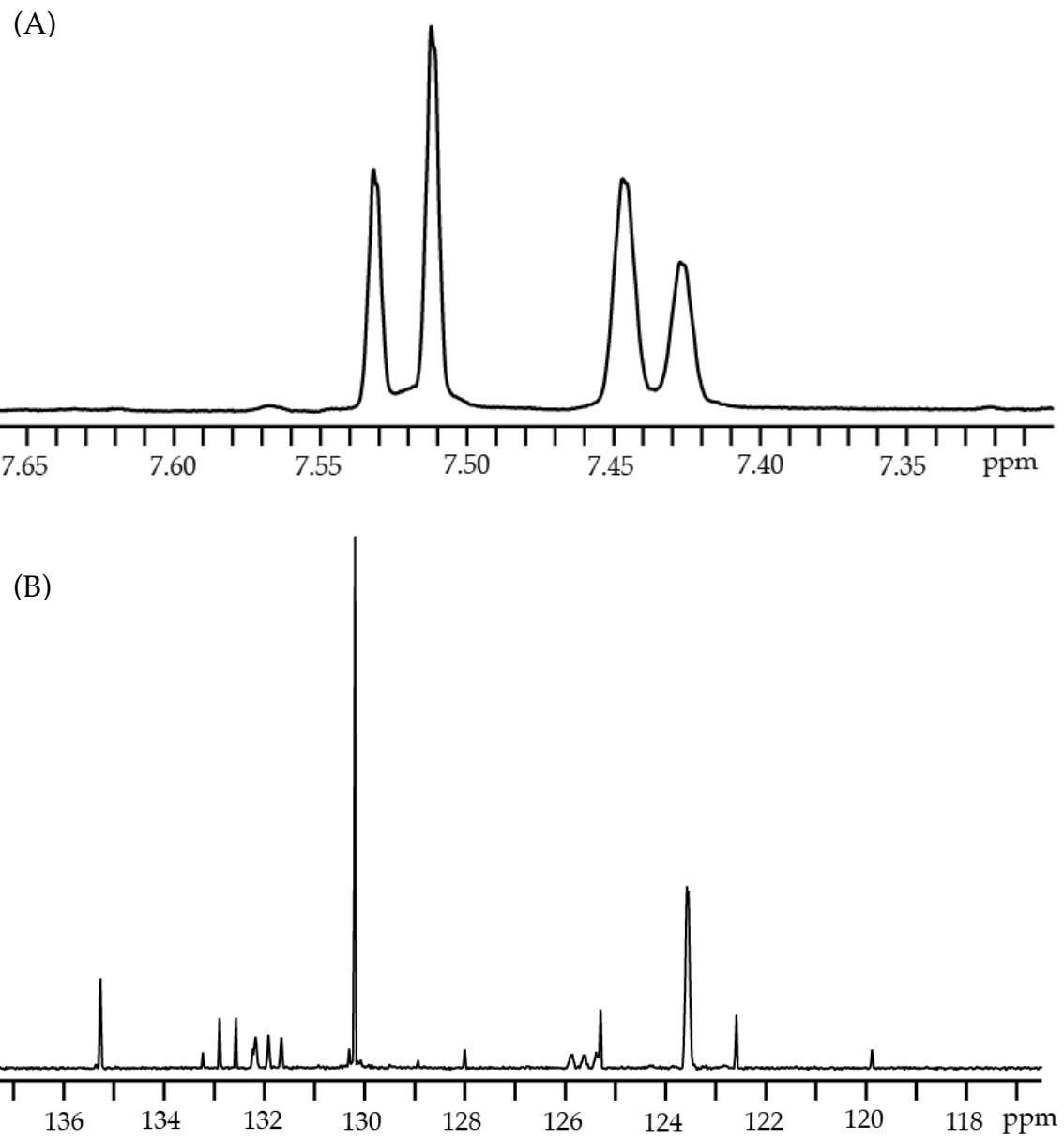


Figure 12. ^1H and ^{13}C NMR spectra of **1-2,6-*d*₂** in CDCl_3 . The compound was prepared as described in Part 1: (A) ^1H NMR δ 7.52 (m, 1H), 7.43 (m, 1H); (B) ^{13}C NMR δ 135.3 (s), 132.6 (q, $^2J_{\text{C}-\text{F}} = 33$ Hz), 131.9 (t, $^2J_{\text{C}-\text{D}} = 26$ Hz), 130.2 (s), 125.8 (tq,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

Part 3: Rate Studies

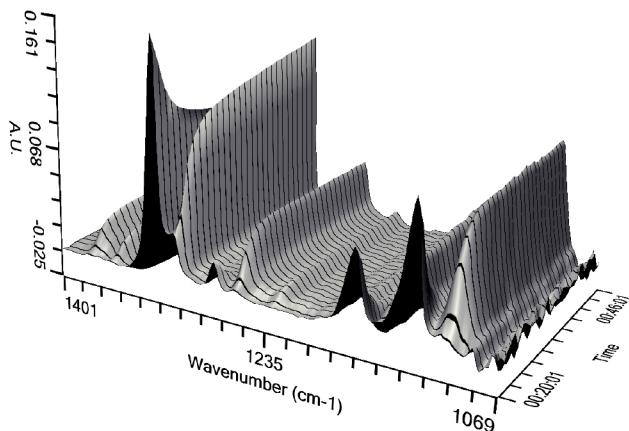


Figure 13. Representative in situ IR trace for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) in THF at -78 °C. Compounds **1**, **2**, and **3** exhibit the IR absorptions listed for the four possible isotopomers. The IR spectra were deconvoluted using ConcIRT®. Deconvolution of the product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

1: 1428 cm⁻¹, 1325 cm⁻¹, 1276 cm⁻¹, 1171 cm⁻¹, 1131 cm⁻¹

2: 1378 cm⁻¹, 1306 cm⁻¹, 1260 cm⁻¹, 1140 cm⁻¹, 1104 cm⁻¹

3: 1378 cm⁻¹, 1324 cm⁻¹, 1258 cm⁻¹, 1154 cm⁻¹, 1109 cm⁻¹

1-2-d₁: 1325 cm⁻¹, 1215 cm⁻¹, 1170 cm⁻¹, 1132 cm⁻¹

2+3: 1322 cm⁻¹, 1245 cm⁻¹, 1176 cm⁻¹, 1140 cm⁻¹, 1108 cm⁻¹

1-6-d₁: 1401 cm⁻¹, 1326 cm⁻¹, 1173 cm⁻¹, 1131 cm⁻¹

2+3: 1378 cm⁻¹, 1329 cm⁻¹, 1299 cm⁻¹, 1260 cm⁻¹, 1146 cm⁻¹, 1121 cm⁻¹, 1104 cm⁻¹

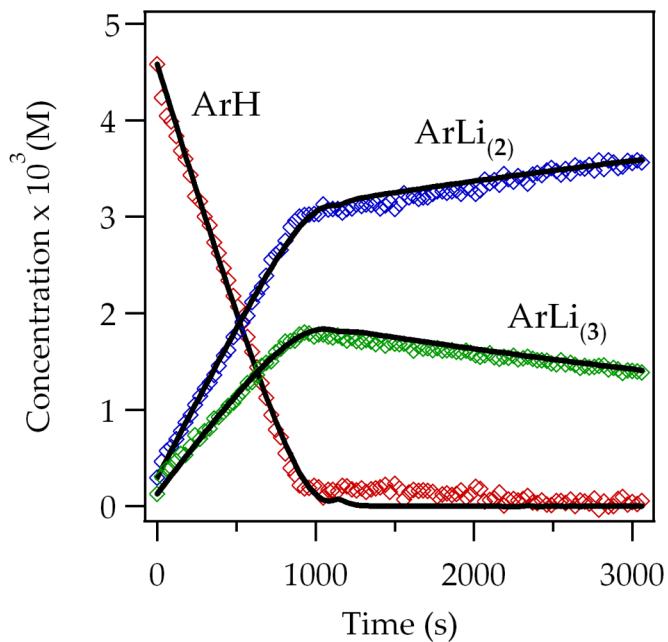
1-2,6-d₂: 1383 cm⁻¹, 1324 cm⁻¹, 1181 cm⁻¹, 1161 cm⁻¹, 1131 cm⁻¹

2+3: 1322 cm⁻¹, 1297 cm⁻¹, 1260 cm⁻¹, 1245 cm⁻¹, 1212 cm⁻¹, 1176 cm⁻¹, 1108 cm⁻¹

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

Figure 14 (continued).

(A)



$$k_1 = 0.000115 \pm 1\text{e-}006$$

$$k_{-1} = 1000k_1$$

$$k_2 = 0$$

$$k_{-2} = 0$$

$$k_3 = 220 \pm 20$$

$$k_4 = 150 \pm 13$$

$$k_5 = 0$$

$$k_6 = 0$$

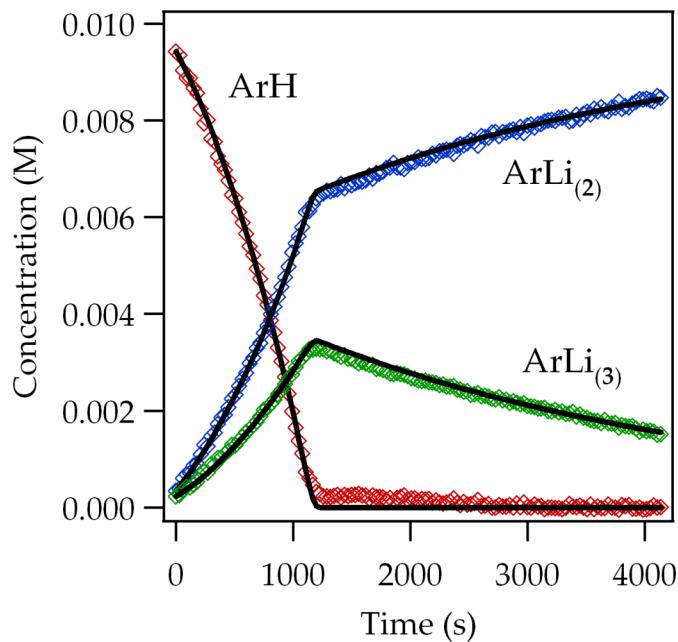
$$k_7 = 0.0010 \pm 0.0008$$

$$k_{-7} = 0.30 \pm 0.002$$

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

Figure 14 (continued).

(B)



$$k_1 = 0.00022 \pm 3\text{e-}005$$

$$k_{-1} = 1000k_1$$

$$k_2 = 0.020 \pm 0.0004$$

$$k_{-2} = 1000k_2$$

$$k_3 = 9.0 \pm 0.9$$

$$k_4 = 4.2 \pm 0.5$$

$$k_5 = 152 \pm 50$$

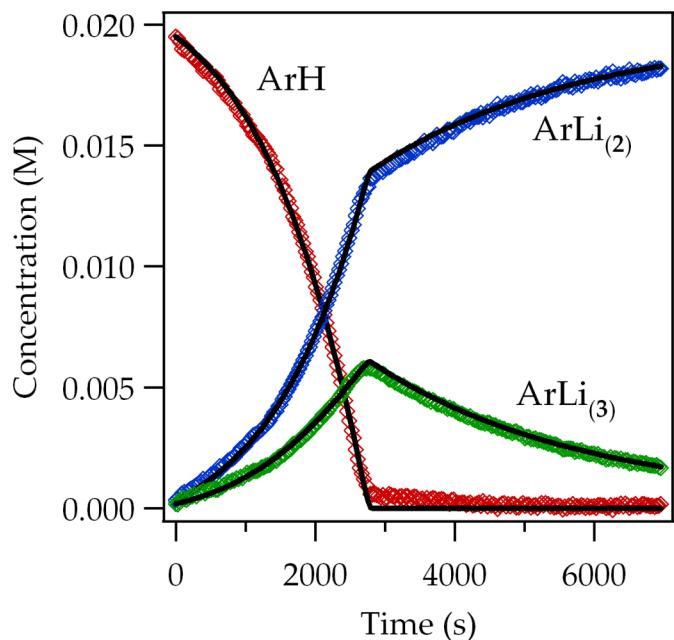
$$k_6 = 105 \pm 30$$

$$k_7 = 0.0001 \pm 0.0004$$

$$k_{-7} = 0.028 \pm 0.001$$

Figure 14 (continued).

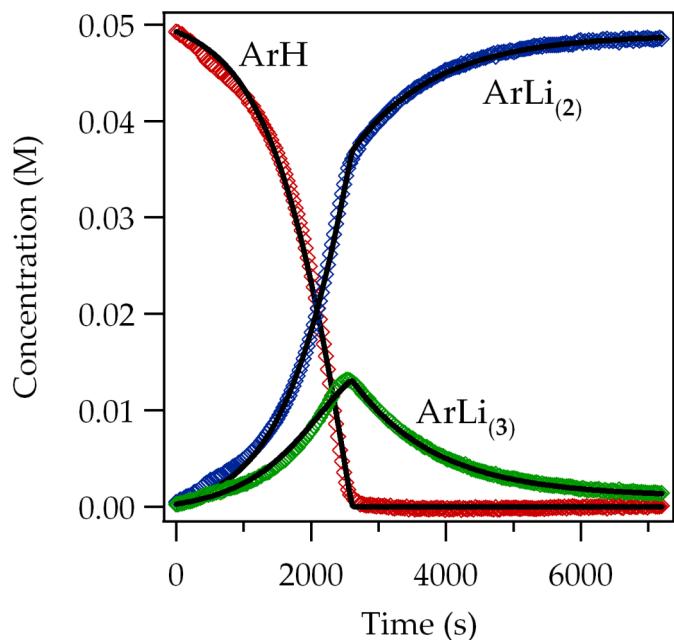
(C)



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

Figure 14 (continued).

(D)



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

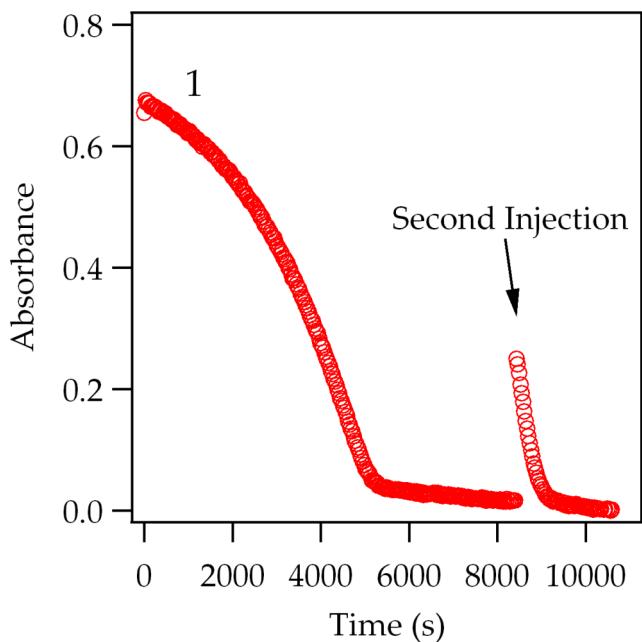


Figure 15. Representative plot showing absorbance of arene **1** vs time for the ortholithiation of **1** (0.010 M) with LDA (0.10 M) in THF (12.20 M) at -78°C . After completion of the reaction a second aliquot of **1** (0.005) was injected.

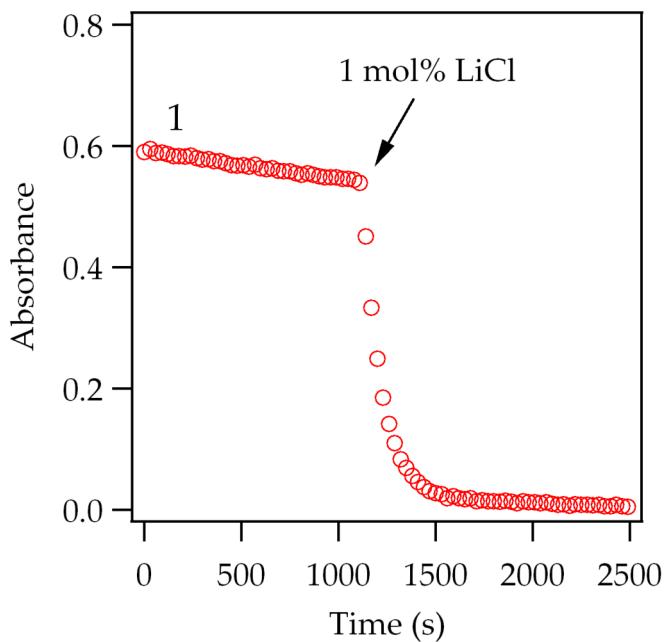


Figure 16. Ortholithiation of **1** (0.010 M) with LDA (0.10 M) in THF (12.2 M) at -78°C monitored by IR spectroscopy (1325 cm^{-1}) with injection of 1.0 mol % LiCl.

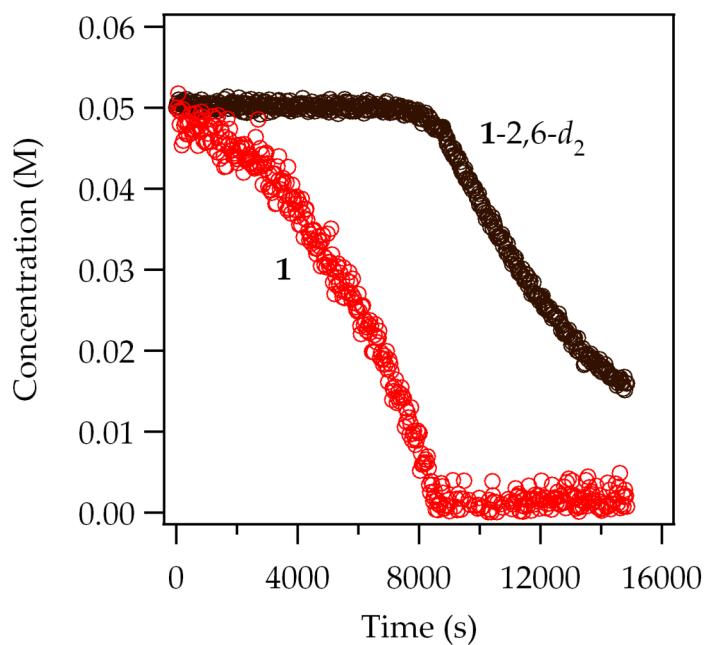


Figure 17 Competitive ortholithiation of **1** (0.050 M) and **1-2,6-d**₂ (0.050 M) with LDA (0.10 M) in THF (12.2 M) at -78 °C monitored by IR spectroscopy.

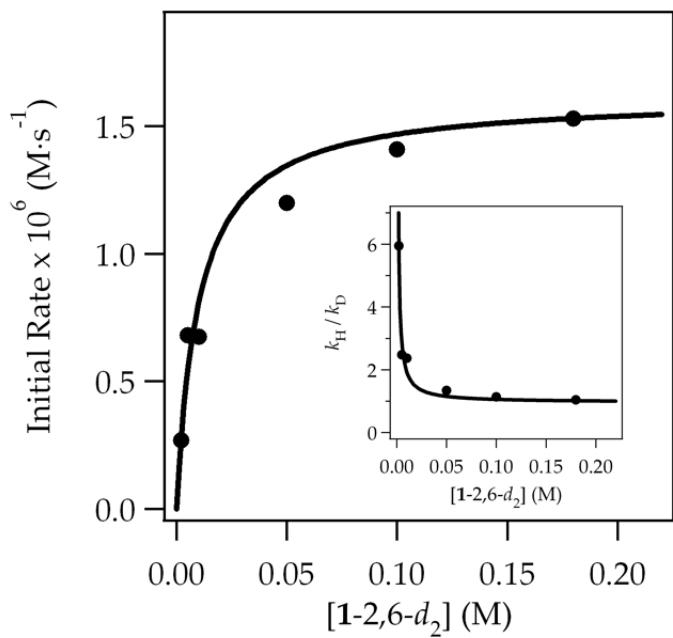


Figure 18. Plot of initial rate versus **1-2,6-d₂** for the ortholithiation of **1-2,6-d₂** by 0.10 M LDA in 12.2 M THF at -78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to a first-order saturation function: $-\Delta[\text{ArH}]/\Delta t|_{t=0} = (a[\text{ArH}])/(1+b[\text{ArH}])$ where ArH is **1-2,4-d₂**. The ratio a/b was constrained to $1.6 \times 10^{-6} \text{ M}\cdot\text{s}^{-1}$ to ensure saturation at the initial rate of 1 ($1.6 \times 10^{-6} \text{ M}\cdot\text{s}^{-1}$). [$b = (2.62 \pm 0.08) \times 10^{-6}$]

[1-2,6-d₂] (M)	$-\Delta[\text{ArH}]/\Delta t$ (M·s ⁻¹)
0.002	$2.69 \text{ e-7} \pm 2 \text{ e-8}$
0.005	$6.46 \text{ e-7} \pm 4 \text{ e-8}$
0.010	$6.74 \text{ e-6} \pm 1 \text{ e-7}$
0.050	$1.96 \text{ e-6} \pm 3 \text{ e-7}$
0.10	$1.41 \text{ e-6} \pm 6 \text{ e-7}$
0.18	$1.53 \text{ e-6} \pm 4 \text{ e-7}$
0.38	$2.62 \text{ e-6} \pm 2 \text{ e-7}$

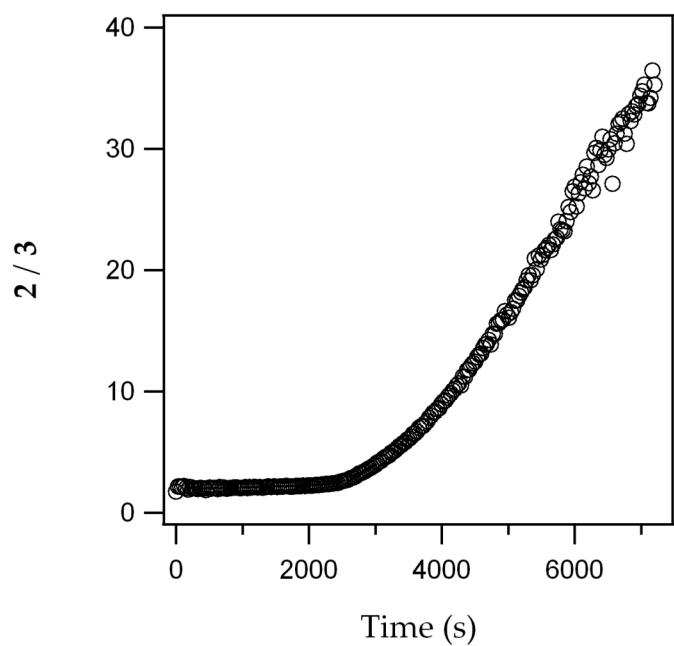


Figure 19. Plot of $2/3$ versus time for the ortholithiation of **1** by LDA in THF (12.2 M) at $-65\text{ }^{\circ}\text{C}$ measured by ^{19}F NMR spectroscopy.

Table 1. Relative initial rates for the formation of **2** and **3** for the ortholithiation of **1**, **1-2-d**, **1-6-d**, and **1-2,6-d₂** (0.050 M each) by LDA (0.10 M) in THF (12.2 M) at -78 °C measured by ¹⁹F NMR spectroscopy (A) in the absence of LiCl and (B) with 5 mol% LiCl.

No LiCl	(Δ 2 /Δ 3)
1	1.65
1-2-d	0.057
1-6-d	34.0
1-2,6-d₂	0.70

5 mol% LiCl	(Δ 2 /Δ 3)
1	0.78
1-2-d	0.016
1-6-d	26.0
1-2,6-d₂	0.30

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

Lithium salt	$(\Delta \mathbf{2} / \Delta t) / (\Delta \mathbf{3} / \Delta t)$
LiCl	0.78
2	0.84
34	0.72
35	0.73
36	0.49

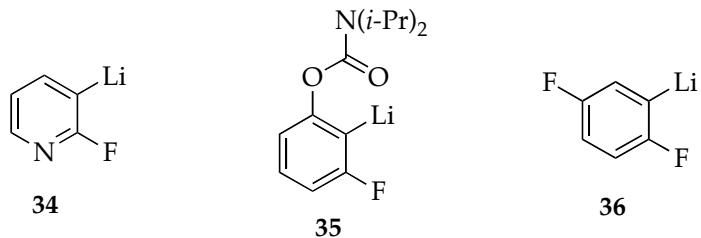


Table 3. Table showing regioselectivity at equilibrium for the ortholithiation of **1** by *sec*-BuLi (0.11 M) and *n*-BuLi (0.11 M) in 12.2 M THF at -90 °C measured by ¹⁹F NMR spectroscopy.

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

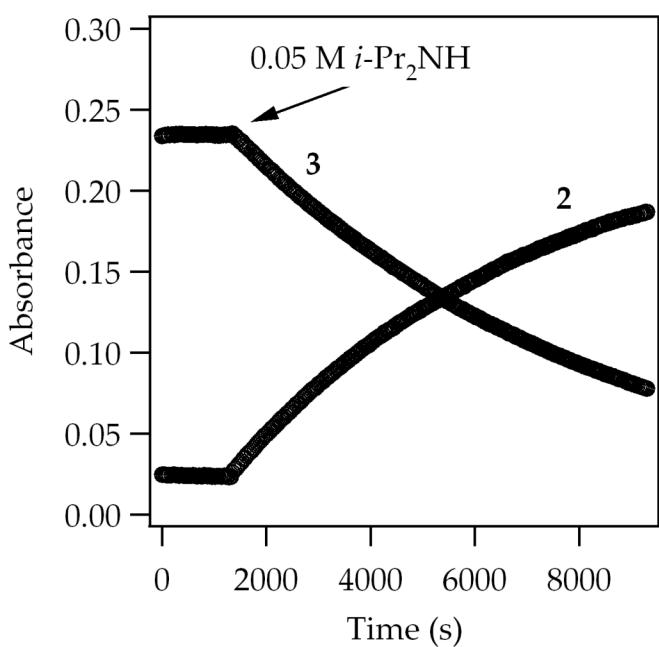


Figure 20. Representative IR plot for the equilibration of **3** (1151 cm^{-1}) to **2** (1306 cm^{-1}) was monitored by IR spectroscopy. Aryllithium **3** was generated by addition of LiTMP (0.050 M) to **1** (0.050 M) in 12.2 M THF at -78 °C. After **3** was produced quantitatively and no observable isomerization was detected, *i*-Pr₂NH (0.050 M) was injected.

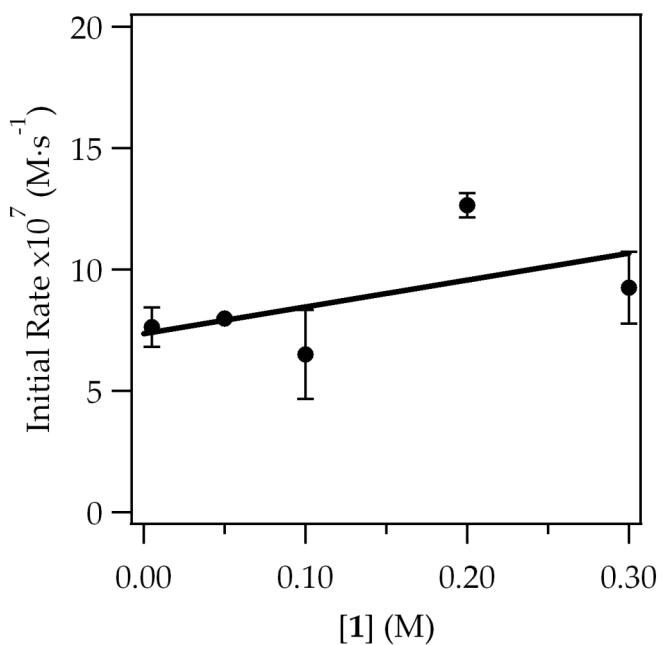


Figure 21. Plot of initial rate vs [1] (initial arene concentration) for the ortholithiation of **1** with LDA (0.10 M) in THF (12.2 M) at $-78\text{ }^\circ\text{C}$ measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{ArH}] + b$. [$a = (9 \pm 1) \times 10^{-7}$,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

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

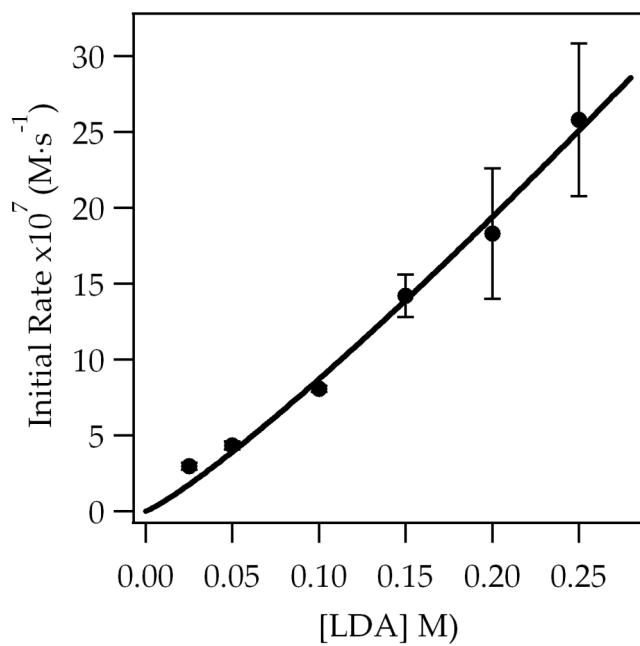


Figure 22. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.050 M) at -78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (1.2 \pm 0.2) \times 10^{-5}$, $n = (1.16 \pm 0.09)$]

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

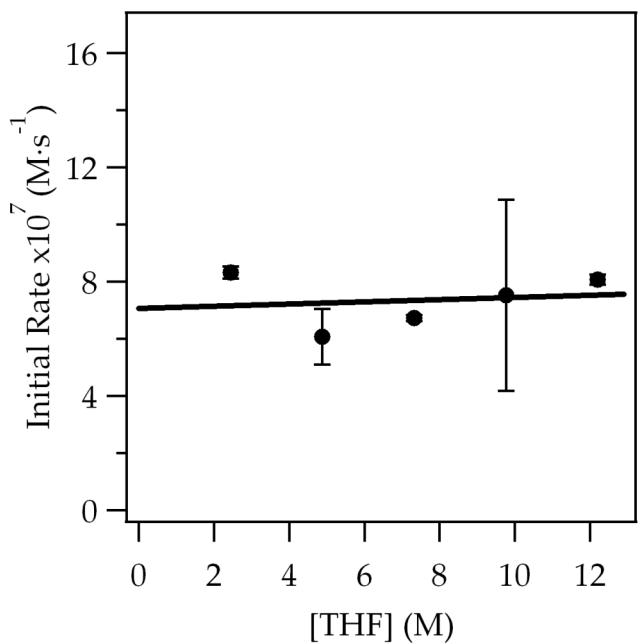


Figure 23. Plot of initial rate versus [THF] for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at -78 °C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [$a = (7 \pm 1) \times 10^{-7}$, $b = (3.9 \pm 0.1) \times 10^{-9}$]

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

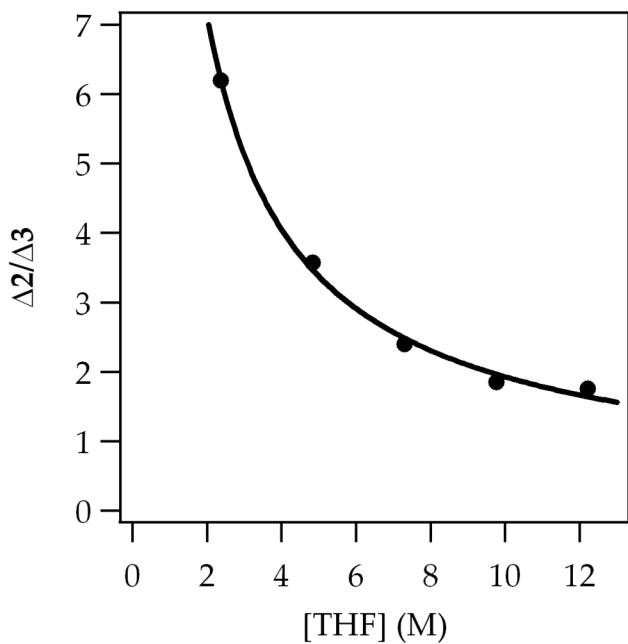


Figure 24. Ratio of relative initial rates of formation **2** and **3**, $(\Delta 2/\Delta t)/(\Delta 3/\Delta t)$, versus [THF] for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) at -65°C measured by ^{19}F NMR. The elevated temperature was used to shorten the duration of the experiments. The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

[THF] (M)	$(\Delta 2/\Delta t)/(\Delta 3/\Delta t)$
2.37	6.20
4.83	3.57
7.30	2.40
9.76	1.85
12.21	1.76

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

[LDA] (M)	$(\Delta 2 / \Delta t) / (\Delta 3 / \Delta t)$
0.020	1.74
0.10	1.76
0.20	1.71

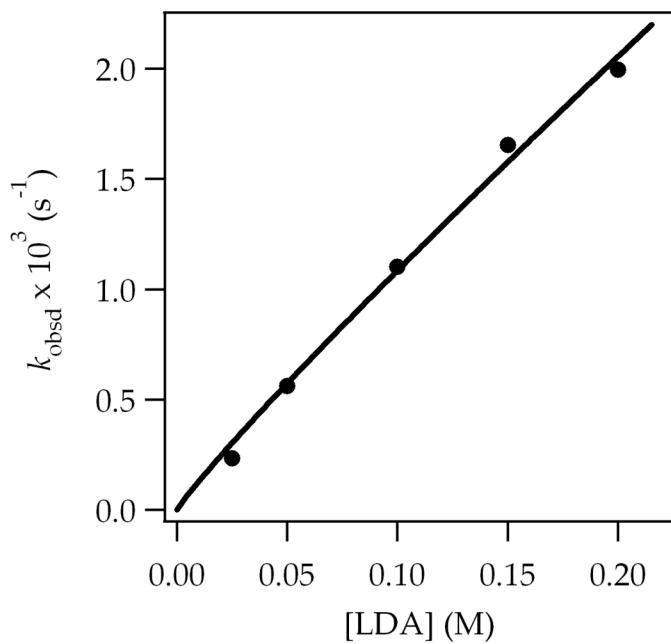


Figure 25. Plot of k_{obsd} versus [LDA] in THF (12.2 M) for the ortholithiation of **1**-*2,6-d*₂ (0.002 M) –65 °C measured by ¹⁹F NMR spectroscopy. The curve depicts an unweighted least-squares fit to $y = k[\text{LDA}]^n$. [$k = (9 \pm 1) \times 10^{-3}$, $n = 0.92 \pm 0.06$]

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

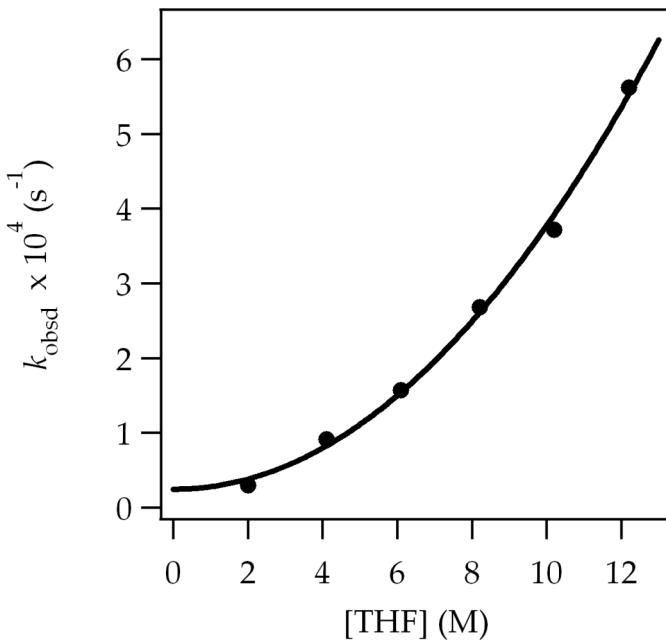


Figure 26. Plot of k_{obsd} versus [THF] in hexanes for the ortholithiation of **1-2,6-d₂** (0.002 M) by LDA (0.050 M) –65 °C measured by ¹⁹F NMR spectroscopy. The rates are not affected by medium effects as measured by the use of 2,6-dimethyltetrahydrofuran as a cosolvent. The curve depicts an unweighted least-squares fit to $y = k[\text{THF}]^n + c$. [$k = (3 \pm 1) \times 10^{-6}$, $n = 2.0 \pm 0.2$, $c = (3 \pm 1) \times 10^{-5}$]

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

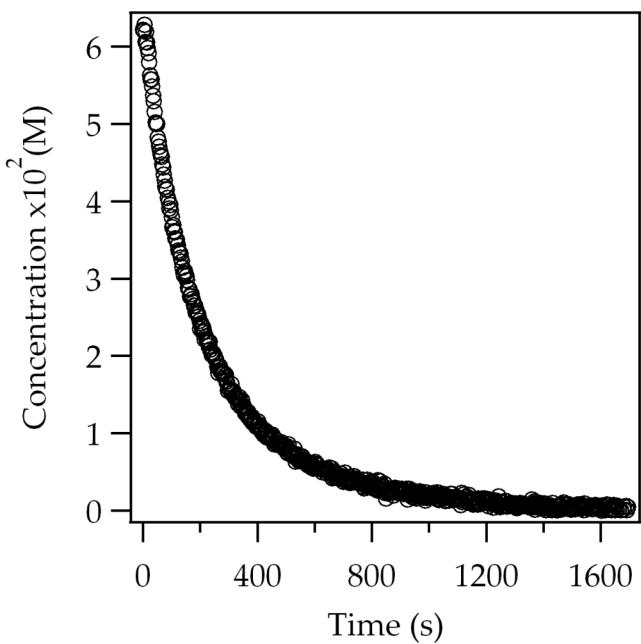


Figure 27. Representative plot of **1** (0.005 M) versus time for the ortholithiation by LDA (0.10 M) in 12.2 M THF in the presence of 5 mol% LiCl at -90 °C.

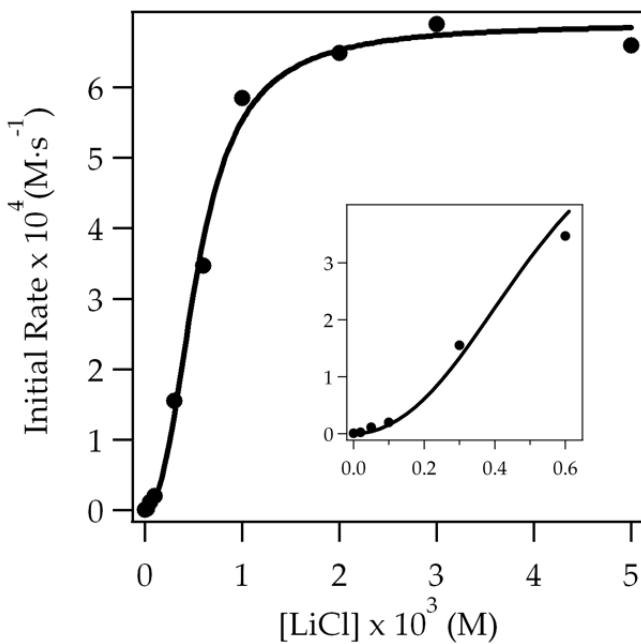


Figure 28. Plot of initial rate versus $[LiCl]$ for the ortholithiation of **1** (0.074 M) by 0.10 M LDA in 12.2 M THF at $-78\text{ }^\circ C$ measured by IR spectroscopy. The inset is a magnified view of the data at low concentrations. The curve depicts an unweighted least-squares fit to eq 17. $[ArH]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

$[LiCl]\text{ (mM)}$	$(\Delta[1]/\Delta t)\text{ (abs}\cdot\text{s}^{-1})$
0.0	$6.08 \text{ e-7} \pm 4 \text{ e-7}$
0.02	$2.37 \text{ e-6} \pm 2 \text{ e-7}$
0.05	$1.15 \text{ e-5} \pm 9 \text{ e-7}$
0.10	$1.99 \text{ e-5} \pm 5 \text{ e-7}$
0.30	$1.55 \text{ e-4} \pm 4 \text{ e-6}$
0.60	$3.47 \text{ e-4} \pm 2 \text{ e-5}$
1.0	$6.08 \text{ e-4} \pm 1 \text{ e-5}$
2.0	$6.49 \text{ e-4} \pm 2 \text{ e-5}$
3.0	$6.90 \text{ e-4} \pm 2 \text{ e-5}$
5.0	$6.602 \text{ e-4} \pm 2 \text{ e-5}$

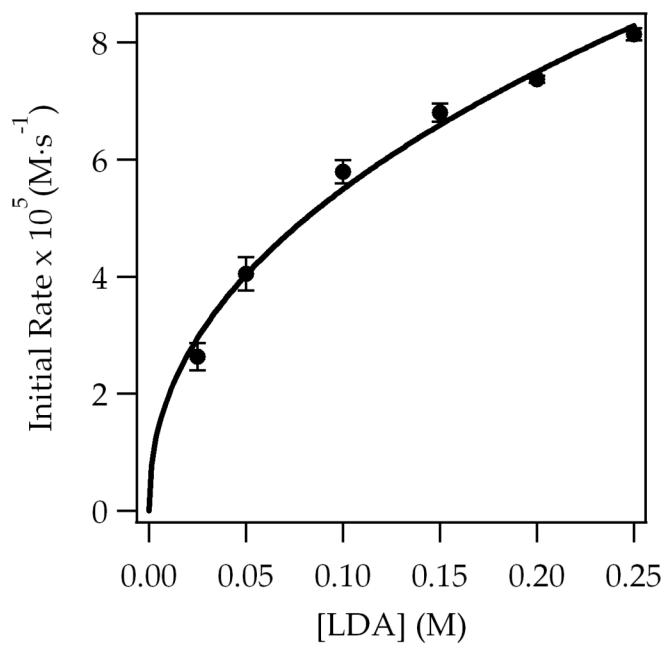


Figure 29. Plot of initial rate versus [LDA] in THF (12.2 M) for the ortholithiation of **1** (0.075 M) in the presence of 5 mol% LiCl at $-78\text{ }^\circ\text{C}$ measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{LDA}]^n$. [$a = (154 \pm 9) \times 10^{-6}$,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

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

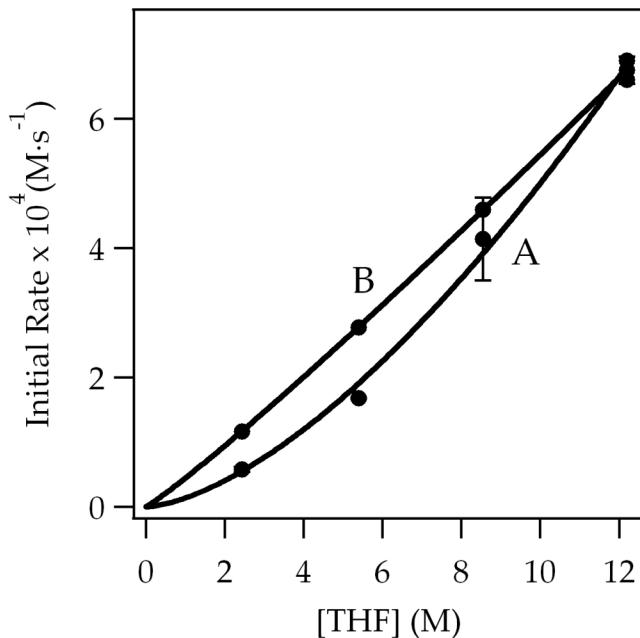


Figure 30. Plot of initial rate versus [THF] in hexanes (curve A) and 2,5-dimethyltetrahydrofuran (curve B) cosolvent for the ortholithiation of **1** (0.075 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at -78 °C. The data was measured by IR spectroscopy. The curve depicts an unweighted least-squares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

[THF] (M)	y1 (Ms ⁻¹)	y2 (Ms ⁻¹)
2.44	6.08 e-5 ± 8 e-7	5.5 e-5 ± 7 e-7
5.39	1.68 e-4 ± 3 e-6	1.67 e-4 ± 2 e-6
8.54	3.69 e-4 ± 1 e-5	3.40 e-4 ± 7 e-6
12.2	6.08 e-4 ± 4 e-6	5.51 e-4 ± 3 e-6

[Me ₂ -THF] (M)	y (Ms ⁻¹)
2.44	1.17 e-4 ± 4 e-6
5.39	2.77 e-4 ± 8 e-6
8.54	4.59 e-4 ± 2 e-5

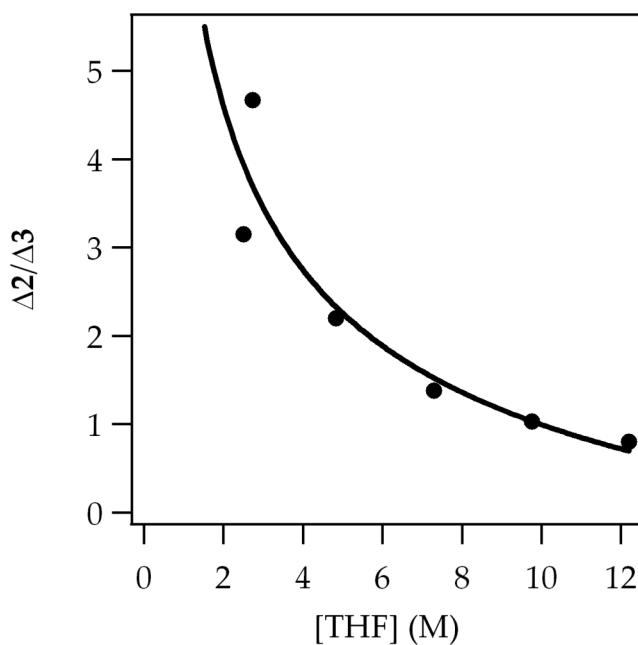


Figure 31. Plot of relative initial rate versus [THF] in 2,5-dimethyltetrahydrofuran cosolvent for the ortholithiation of **1** (0.050 M) by LDA (0.10 M) in the presence of 5 mol% LiCl at -78°C . The concentrations of **2** and **3** were monitored by ^{19}F NMR spectroscopy. The curve depicts an unweighted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

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

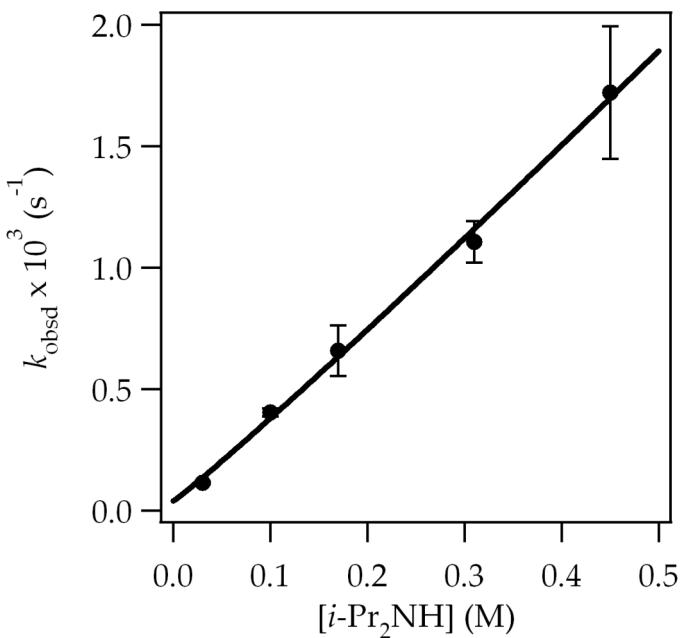


Figure 32. Plot of k_{obsd} vs $[i\text{-Pr}_2\text{NH}]$ for the isomerization of **3** (0.050 M) to **2** in 12.2 M THF at -78°C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = k[i\text{-Pr}_2\text{NH}]^n + c$. [$k = (3.8 \pm 0.3) \times 10^{-3}$, $n = 1.1 \pm 0.1$, $c = (2 \pm 1) \times 10^{-5}$]

$[i\text{-Pr}_2\text{NH}]$ (M)	$y1$ (s^{-1})	$y2$ (s^{-1})
0.030	$1.12 \text{ e-}4 \pm 4 \text{ e-}6$	$1.18 \text{ e-}4 \pm 1 \text{ e-}6$
0.10	$3.92 \text{ e-}4 \pm 3 \text{ e-}6$	$4.15 \text{ e-}4 \pm 3 \text{ e-}6$
0.17	$7.33 \text{ e-}4 \pm 5 \text{ e-}6$	$5.86 \text{ e-}4 \pm 3 \text{ e-}6$
0.31	$1.17 \text{ e-}3 \pm 7 \text{ e-}6$	$1.05 \text{ e-}3 \pm 8 \text{ e-}6$
0.45	$1.91 \text{ e-}3 \pm 2 \text{ e-}5$	$1.53 \text{ e-}3 \pm 1 \text{ e-}5$

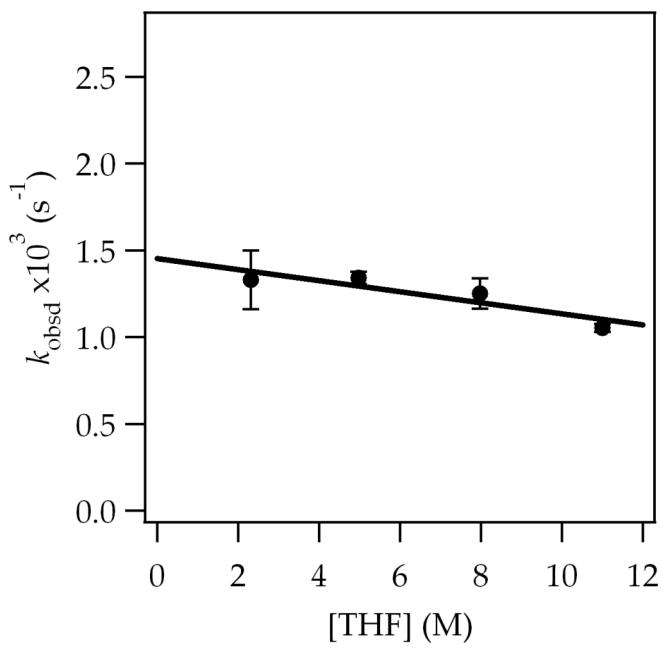


Figure 33. Plot of k_{obsd} versus [THF] for the isomerization of **3** (0.050 M) to **2** in 12.2 M THF at -78°C measured by IR spectroscopy. The curve depicts an unweighted least-squares fit to $y = a[\text{THF}] + b$. [$a = (1.45 \pm 0.08) \times 10^{-3}$, $b = (3.2 \pm 1.1) \times 10^{-5}$]

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

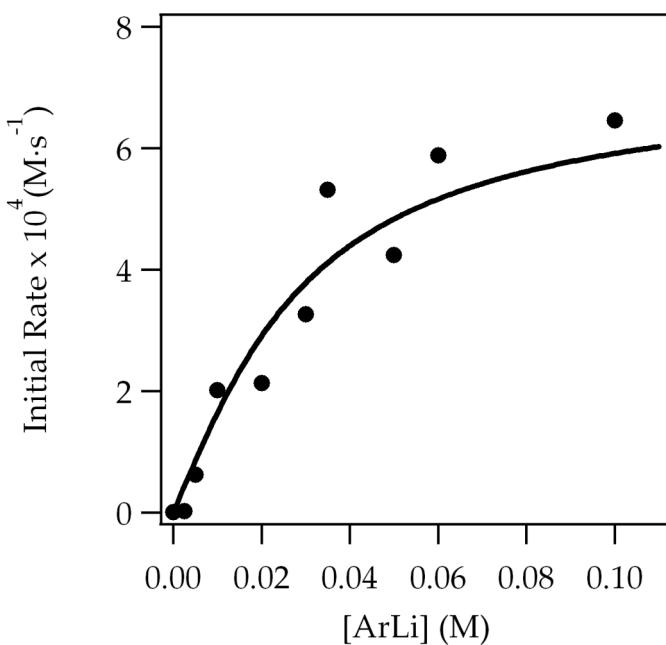
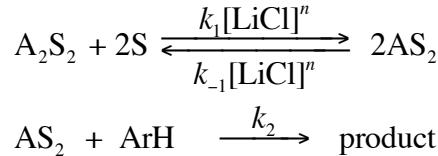


Figure 34. Plot of initial rate versus aryllithium **2-6-d** for the ortholithiation of **1** (0.075 M) by 0.10 M LDA in 12.2 M THF at -78 °C measured by IR spectroscopy. Aryllithium **2** was generated from **1-6-d** with one equivalent LDA at -40 °C prior to injection **1**. The curve depicts an unweighted least-squares fit a simple first-order saturation function: $-\Delta[\text{ArH}] / \Delta t|_{t=0} = (k_1 k_2 [\text{A}_2\text{S}_2][\text{ArH}]) / (k_{-1} + k_2[\text{ArH}])$ where $[\text{ArH}] = 0.075 \text{ M}$, $[\text{A}_2\text{S}_2] = 0.050 \text{ M}$. k_2 was constrained to the same value corresponding to lithium chloride saturation (see Figure 13). $[k_1 = (0.18 \pm 0.02); k_{-1} = (1.97 \pm 0.01) \times 10^9]$

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

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



The initial rate of consumption of ArH is defined as:

$$-\Delta[\text{ArH}] / \Delta t|_{t=0} = k_2[\text{AS}_2]_0[\text{ArH}]_0 \quad (1)$$

Applying the steady-state approximation to monomer AS_2 gives

$$\frac{d[\text{AS}_2]}{dt} = 2k_1[\text{A}_2\text{S}_2][\text{LiCl}]^n - 2k_{-1}[\text{AS}_2]^2[\text{LiCl}]^n - k_2[\text{AS}_2][\text{ArH}] = 0 \quad (2)$$

solving for $[\text{AS}_2]$ using the quadratic equation gives

$$[\text{AS}_2] = \frac{1}{4k_{-1}[\text{LiCl}]^n} (\sqrt{k_2^2[\text{ArH}]^2 + 16k_1k_{-1}[\text{A}_2\text{S}_2][\text{LiCl}]^{2n}} - k_2[\text{ArH}]) \quad (3)$$

Substituting eq 3 into eq 1 gives

$$-\Delta[\text{ArH}] / \Delta t|_{t=0} = \frac{k_2[\text{ArH}]}{4k_{-1}[\text{LiCl}]^n} (\sqrt{k_2^2[\text{ArH}]^2 + 16k_1k_{-1}[\text{A}_2\text{S}_2][\text{LiCl}]^{2n}} - k_2[\text{ArH}]) \quad (4)$$

where $[\text{ArH}]$ and $[\text{A}_2\text{S}_2]$ are evaluated at $t=0$. To account for the LiCl-free pathway, we add a constant c to eq 4 that reflects the initial rate without LiCl. The constant is determined experimentally rather than as an adjustable parameter.

$$-\Delta[\text{ArH}] / \Delta t|_{t=0} = \frac{k_2[\text{ArH}]}{4k_{-1}[\text{LiCl}]^n} (\sqrt{k_2^2[\text{ArH}]^2 + 16k_1k_{-1}[\text{A}_2\text{S}_2][\text{LiCl}]^{2n}} - k_2[\text{ArH}]) + c \quad (5)$$

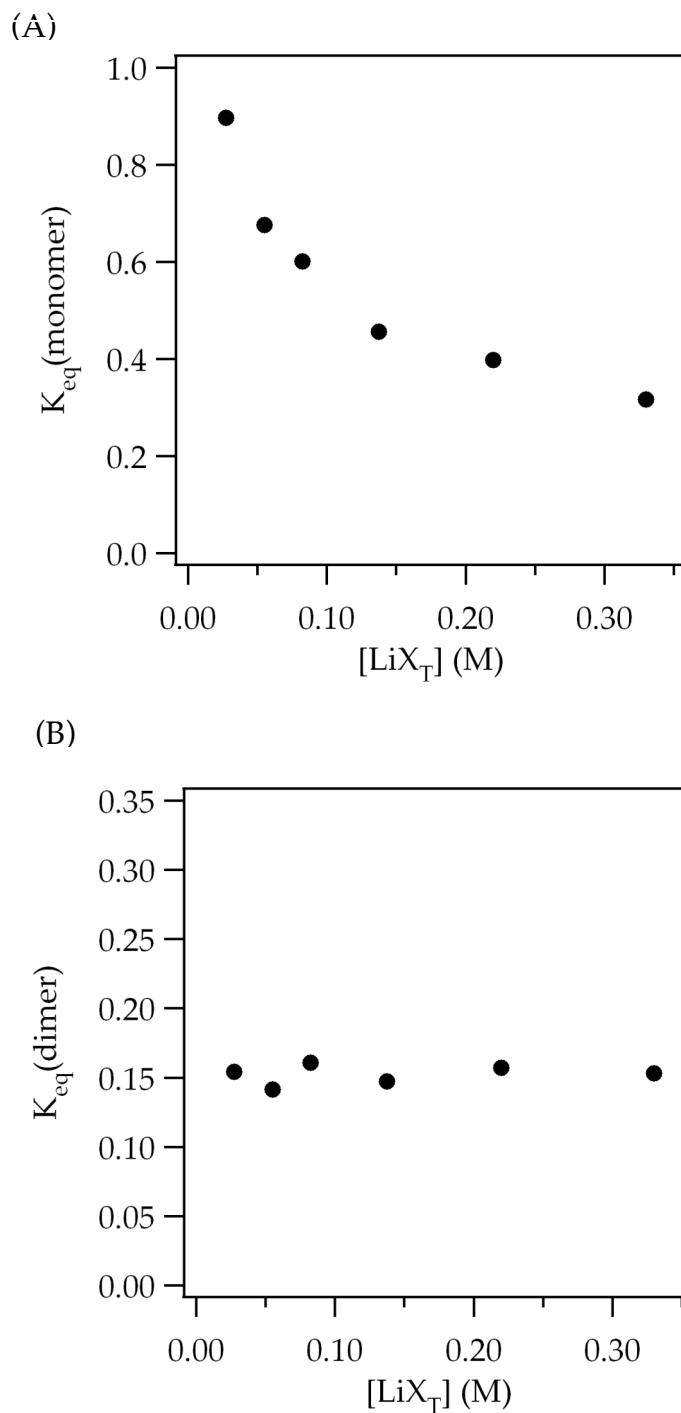


Figure 35. Plot of the equilibrium constant (K_{eq}) versus total concentration of lithium titer LiX_T (=LDA+LiCl) assuming (A) monomeric lithium chloride and (B) dimeric lithium chloride. Amounts of LDA-LiCl mixed dimer AX and mixed trimer A_2X and lithium chloride X_n are measured by ^6Li NMR for solutions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

Figure 35 (continued).

$$K_{\text{equ}}(\text{monomer}) = [\text{AX}]^2 / ([\text{X}][\text{A}_2\text{X}])$$

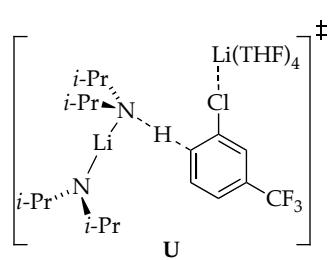
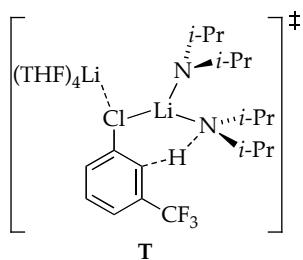
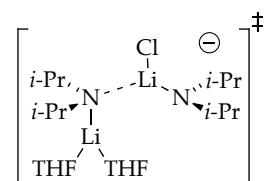
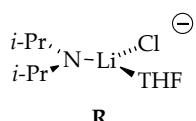
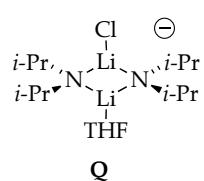
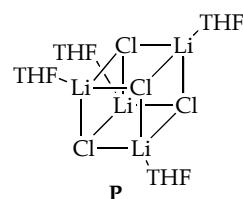
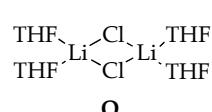
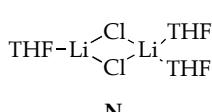
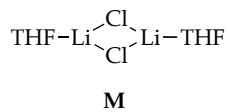
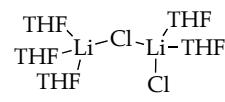
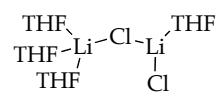
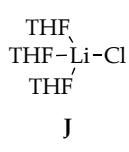
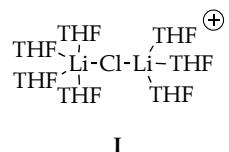
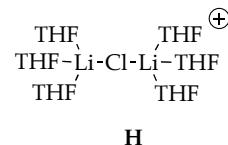
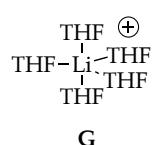
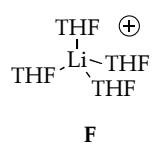
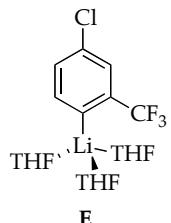
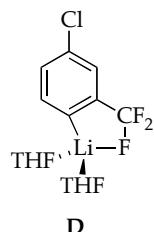
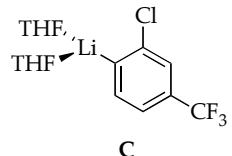
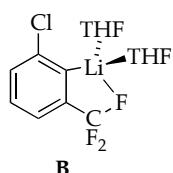
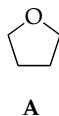
$$K_{\text{equ}}(\text{dimer}) = [\text{AX}]^2 / ([\text{X}_2]^{0.5}[\text{A}_2\text{X}])$$

where values of AX, X_n and A₂X are expressed in units of molarity.

[LiX _T] (M)*	K _{equ} (monomer)	K _{equ} (dimer)
0.023	0.90	0.15
0.055	0.68	0.14
0.083	0.60	0.16
0.14	0.46	0.16
0.22	0.40	0.16
0.33	0.32	0.15

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

Part 4: Computational Studies



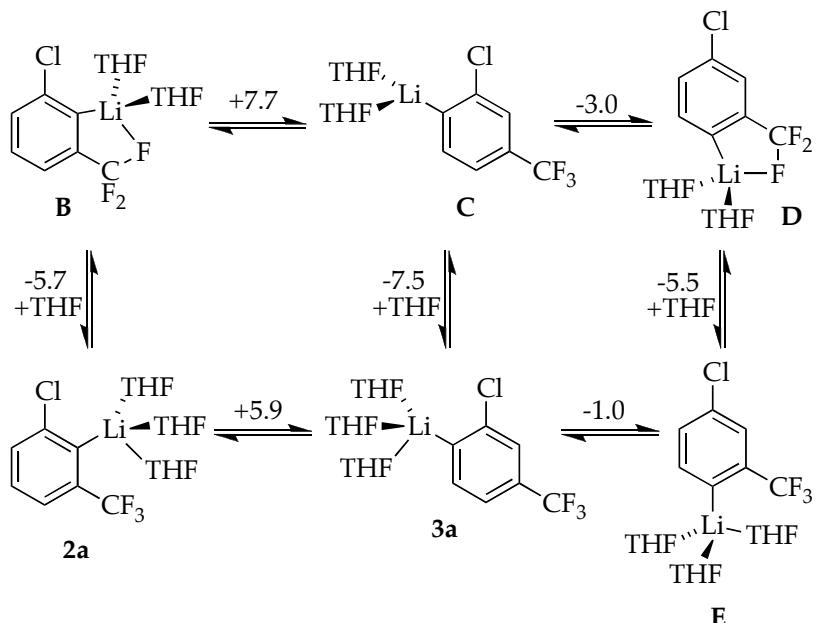


Figure 36. Relative free energies for the solvation (ΔG , kcal / mol) of of **2**, **3**, and **4**-lithio-1-chloro-3-(trifluoromethyl)benzene at -78 °C calculated at the MP2 level of theory with the 6-31G(d) basis set. Relative free energies are given in kcal / mol.

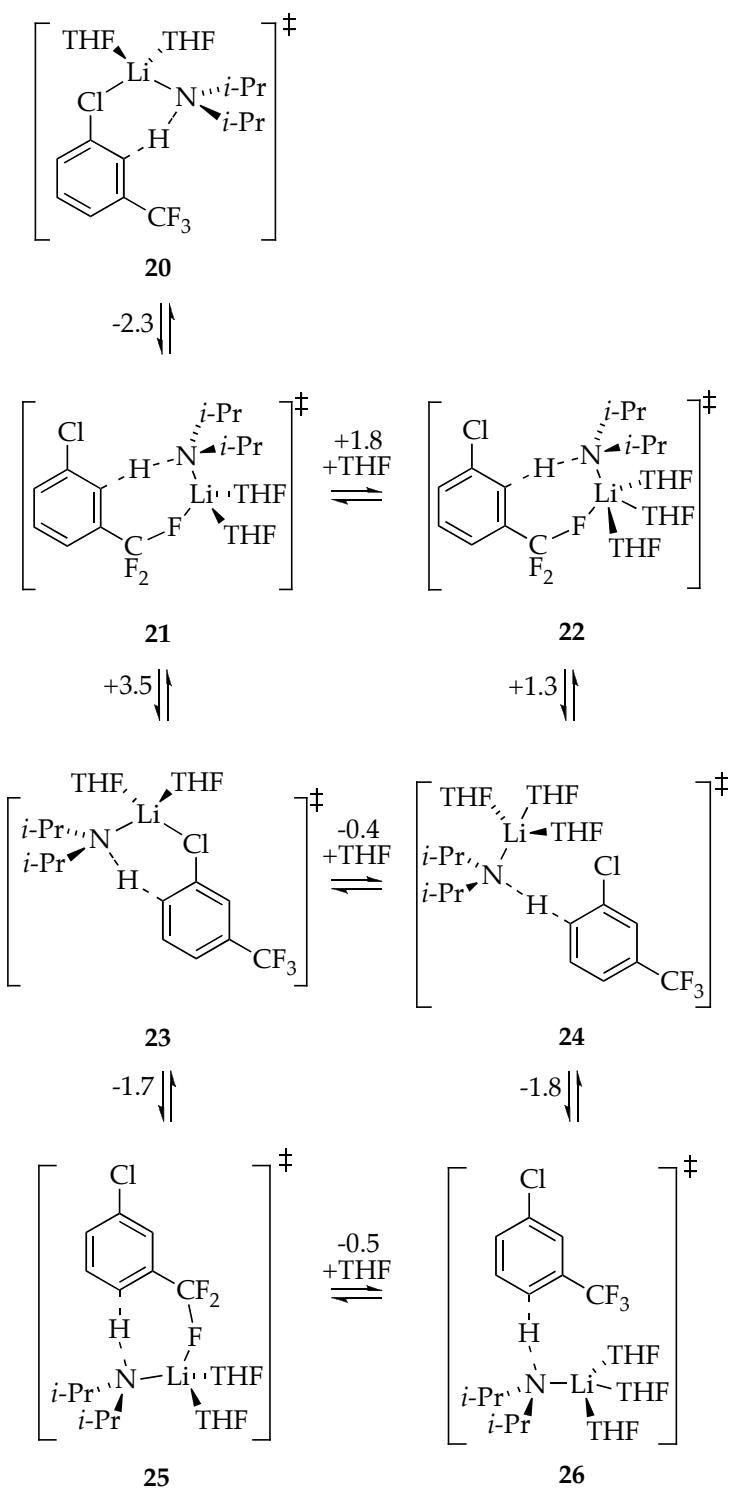


Figure 37. DFT computations [MP2/6-31G(d)/B3LYP/6-31G(d)] of monomer-based transition structures for the metalation of **1**. The free energy of activation for the formation of **18** (ΔG^\ddagger) is 14.5 kcal/mol calculated at -78°C . The numbers affiliated with the arrows represent the relative free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

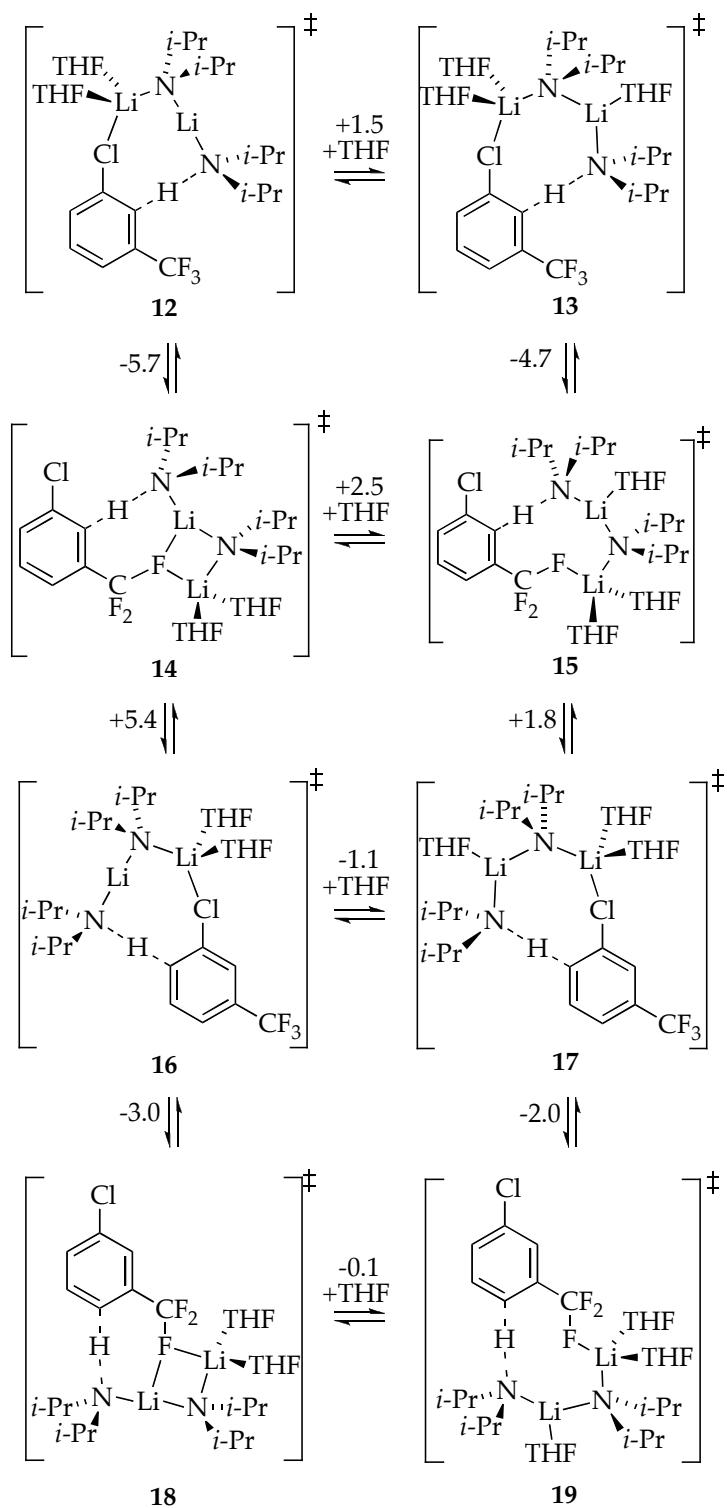
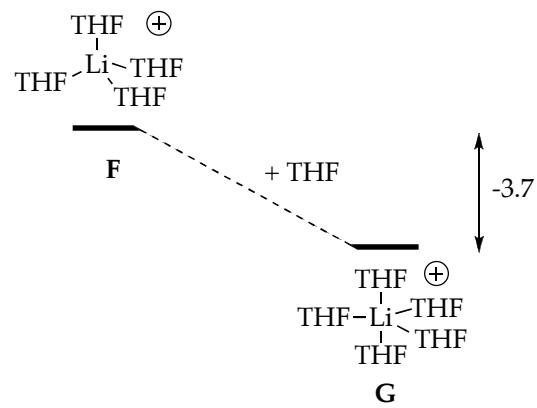
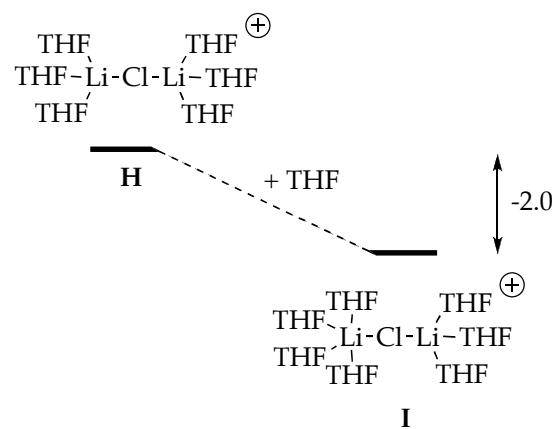


Figure 38. DFT computations [MP2/6-31G(d) / B3LYP/6-31G(d)] of dimer-based transition structures for the metalation of **1**. The free energy of activation for the formation of **12** (ΔG^\ddagger) is 19.3 kcal/mol calculated at -78 °C. The numbers affiliated with the arrows represent the relative free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

(A)



(B)



(C)

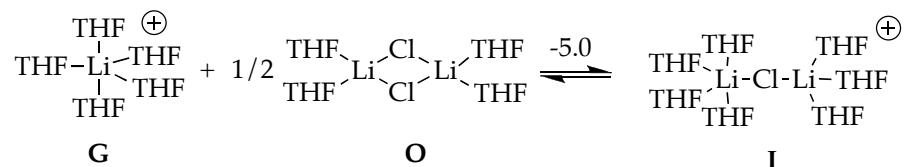
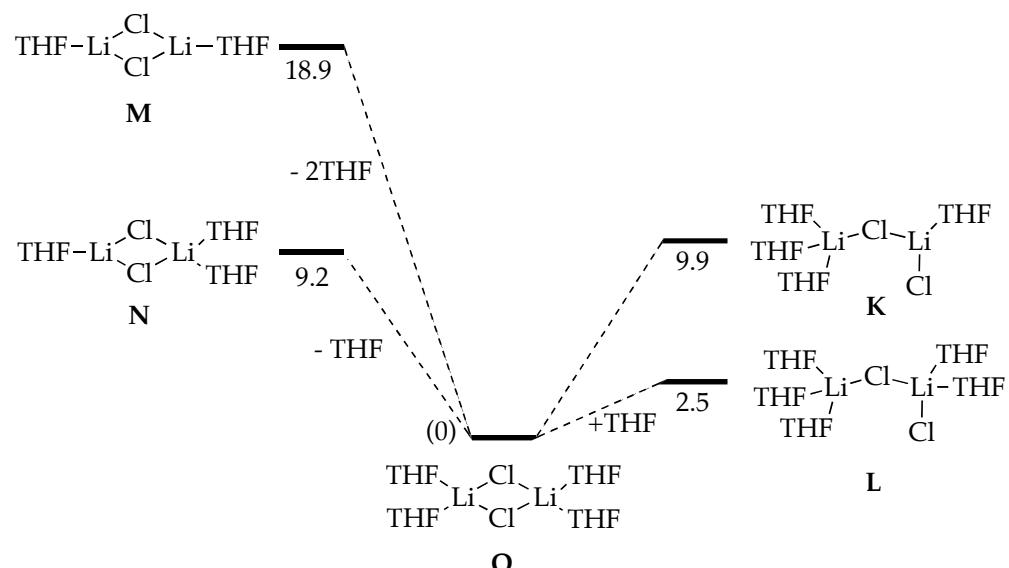


Figure 39. Relative free energies (ΔG , kcal / mol) at -78 °C for the solvation of (A) THF-tetrasolvated lithium ion and (B) THF-hexasolvated LiCl triple ion. (C) Relative free energy (ΔG , kcal / mol) at -78 °C showing the relative propensity of the lithium ion to exist in the triple-ion form rather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

(A)



(B)

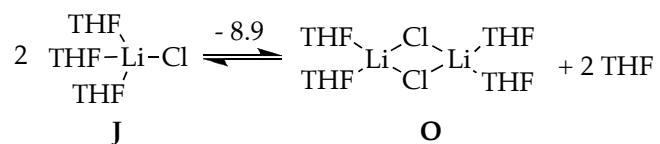


Figure 40. Relative free energies (ΔG , kcal / mol) at -78°C of (A) dimeric LiCl and relative free energy of monomeric and dimeric LiCl at -78°C . Tetrasolvated monomeric LiCl failed to minimize.

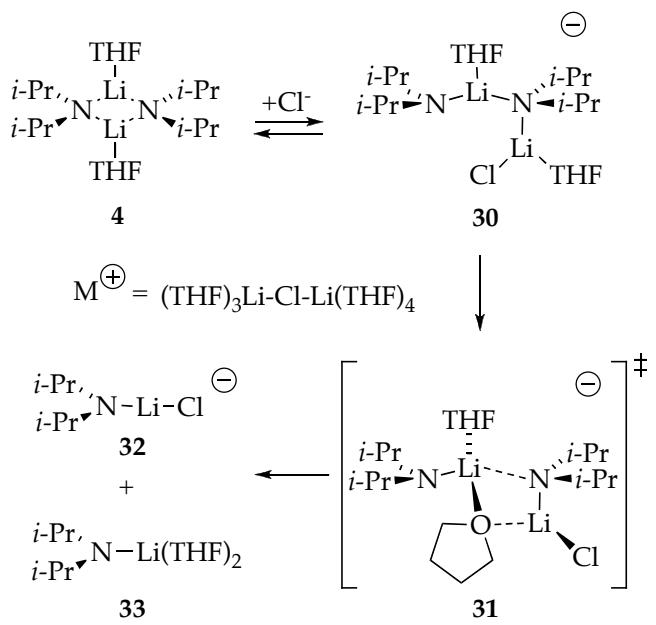
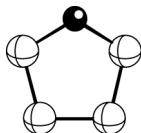


Figure 41. Reaction scheme showing lithium chloride deaggregating THF-disolvated closed dimer. The free energy of **31** is + 5.0 kcal/mol at -78 °C relative to chloride-solvated opendimer **30**. The left side of the equation could, in principle, be balanced by the inclusion of LDA-LiCl mixed aggregates.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

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



A

$G = -232.349385$

$G_{MP2} = -231.669937$

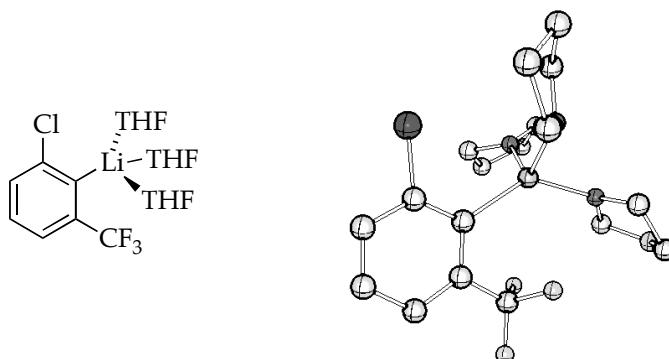
Atom	X	Y	Z
<hr/>			
C	-0.77676	0.78926	-0.12614
C	-1.13241	-0.69941	0.08086
O	-0.00028	-1.43271	-0.37154
C	1.13192	-0.69999	0.08156
C	0.77743	0.78860	-0.12707
H	-1.99954	-1.03544	-0.49441
H	-1.32099	-0.90818	1.14790
H	1.99943	-1.03711	-0.49250
H	1.31917	-0.90803	1.14900
H	1.16400	1.14893	-1.08517
H	1.20108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

Table 5 (Continued).

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

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

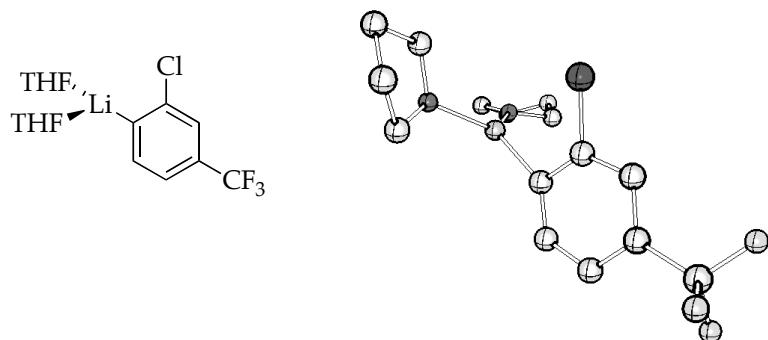
Table 5 (Continued).



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

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

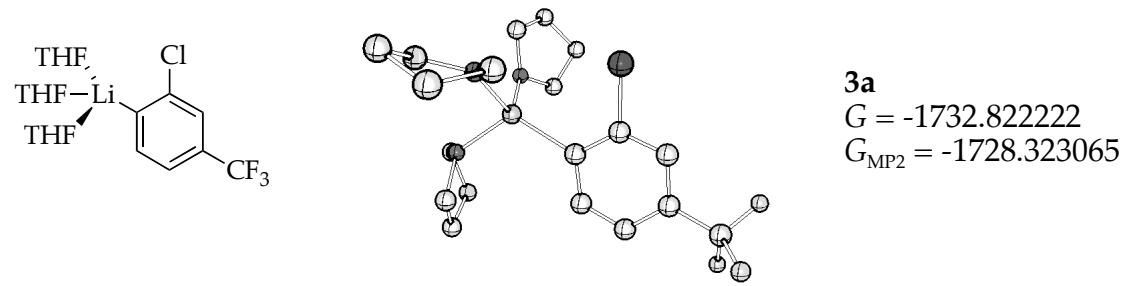
Table 5 (Continued).



The figure shows the chemical structure of a lithium salt in THF. On the left, a chemical structure is shown with a central lithium atom bonded to two THF molecules. This lithium atom is also bonded to a phenyl ring substituted with a chlorine atom at the para position and a trifluoromethyl group at the meta position. To the right, a 3D ball-and-stick model of the same molecule is shown, illustrating the spatial arrangement of atoms.

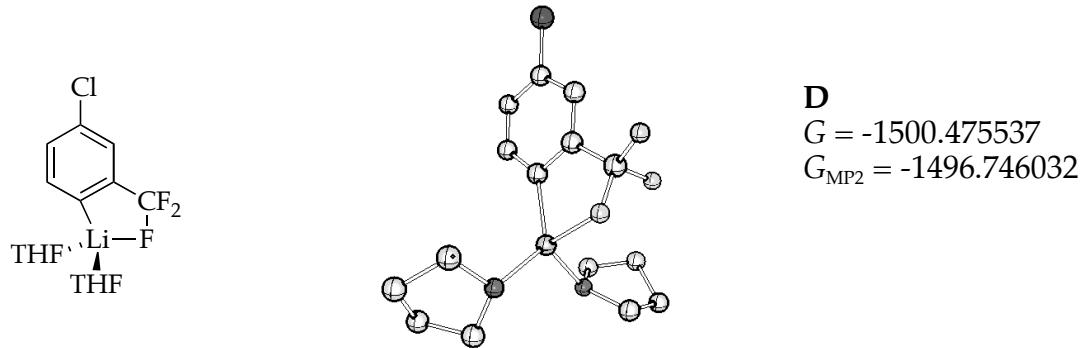
Atom	X	Y	Z	Atom	X	Y	Z
C	4.228498	-1.630255	-0.619511	C	1.726562	2.794350	-1.282569
O	2.877050	-1.419008	-0.152078	H	2.273506	3.163010	-2.160724
Li	1.656774	0.036753	-0.472780	H	0.794132	2.322429	-1.600537
C	-0.387058	-0.159538	-0.721856	H	1.332794	4.859306	-0.663125
C	-1.331327	-0.362525	-1.756929	H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

Table 5 (Continued).



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

Table 5 (Continued).



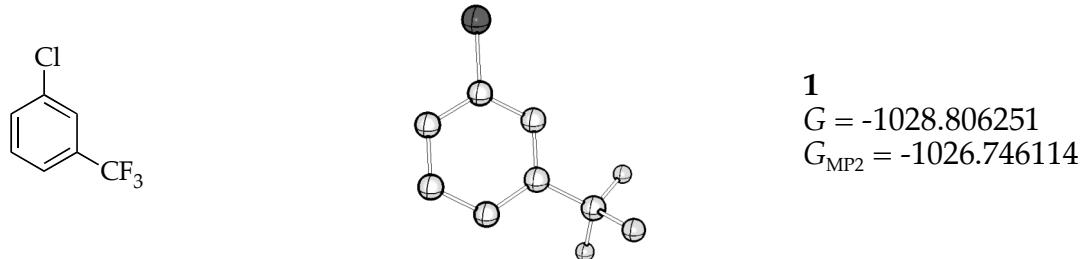
Atom	X	Y	Z	Atom	X	Y	Z
C	0.928658	-1.012816	1.482744	O	-2.299268	-1.328246	-0.680100
C	1.584391	-0.172928	0.426750	C	-1.748621	-1.930597	-1.881721
C	2.986545	-0.101788	0.456051	C	-1.412668	-3.363833	-1.483259
C	3.615938	0.617026	-0.550917	C	-2.559332	-3.697790	-0.515193
C	2.873361	1.242314	-1.552503	C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

Table 5 (Continued).

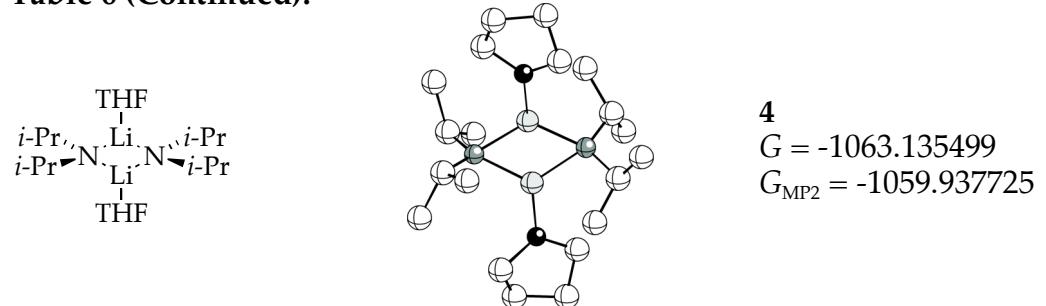
E
 $G = -1732.822473$
 $G_{MP2} = -1728.324732$

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

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

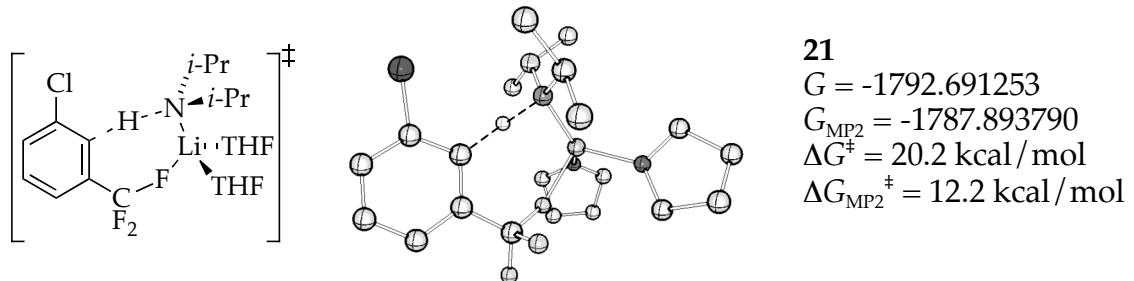


Atom	X	Y	Z
C	-2.022802	-0.354078	-0.001457
C	-0.643328	0.251689	-0.033108
C	-0.495501	1.640876	-0.019701
C	0.783061	2.195416	0.003163
C	1.912125	1.375235	0.012535
C	1.743556	-0.009039	-0.002061
C	0.475114	-0.584206	-0.024773
H	0.360420	-1.661422	-0.043478
Cl	3.156784	-1.051435	0.002466
H	2.910210	1.799814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

Table 6 (Continued).

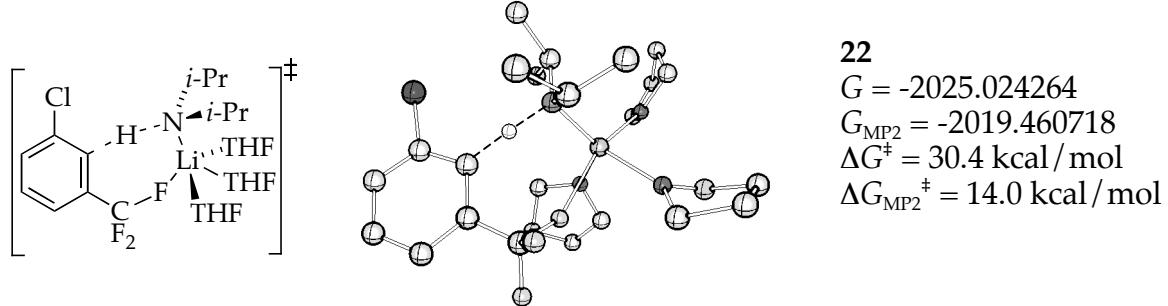
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.19464	-0.00774	0.01421	H	1.83816	-3.21720	1.36630
O	-3.18299	0.01572	-0.13583	H	-2.15959	-1.60468	1.84082
C	-3.98409	-1.09503	-0.60154	H	-1.26327	-2.26497	3.22164
C	-5.41144	-0.77445	-0.16155	H	-0.80287	-0.70251	2.54173
C	-5.43839	0.75767	-0.27769	H	-0.65863	-3.39245	1.09537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

Table 6 (Continued).



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

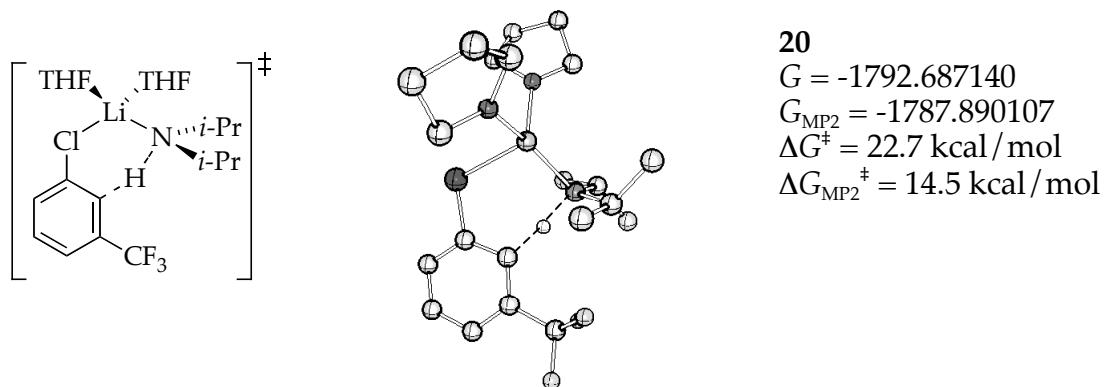
Table 6 (Continued).



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

Table 6 (Continued).

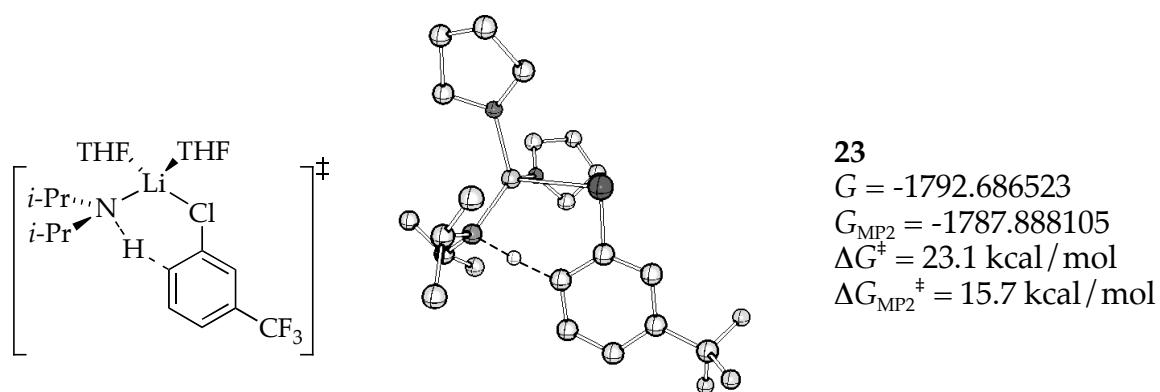
H	-1.144990	-2.649350	1.620721	H	1.382920	0.713329	-4.145369
H	-0.779998	-2.028100	4.594453	H	1.299741	2.353039	-3.495115
H	-0.251091	-3.473827	3.714990	H	2.299350	1.135743	-2.689473
H	1.589725	-1.511824	4.206616	H	1.415445	0.841583	-0.453604



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

Table 6 (Continued).

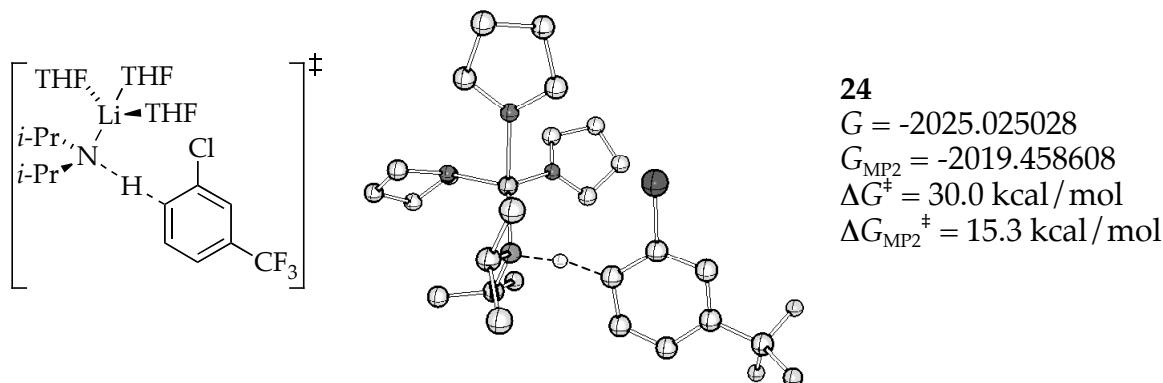
C	1.734404	2.975449	0.714586	H	-5.291907	1.470665	-1.106013
C	2.869272	3.823845	1.284377	C	-4.144560	-0.297623	0.535928
C	3.484261	2.870514	2.321018	F	-3.450122	-0.410314	1.690587
C	3.367008	1.510400	1.624488	F	-4.362677	-1.564912	0.091579
H	3.186662	0.684131	2.319223	F	-5.364027	0.198725	0.864650
H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



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

Table 6 (Continued).

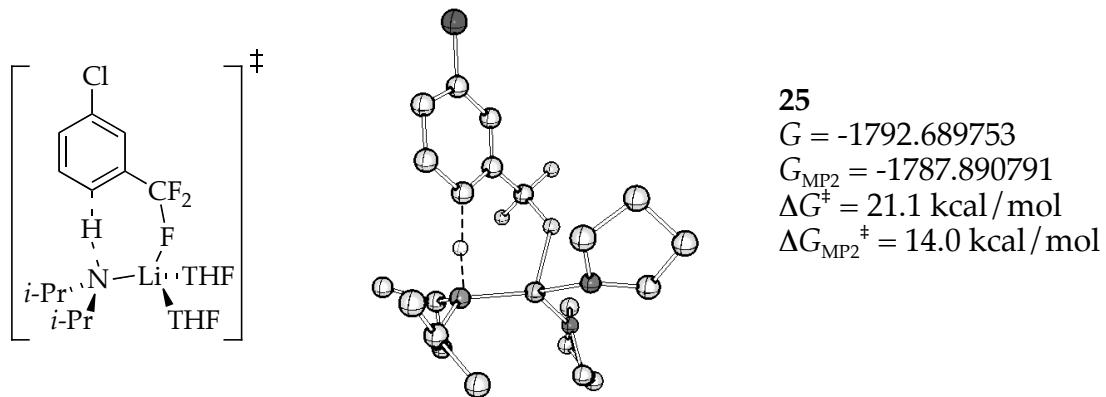
H	2.100926	-1.690383	-1.841922	Cl	-0.331664	0.960654	-1.375104
H	1.454356	-3.253822	-2.375538	H	-3.136445	1.375044	-1.577256
O	1.668402	1.657810	1.372684	C	-5.476277	0.371613	-0.596472
C	0.465850	2.248209	1.906611	F	-6.311780	0.306098	0.467187
C	0.505941	3.684437	1.390487	F	-5.531856	1.638364	-1.072852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



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

Table 6 (Continued).

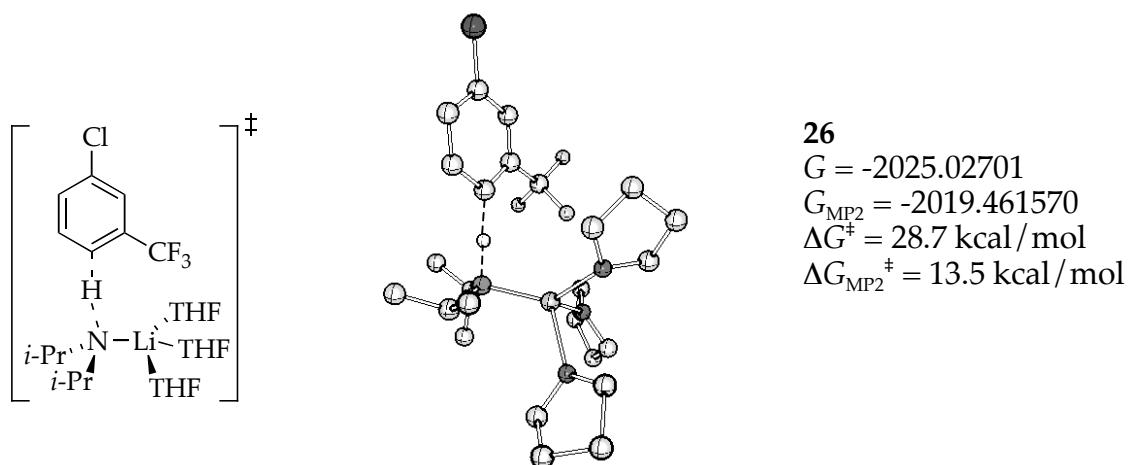
H	-0.293307	0.126406	-2.761327	H	1.196789	3.941830	2.150438
H	1.466992	0.249737	-2.618973	H	1.388123	3.389426	3.813116
H	4.032885	0.850155	-2.256263	H	2.672501	1.531401	3.187258
C	3.887886	1.738878	-1.633315	H	2.870467	2.306750	1.594616
O	2.613618	1.634694	-0.958800	C	-2.862419	-1.721783	0.104666
C	1.799790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



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

Table 6 (Continued).

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

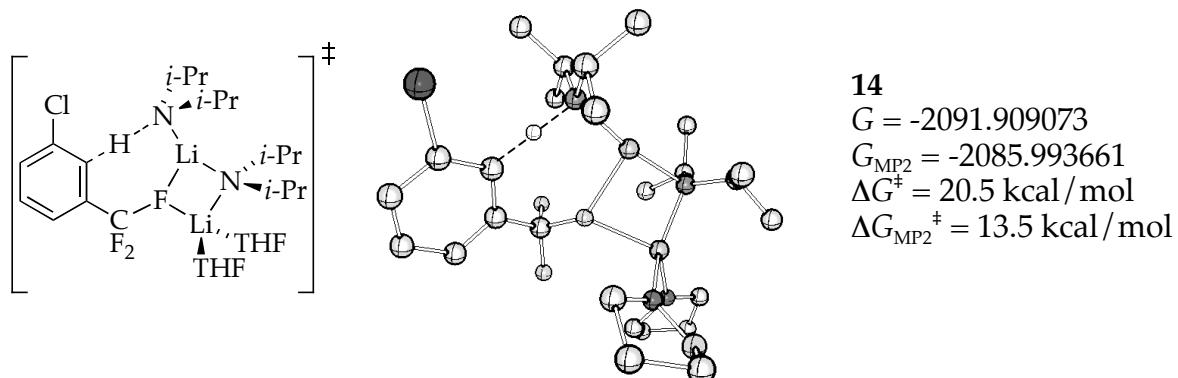


Atom	X	Y	Z	Atom	X	Y	Z
C	2.099262	-1.624323	-0.721682	H	1.728408	-1.635521	2.639896
C	2.891387	-0.407130	-0.340558	H	0.931180	0.500589	1.876597
C	4.250683	-0.583469	-0.043147	H	-0.013717	0.767339	3.371211

Table 6 (Continued).

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

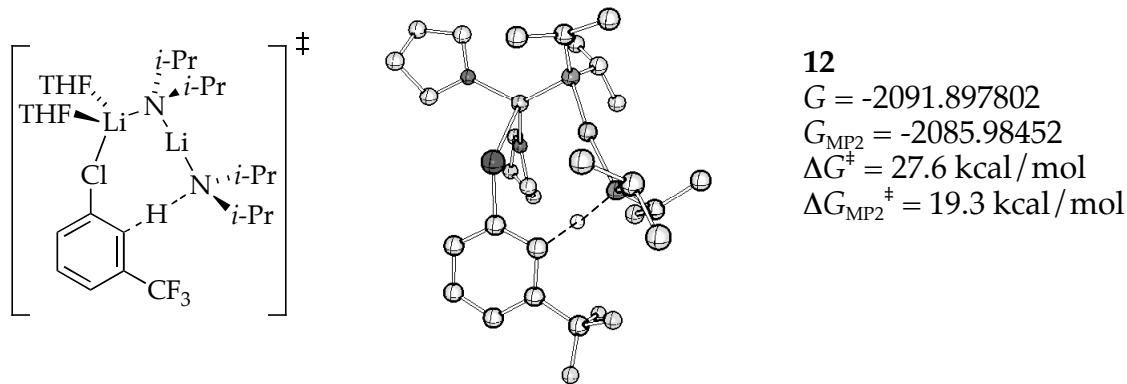
Table 7. Optimized geometries of reactants and dimer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the ortholithiation of **1** at -78 °C with free energies (Hartrees), and cartesian coordinates (X,Y,Z). (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d)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



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

Table 7 (Continued).

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

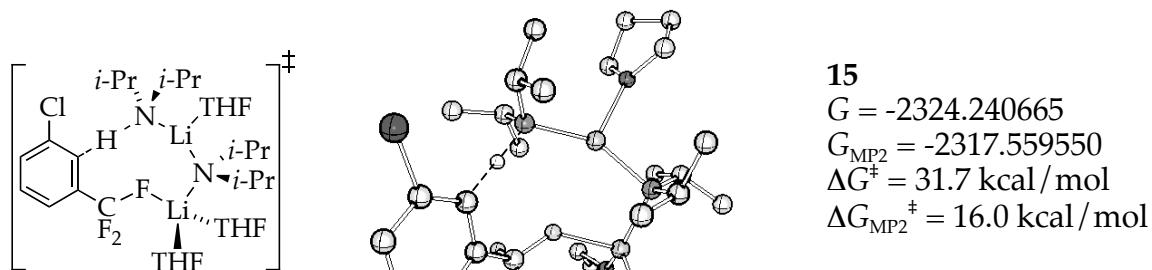


Atom	X	Y	Z	Atom	X	Y	Z
N	1.999882	1.967933	0.292844	H	-2.006141	1.319855	-2.783326
Li	2.393813	0.005958	0.226267	H	-1.996502	3.031866	-3.249239
O	1.876794	-1.403614	1.532529	H	-0.633496	2.351113	-2.358615
C	2.838468	-1.990841	2.440064	C	-3.949484	2.755344	-1.400180
C	2.130009	-3.190306	3.068961	H	-4.335502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

Table 7 (Continued).

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

Table 7 (Continued).



15

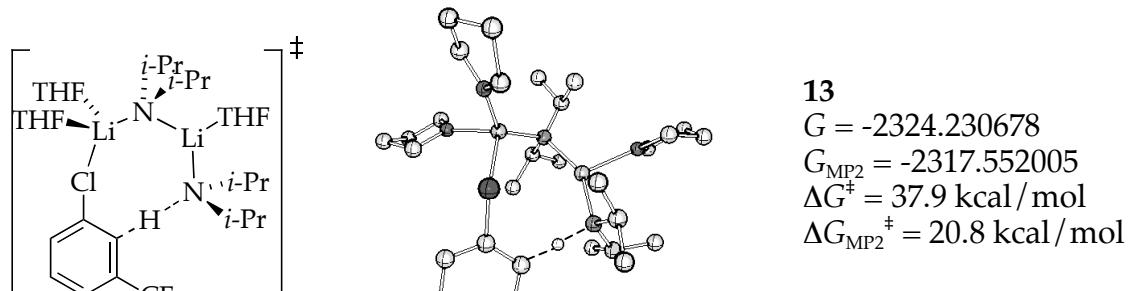
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 $G_{MP2} = -2317.559550$
 $\Delta G^\ddagger = 31.7 \text{ kcal/mol}$
 $\Delta G_{MP2}^\ddagger = 16.0 \text{ kcal/mol}$

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

Table 7 (Continued).

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

Table 7 (Continued).

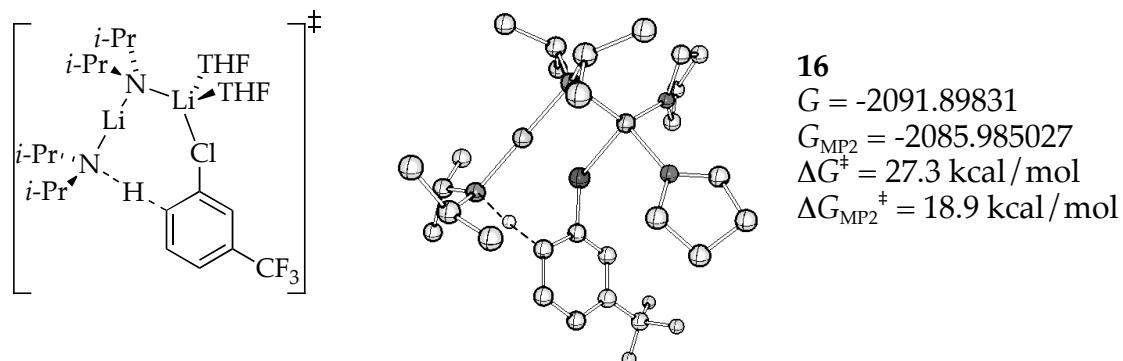


Atom	X	Y	Z	Atom	X	Y	Z
C	3.382045	1.015891	-0.332080	H	-2.824007	3.851274	0.707015
N	2.203611	0.714380	0.519915	H	-2.979647	2.124380	1.081464
Li	0.466508	1.561708	-0.285372	O	0.762616	3.802775	-0.250152
N	-1.467645	1.287755	-1.107929	C	0.909357	4.662765	-1.404321
Li	-2.300505	-0.239856	-0.118292	C	1.043327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

Table 7 (Continued).

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

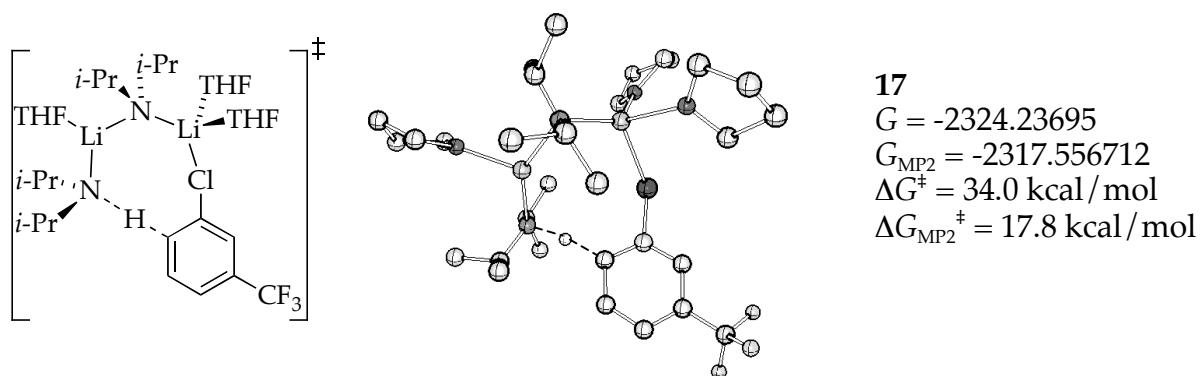
Table 7 (Continued).



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

Table 7 (Continued).

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

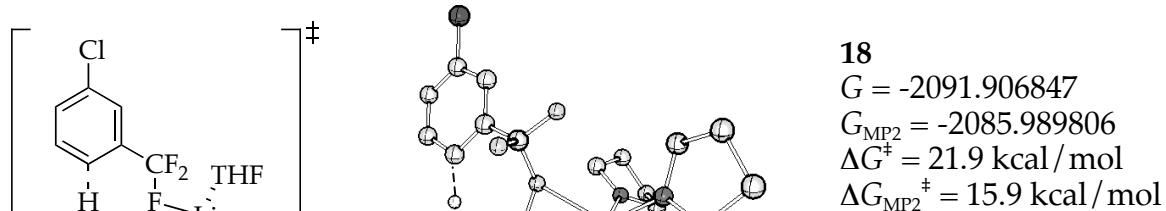


Atom	X	Y	Z	Atom	X	Y	Z
N	1.718676	1.115895	-1.084696	H	-0.555634	-3.224665	2.672606
Li	0.233451	1.974734	-0.017449	O	4.184641	-1.235028	-0.394244
O	0.384983	3.018609	1.752338	C	4.995955	-1.435919	-1.575260
C	0.113239	4.436696	1.831944	C	6.429202	-1.635428	-1.074709
C	-0.080454	4.735645	3.318099	C	6.203164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

Table 7 (Continued).

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

Table 7 (Continued).



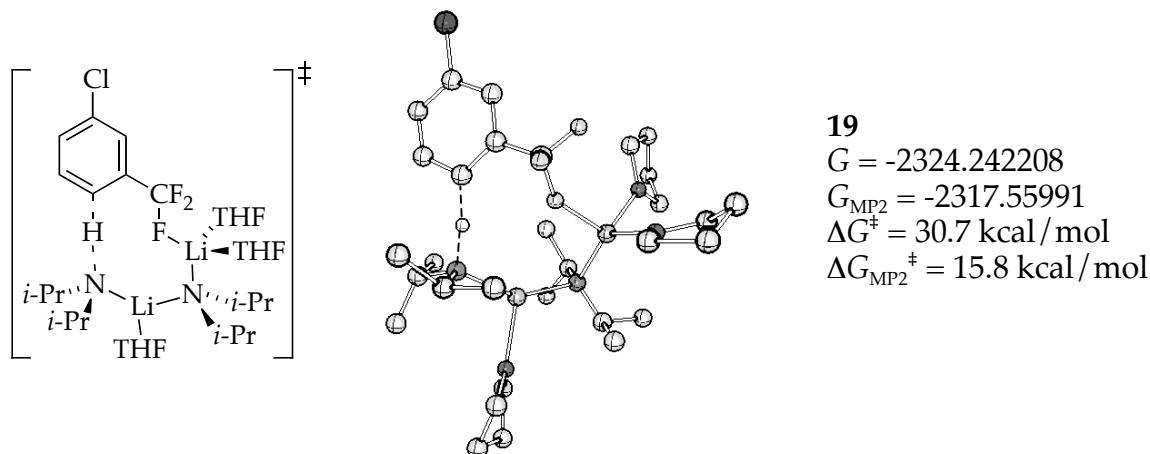
18

$G = -2091.906847$
 $G_{MP2} = -2085.989806$
 $\Delta G^\ddagger = 21.9 \text{ kcal/mol}$
 $\Delta G_{MP2}^\ddagger = 15.9 \text{ kcal/mol}$

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

Table 7 (Continued).

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

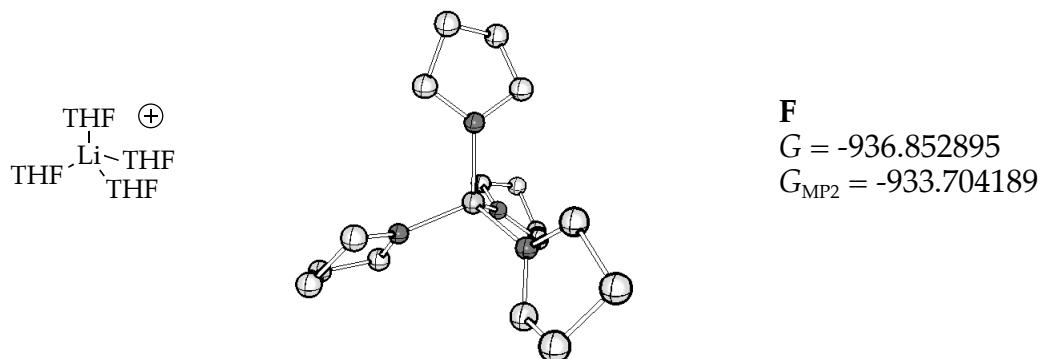


Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.272486	1.933725	-0.045018	H	6.705227	0.601706	-0.476194
F	-1.066358	0.176203	0.617594	H	7.252240	-0.838950	-1.354867
C	-2.210185	-0.412128	1.124240	H	4.979452	-1.470722	-1.924707
F	-3.176513	0.539150	1.036513	H	4.802161	0.301060	-1.938842
F	-1.968428	-0.564587	2.453434	C	1.103494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

Table 7 (Continued).

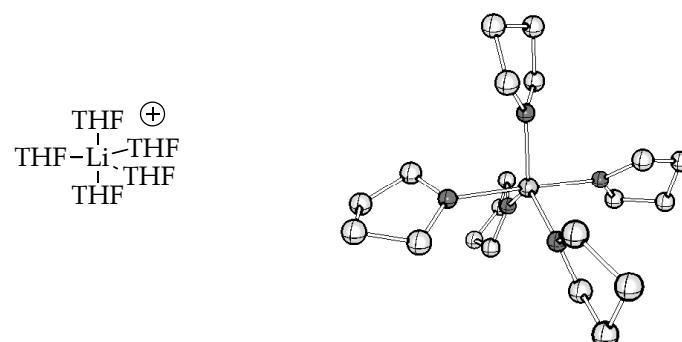
H	-1.205990	-4.501911	-0.841668	C	2.379802	3.736995	-1.269331
N	1.417860	1.380141	-1.022053	H	2.251418	3.778989	-2.356398
Li	1.950534	-0.540460	-0.320384	H	1.506997	4.220568	-0.807015
N	1.269358	-2.400283	0.344700	H	3.262775	4.341872	-1.023984
C	1.638588	-3.543957	-0.521899	C	2.814269	2.352699	0.759648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

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



Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.006449	0.001038	-0.009157	O	1.191545	1.220605	-0.970730
O	-1.077777	-1.026060	-1.295317	C	2.297282	1.933630	-0.357946
C	-0.989910	-2.462953	-1.508784	C	3.270383	2.229150	-1.496696
C	-2.132747	-2.816892	-2.464896	C	2.314055	2.442198	-2.680370
C	-3.164470	-1.715775	-2.173973	C	1.225143	1.399943	-2.415227
C	-2.268061	-0.502979	-1.939270	H	1.461585	0.432429	-2.872967
H	-2.697261	0.253434	-1.276585	H	0.230932	1.713191	-2.746231
H	-1.979832	-0.025559	-2.884933	H	2.793140	2.300813	-3.652757
H	-3.3737433	-1.950673	-1.269413	H	1.893118	3.453407	-2.654471
H	-3.871172	-1.560270	-2.993477	H	3.923574	1.367847	-1.678120
H	-2.518079	-3.825188	-2.292093	H	3.901818	3.097306	-1.290120
H	-1.795718	-2.758029	-3.505587	H	1.915196	2.857533	0.095229
H	0.000191	-2.692371	-1.913886	H	2.708844	1.297860	0.430975
H	-1.097298	-2.956151	-0.535998	O	-1.236654	1.033713	1.121026
O	1.102928	-1.230097	1.050946	C	-2.269354	0.461832	1.968338
C	2.270584	-1.905345	0.513630	C	-3.249489	1.600110	2.249196
C	3.181542	-2.153074	1.713094	C	-2.324461	2.827204	2.240319
C	2.162391	-2.403646	2.835346	C	-1.344388	2.484692	1.118917
C	1.044761	-1.414890	2.493348	H	-0.344441	2.901385	1.265602
H	1.200174	-0.438633	2.967237	H	-1.719882	2.801928	0.138394
H	0.047388	-1.780647	2.754423	H	-1.797773	2.917682	3.196897
H	2.571312	-2.234846	3.834979	H	-2.854323	3.765320	2.055151
H	1.791464	-3.433513	2.791200	H	-3.780163	1.466271	3.195494
H	3.784018	-1.263155	1.929201	H	-3.995082	1.673546	1.449237
H	3.861908	-2.993687	1.553117	H	-2.712408	-0.385399	1.436410
H	1.951993	-2.846493	0.047474	H	-1.800550	0.096006	2.889973
H	2.704206	-1.258975	-0.254455				

Table 8 (Continued).

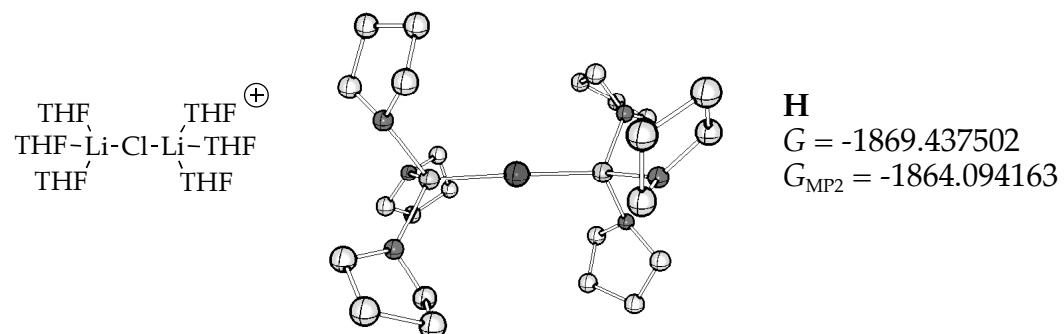


THF^+
 $\text{THF}-\text{Li}^+-\text{THF}$
 THF

G
 $G = -1169.19433$
 $G_{\text{MP2}} = -1165.279988$

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

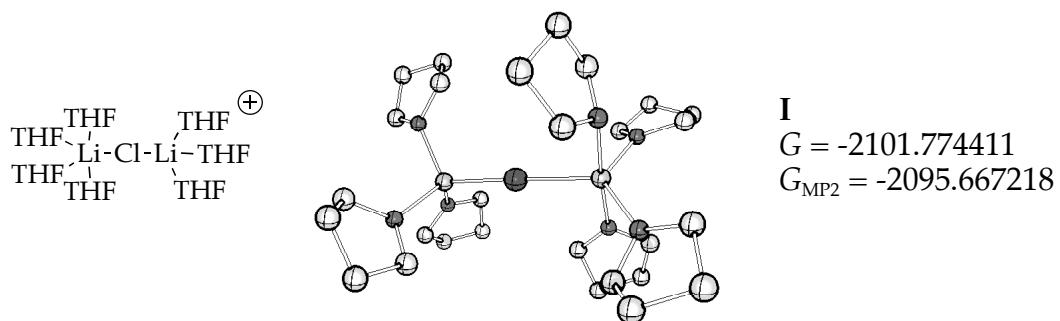
Table 8 (Continued).



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

Table 8 (Continued).

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

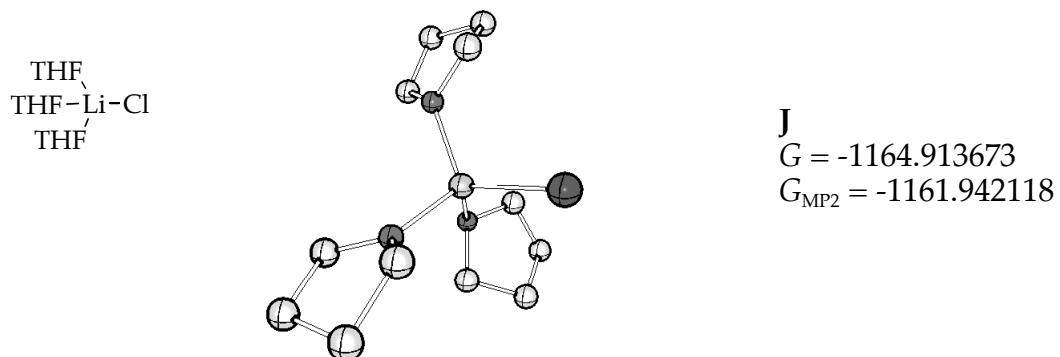


Atom	X	Y	Z	Atom	X	Y	Z
Li	2.092644	-0.204286	0.158816	C	-2.657925	4.258283	-0.147982
Cl	-0.389978	-0.130696	-0.001816	C	-2.534004	2.970481	0.664104
Li	-2.704165	0.088780	-0.123903	H	-2.977136	3.081723	1.662926
O	-3.635244	-0.787110	1.398964	H	-1.513522	2.593050	0.764508
C	-4.856790	-0.239895	1.965413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

Table 8 (Continued).

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

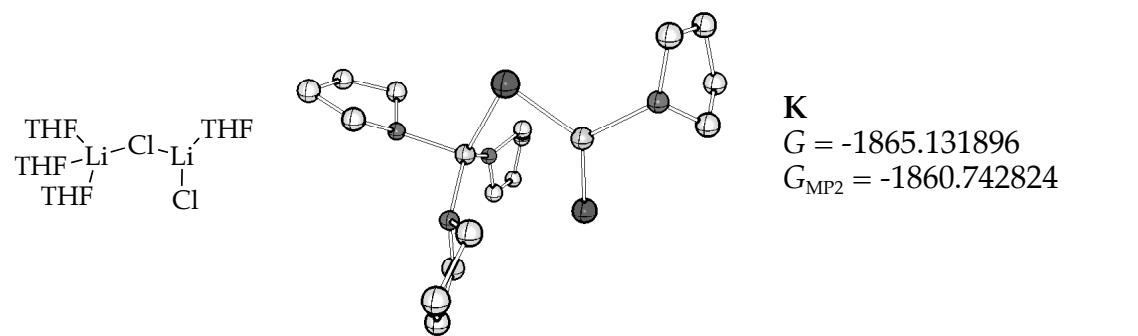
Table 8 (Continued).



* Tetrasolvated lithium chloride monomer fails to minimize.

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

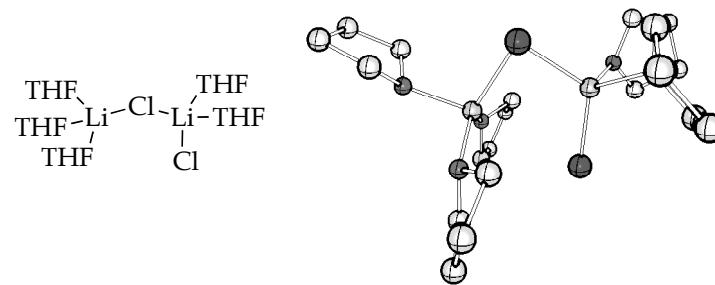
Table 8 (Continued).



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

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

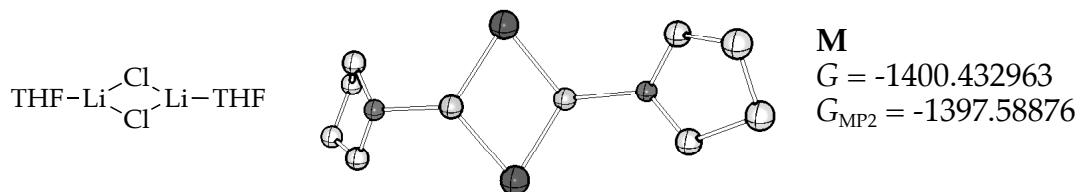
Table 8 (Continued).



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

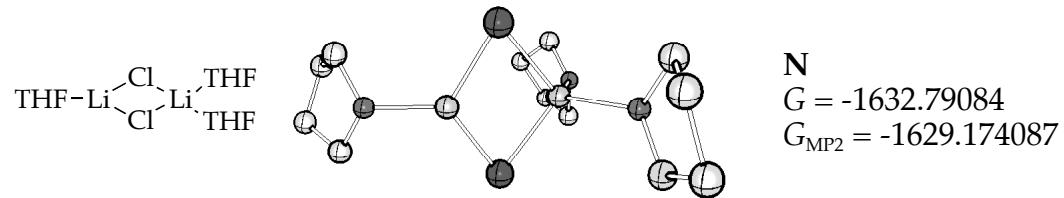
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.645970	-0.147008	-0.040343	H	-2.625812	-1.494039	-2.536674
Cl	-0.091724	0.105549	-1.764153	H	-3.570044	-2.349706	-1.286694
Li	1.683314	0.007390	-0.207878	H	-4.648472	-1.507463	-3.786670
Cl	1.131884	0.172049	2.018032	H	-5.649012	-1.752078	-2.352998
O	2.797808	-1.647805	-0.462347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

Table 8 (Continued).



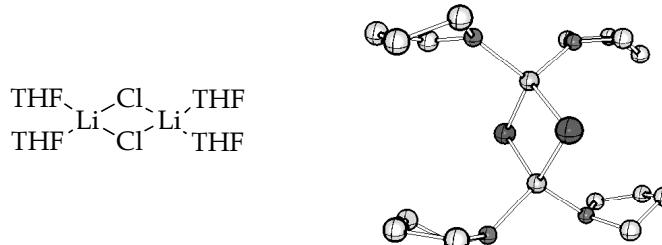
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.224110	0.056448	0.583724	H	-3.288569	1.815396	0.242365
Cl	-0.000071	1.876521	-0.000606	H	-4.147110	1.720238	-1.312896
Li	-1.224402	0.056560	-0.585074	O	3.114196	0.007075	0.737816
Cl	-0.000216	-1.771825	-0.000681	C	3.828251	-1.199145	0.369709
O	-3.114591	0.006934	-0.738054	C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

Table 8 (Continued).



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

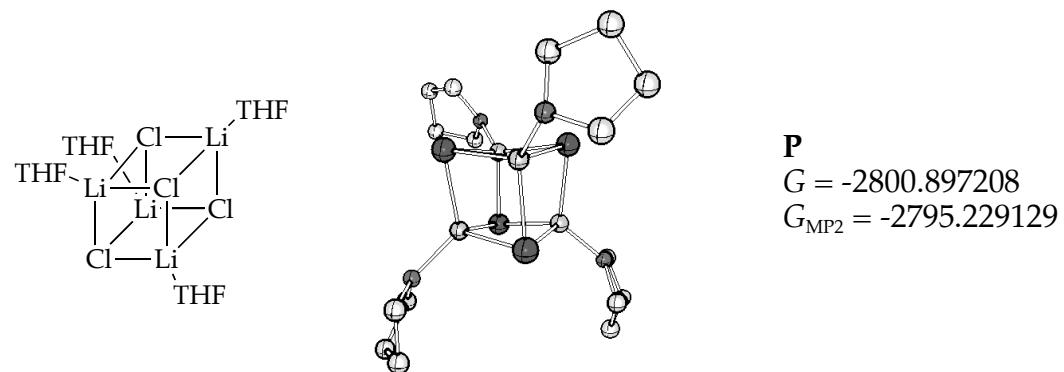
Table 8 (Continued).



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

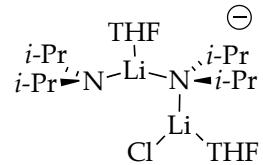
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.032551	-1.524063	0.022267	H	2.632291	3.481070	1.528251
Cl	0.079285	-0.094857	1.893780	H	2.302701	1.731682	1.694753
Li	-0.041459	1.384887	0.065541	O	-1.513441	-2.762613	0.060842
Cl	-0.100281	-0.046379	-1.805635	C	-2.066179	-3.166078	-1.204530
O	-1.659752	2.524905	0.169501	C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

Table 8 (Continued).



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

Table 8 (Continued).



30

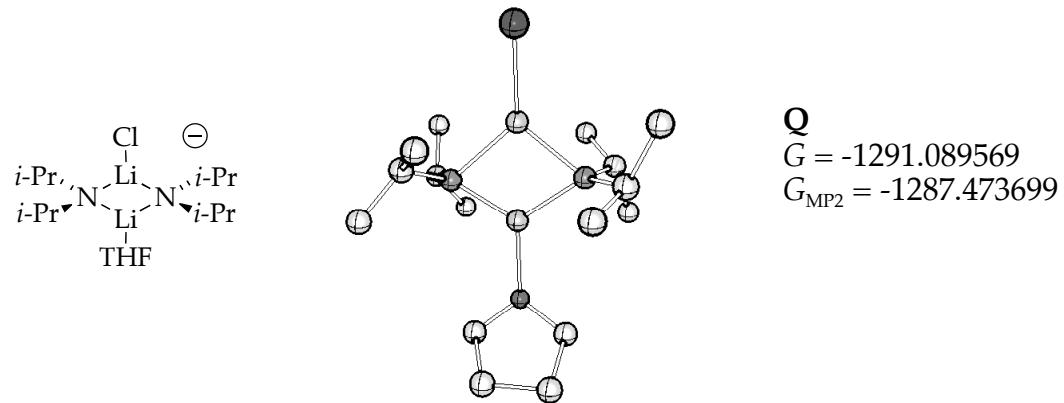
$G = -1523.430812$

$G_{MP2} = -1519.042557$

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

Table 8 (Continued).

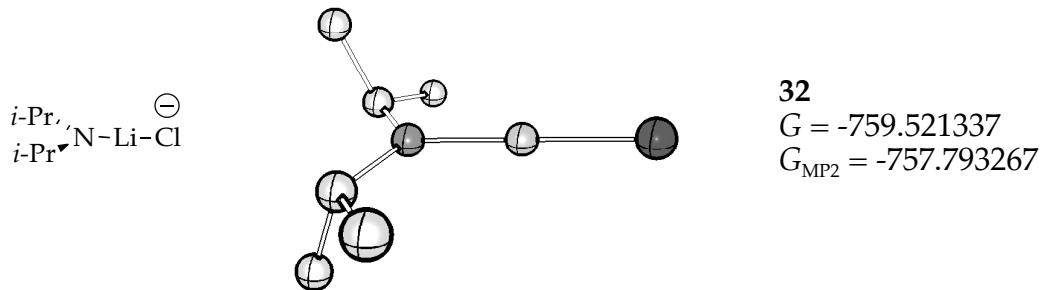
H	1.238809	-3.182141	-0.288835	H	-2.775198	1.472268	-1.035186
O	3.060628	-0.595886	-0.464355	Cl	-3.477198	-1.529859	-1.898789
C	3.855205	-1.762667	-0.261202				



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

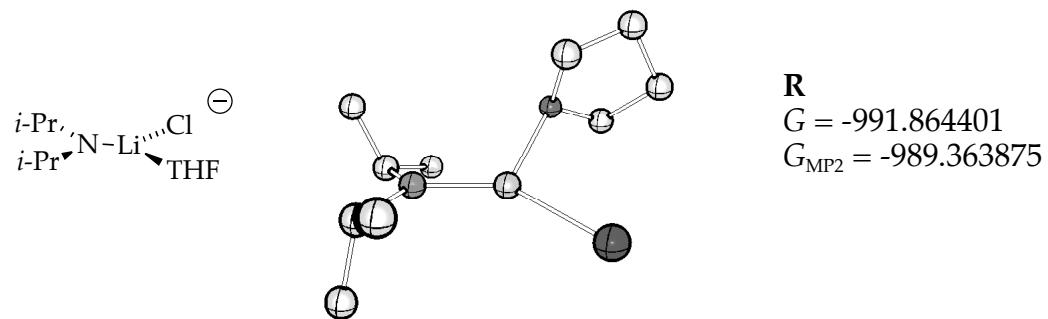
Table 8 (Continued).

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



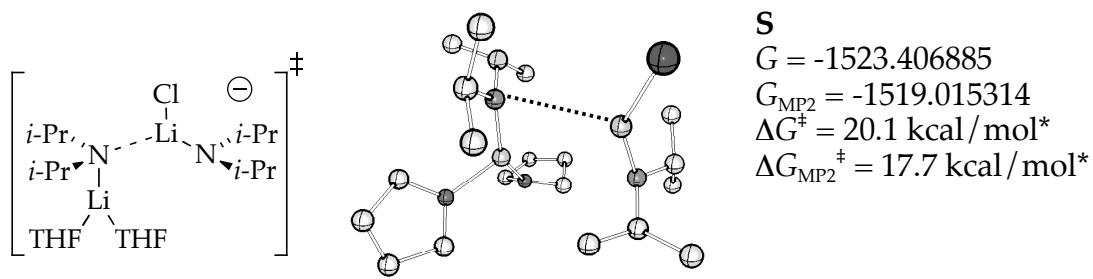
Atom	X	Y	Z	Atom	X	Y	Z
C	1.291509	1.197901	0.158166	H	-0.438698	-2.519497	-0.190255
N	0.500585	-0.000009	-0.000101	H	2.164322	-1.040352	-0.834253
Li	-1.380691	-0.000102	-0.000067	C	0.446290	2.306271	0.806056
Cl	-3.567016	-0.000282	-0.000042	H	0.095684	1.990739	1.795905
C	1.291932	-1.197657	-0.158029	H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

Table 8 (Continued).



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

Table 8 (Continued).

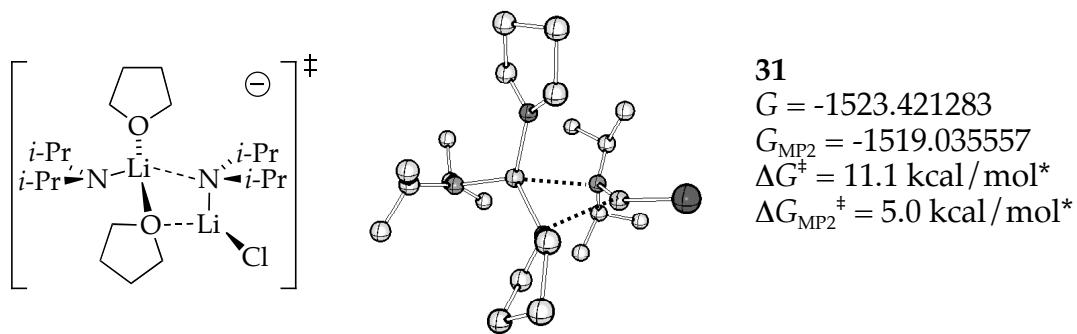


* Activation barrier is measured relative to the ground state energy of open disolvated triple ion xx.

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

Table 8 (Continued).

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



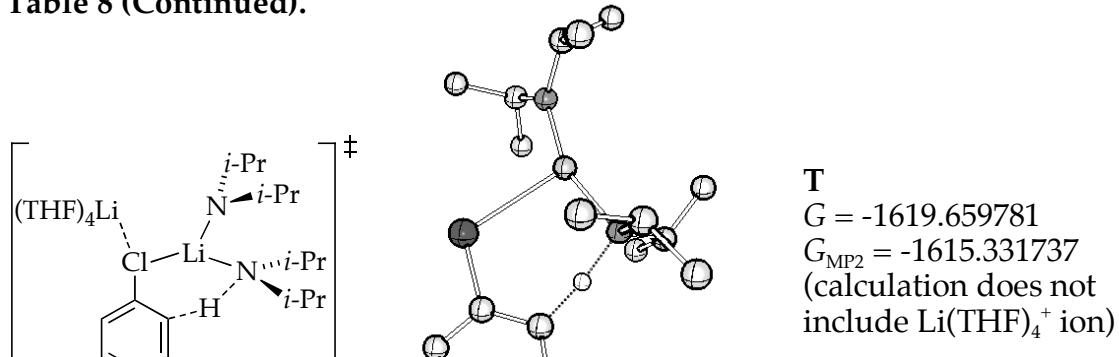
* Activation barrier is measured relative to the ground state energy of open disolvated triple ion xx.

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

Table 8 (Continued).

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

Table 8 (Continued).



T

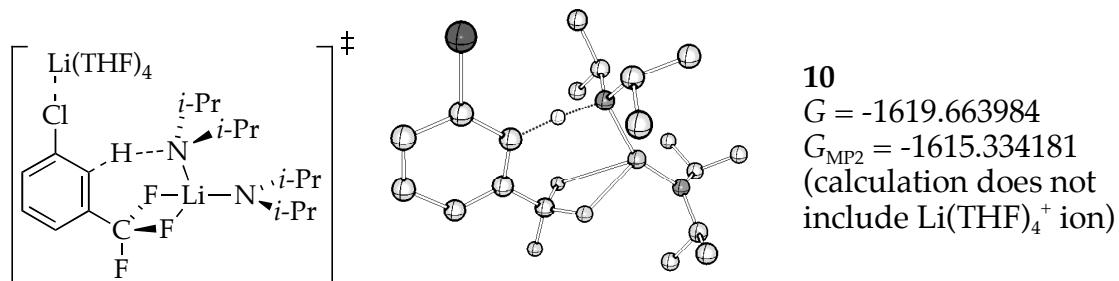
$$G = -1619.659781$$

$$G_{\text{MP2}} = -1615.331737$$

(calculation does not include $\text{Li}(\text{THF})_4^+$ ion)

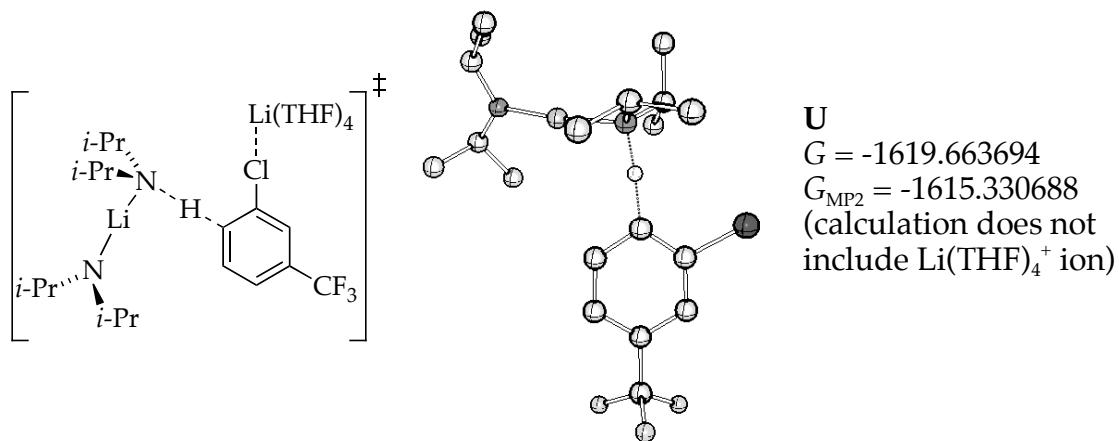
Atom	X	Y	Z	Atom	X	Y	Z
C	0.060727	-2.013382	1.167439	H	-0.915399	-0.443616	-2.495034
N	-0.036174	-1.226121	-0.071550	C	1.218349	-2.983723	-1.433805
Li	-1.707462	-0.067164	-0.020452	H	2.162376	-2.431522	-1.397084
N	-3.552859	0.327947	0.131311	H	1.238369	-3.731041	-0.632587
C	-4.095204	1.416629	0.918751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

Table 8 (Continued).



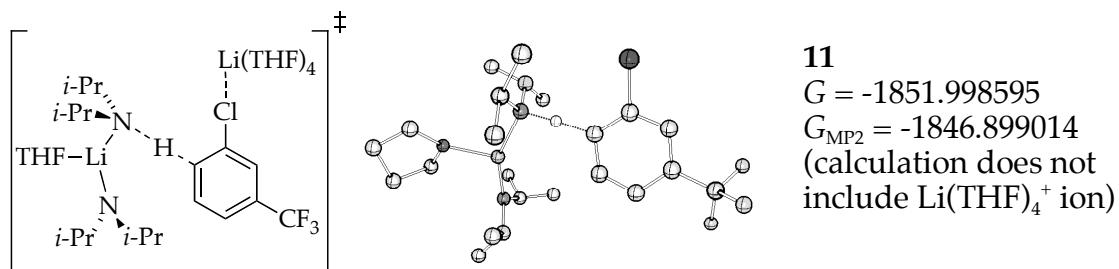
Atom	X	Y	Z	Atom	X	Y	Z
C	-0.623252	-2.109718	-0.480839	H	-0.364569	1.711072	3.401139
F	-0.458024	-3.452268	-0.551905	H	-1.054472	0.463649	2.343218
F	0.189831	-1.682943	0.535875	H	0.706325	0.632872	2.492852
Li	1.411741	0.170956	0.045232	C	0.924972	3.184480	1.465743
N	3.261093	-0.259004	0.112426	H	0.916098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

Table 8 (Continued).



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

Table 8 (Continued).



11
 $G = -1851.998595$
 $G_{MP2} = -1846.899014$
 (calculation does not include Li(THF)₄⁺ ion)

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

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