Anionic Snieckus-Fries Rearrangement:
Solvent Effects and Role of Mixed Aggregates

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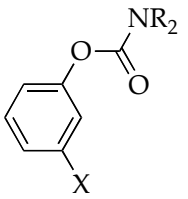
Supporting Information

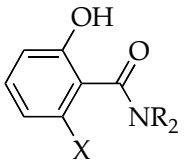
Part I: NMR Spectroscopic Studies

Part III: Computational Studies

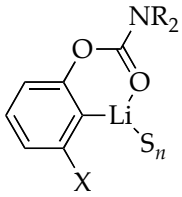
Chart 1



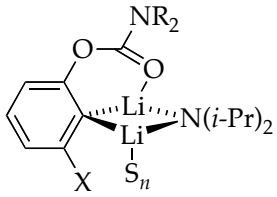
4a; R= Me, X = OMe
4b; R = Et, X = OMe
4c; R = *i*-Pr, X = OMe
4d; R = Me, X = F
4e; R= *i*-Pr, X= F



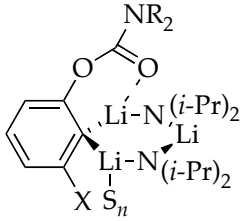
5a; R = Me, X = OMe
5b; R = Et, X = OMe
5c; R = Me, X = F



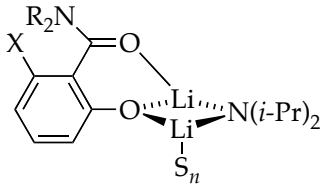
6a; S = THF, R = *i*-Pr, X = F
6b; S = HMPA, R = Et, X = OMe
6c; S = HMPA, R = *i*-Pr, X = OMe
6d; S = HMPA, R = Me, X = F
6e; S = HMPA, R = *i*-Pr, X = F
6f; S = DME, R = *i*-Pr, X = F
6g; S = η^2-TMCDA, R = Et, X = OMe



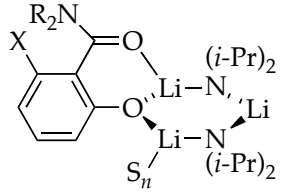
7a; S = THF, R = Me, X = F
7b; S = THF, R = *i*-Pr, X = F
7c; S = *n*-BuOMe, R = Me, X = F
7d; S = *n*-BuOMe, R = Et, X = OMe
7e; S = DME, R = Me, X = F
7f; S = DME, R= *i*-Pr, X= F
7g; S = η^1-TMEDA, R = *i*-Pr, X = OMe
7h; S = Me_2NEt, R = Et, X = OMe



8a; S = η^1-TMEDA, R = *i*-Pr, X = OMe
8b; S = Me_2NEt, R = Et, X = OMe



9a; S = THF, R = Me, X = F
9b; S = *n*-BuOMe, R = Et, X = OMe
9c; S = HMPA, R = Et, X = OMe
9d; S = HMPA, R = Me, X = F



10a; S = *n*-BuOMe, R = Et, X = OMe
10b; S = HMPA, R = Et, X = OMe
10c; S = DME, R = Me, X = F
10d; S = η^1-TMEDA, R = Me, X = OMe
10e; S = Me_2NEt, R = Et, X = OMe

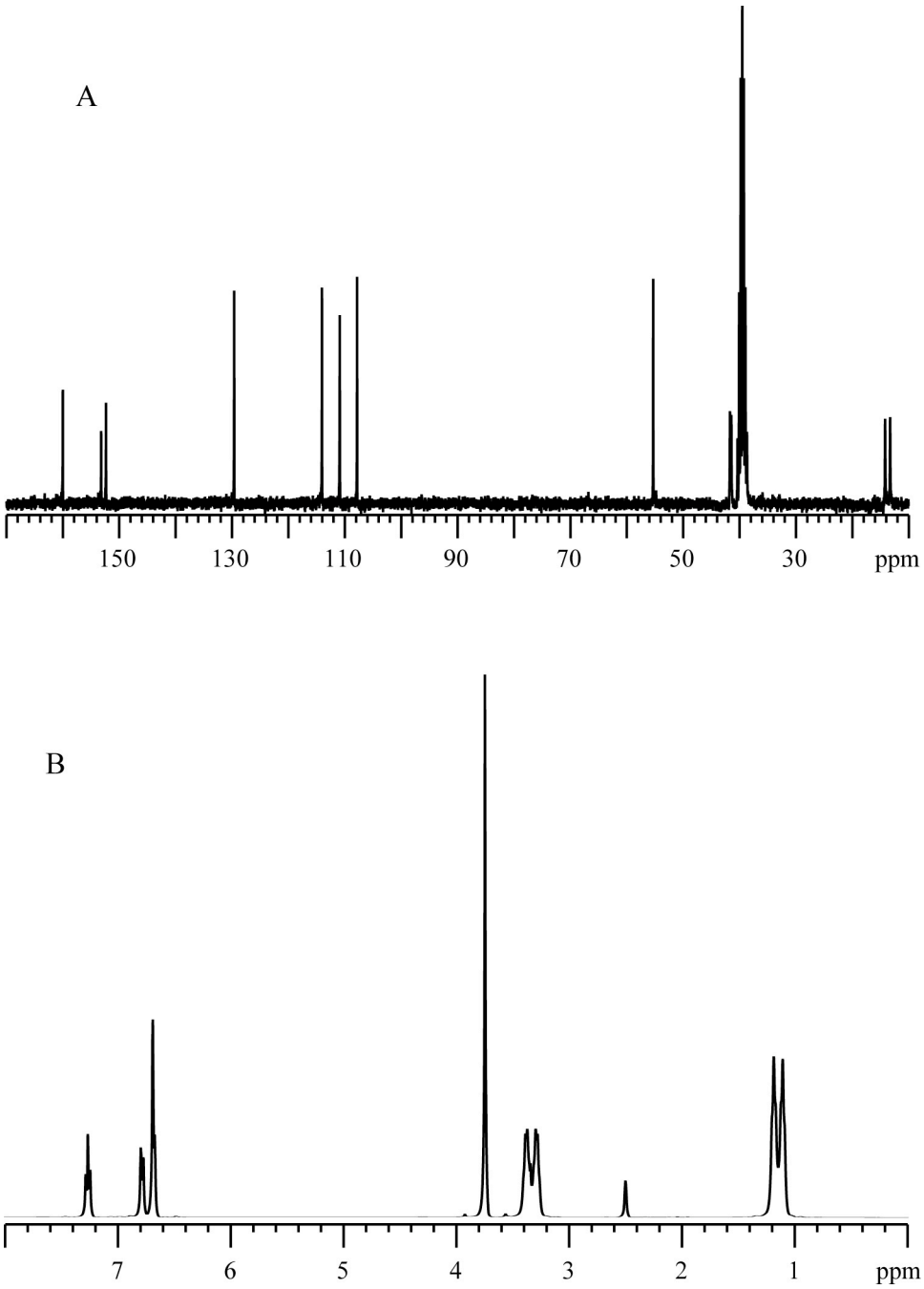


Figure 1. ^{13}C NMR and ^{1}H NMR spectra of **4b**. (A) ^{13}C NMR spectrum, 75 MHz, DMSO-d_6: δ 160.0, 153.2, 152.3, 129.6, 114.0, 110.9, 107.8, 55.3, 41.7, 41.5, 14.2, 13.3; (B) ^{1}H NMR spectrum, 400 MHz, DMSO-d_6: δ 7.28 (t, J = 7.7 Hz, 1H), 6.78 (d, J = 8.5 Hz, 1H), 6.69 (s, 1H), 6.68 (d, J = 7.1 Hz, 1H), 3.75 (s, 3H), 3.4-3.2 (m, 4H), 1.21 (t, J = 7.3 Hz, 3H), 1.11 (t, J = 6.7 Hz, 3H).

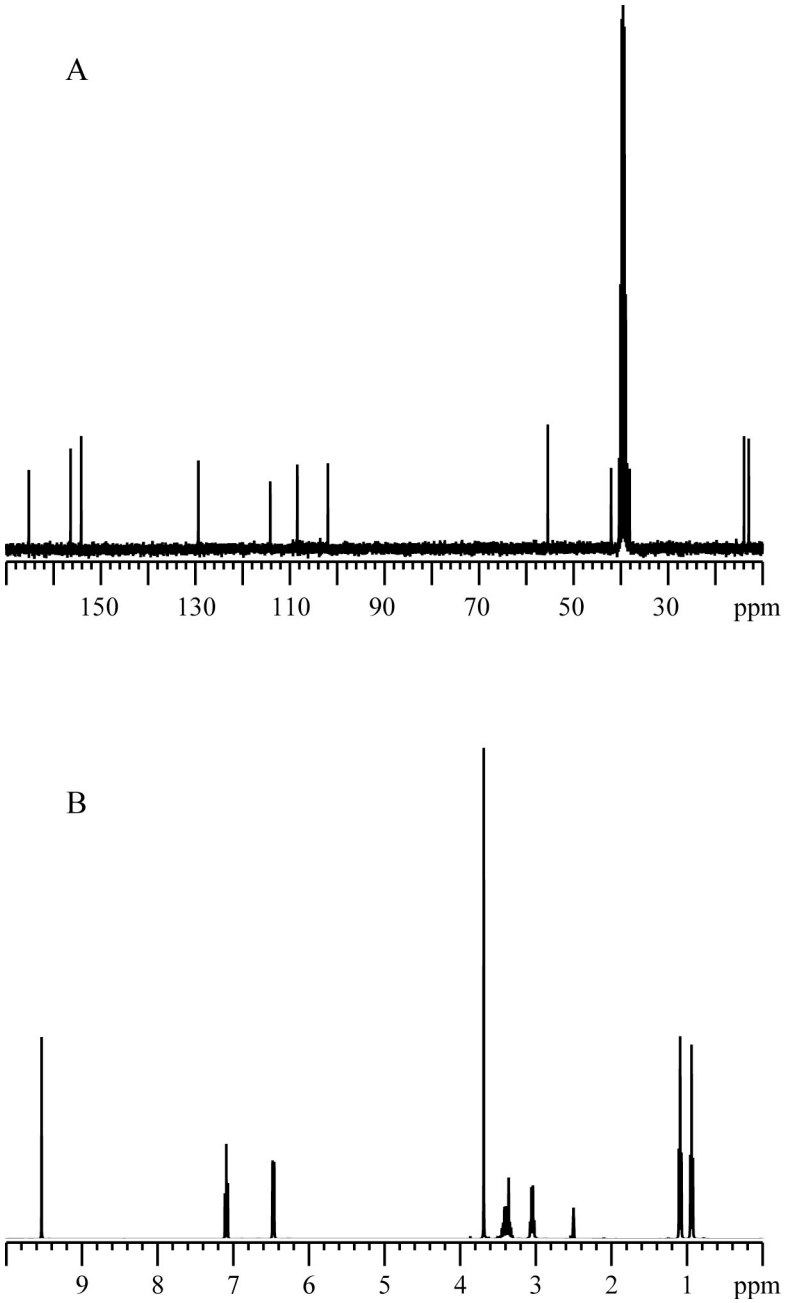


Figure 2. ^{13}C NMR and ^{1}H NMR spectra of **5b**. (A) ^{13}C NMR spectrum, 75 MHz, DMSO-d_6: δ 165.2, 156.4, 154.2, 129.4, 114.2, 108.4, 102.0, 55.4, 42.1, 38.1, 13.9, 12.9; (B) ^{1}H NMR spectrum, 400 MHz, DMSO-d_6: δ 9.53 (s, 1H), 7.09 (t, J = 8.2 Hz, 1H), 6.48 (d, J = 8.3 Hz, 1H), 6.47 (d, J = 8.1 Hz, 1H), 3.69 (s, 3H), 3.38 (10-m, 2H), 3.05 (q, J = 6.5 Hz, 2H), 1.09 (t, J = 6.8 Hz, 3H), 0.94 (t, J = 6.3 Hz, 3H).

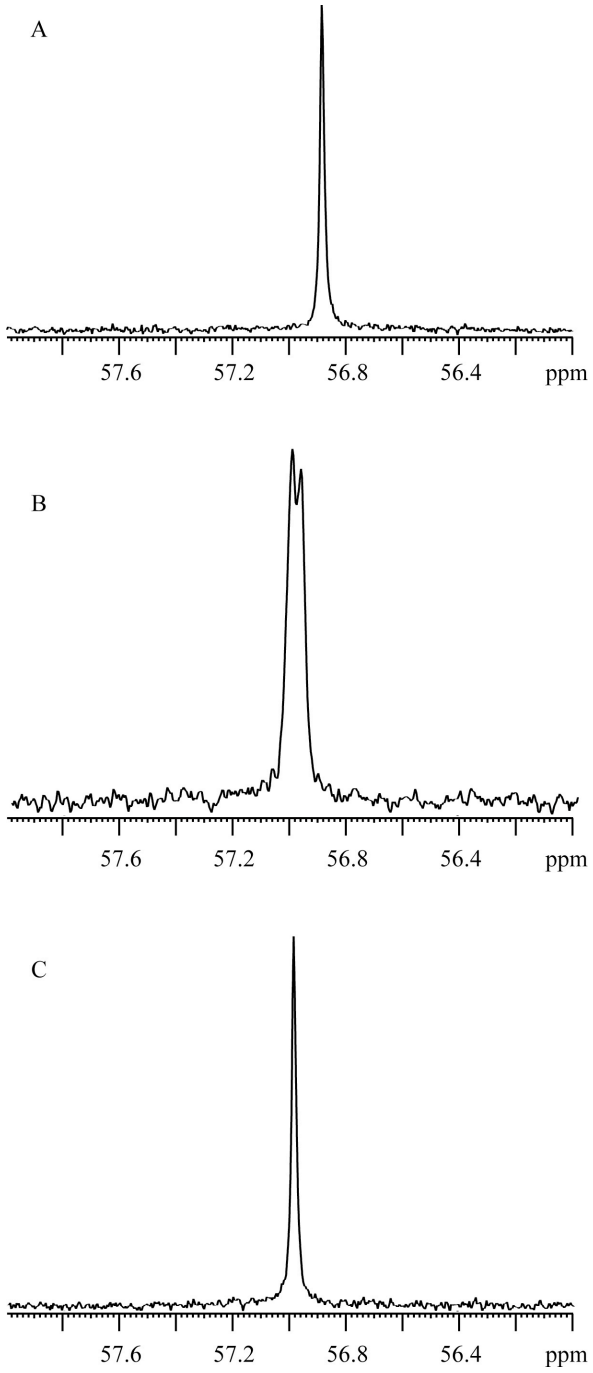


Figure 3. ^{13}C NMR spectra at 75 MHz of 0.21 M (+)-taddol in toluene-d_8 and (A) 0.10 M *R,R*-1,2-cyclohexanediamine; (B) 0.05 M *R,R*-1,2-cyclohexanediamine and 0.05 M *S,S*-1,2-cyclohexanediamine; (C) 0.10 M *S,S*-1,2-cyclohexanediamine.

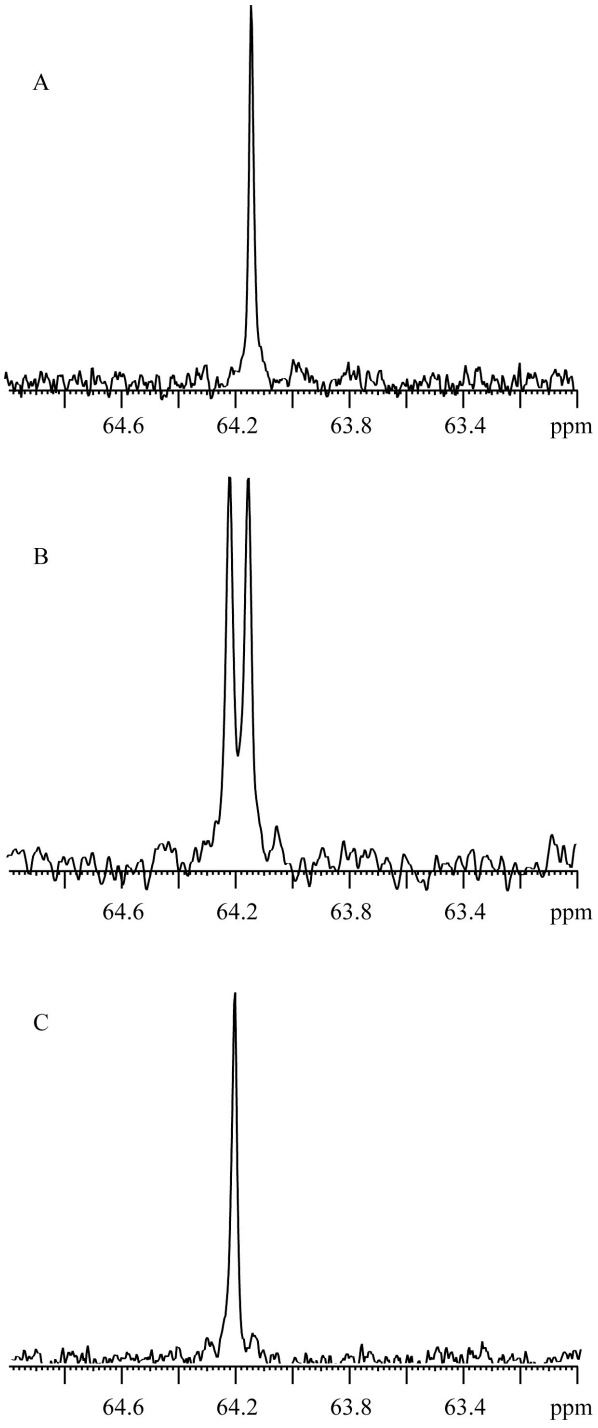


Figure 4. ^{13}C NMR spectra at 75 MHz of 0.21 M (+)-taddol in toluene-d_8 and (A) 0.10 M *R,R*-TMCDA; (B) 0.05 M *R,R*-TMCDA and 0.05 M *S,S*-TMCDA; (C) 0.10 M *S,S*-TMCDA.

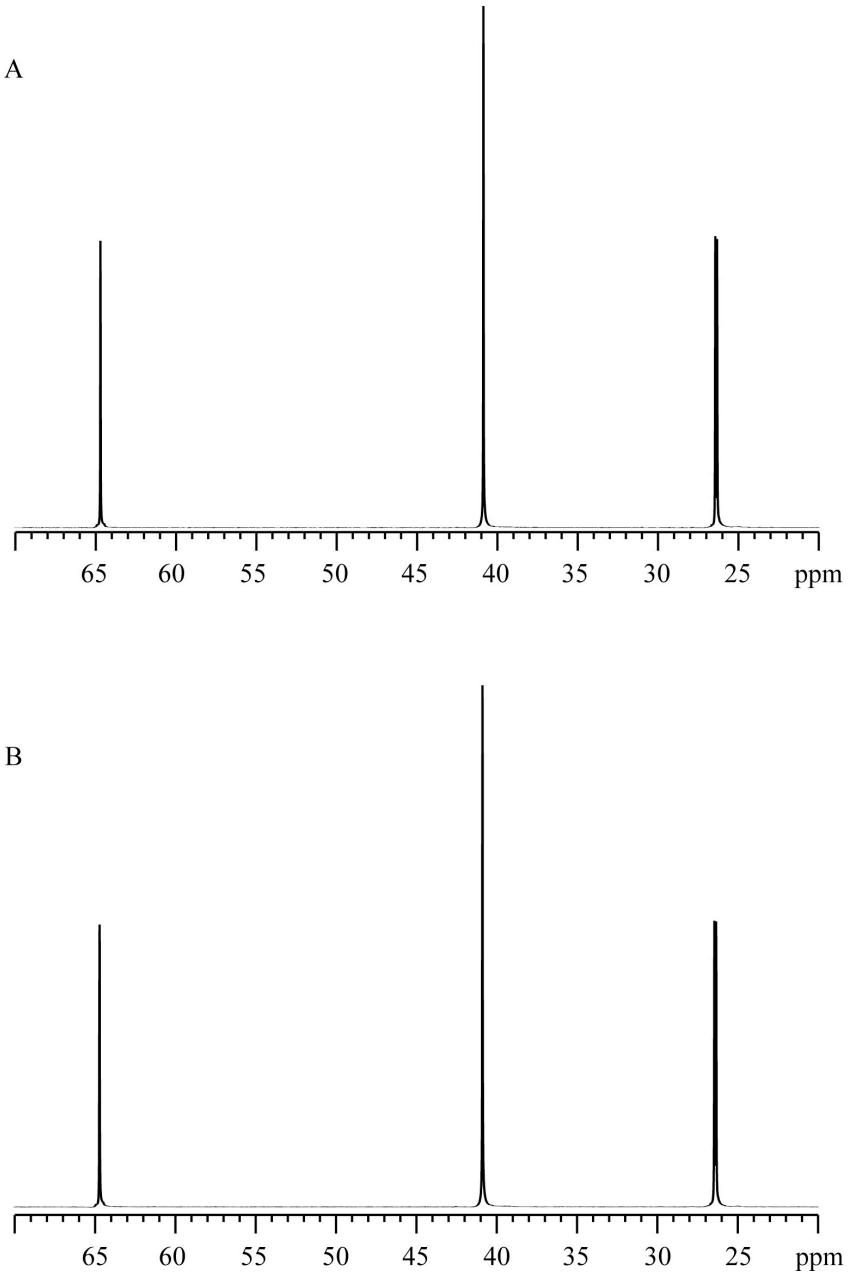


Figure 5. ^{13}C NMR spectra at 75 MHz of (A) neat *R,R*-TMCDA; (B) neat *S,S*-TMCDA.

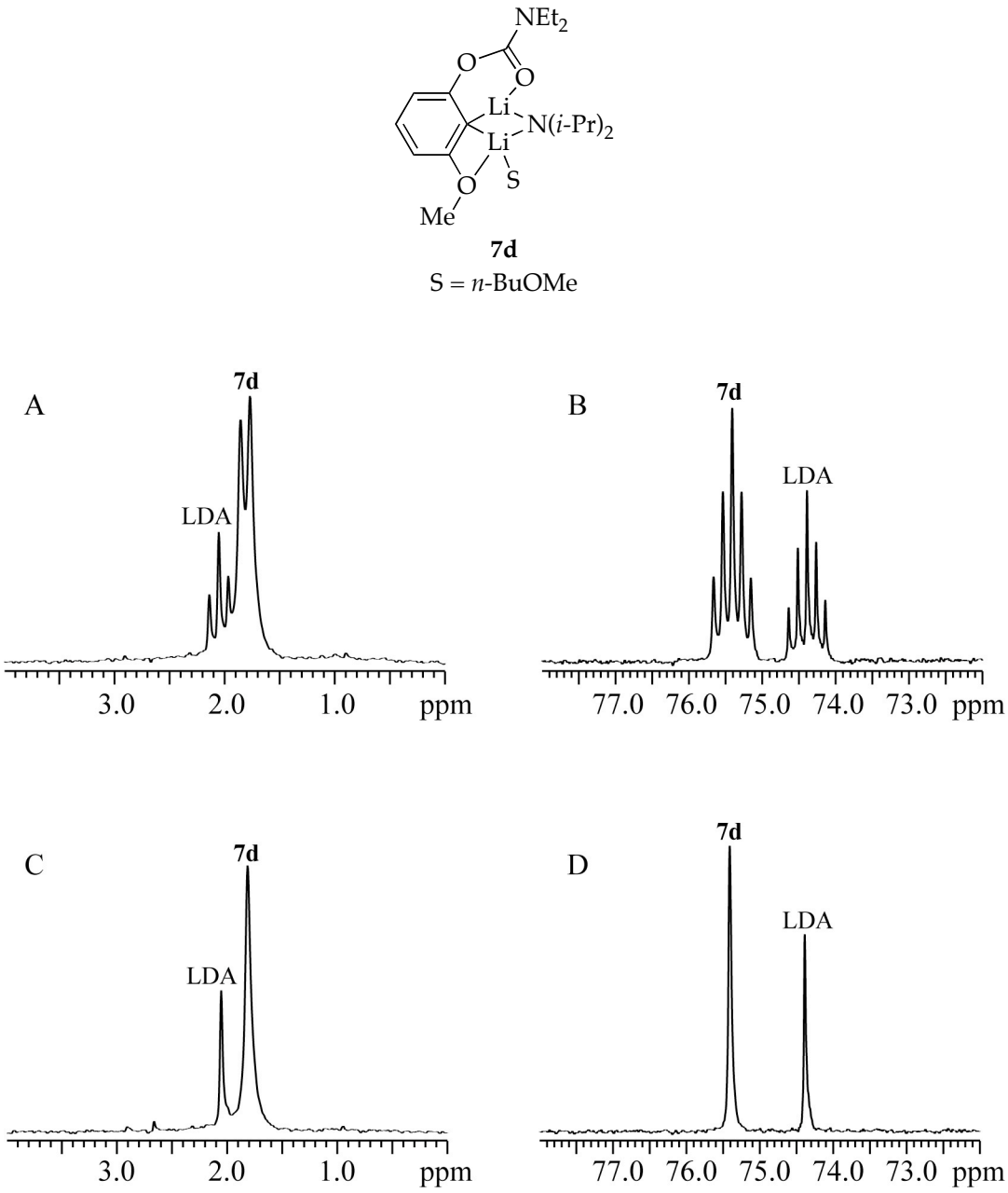


Figure 6. ^{6}Li and ^{15}N NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4b** in 1.0 M *n*-BuOMe/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

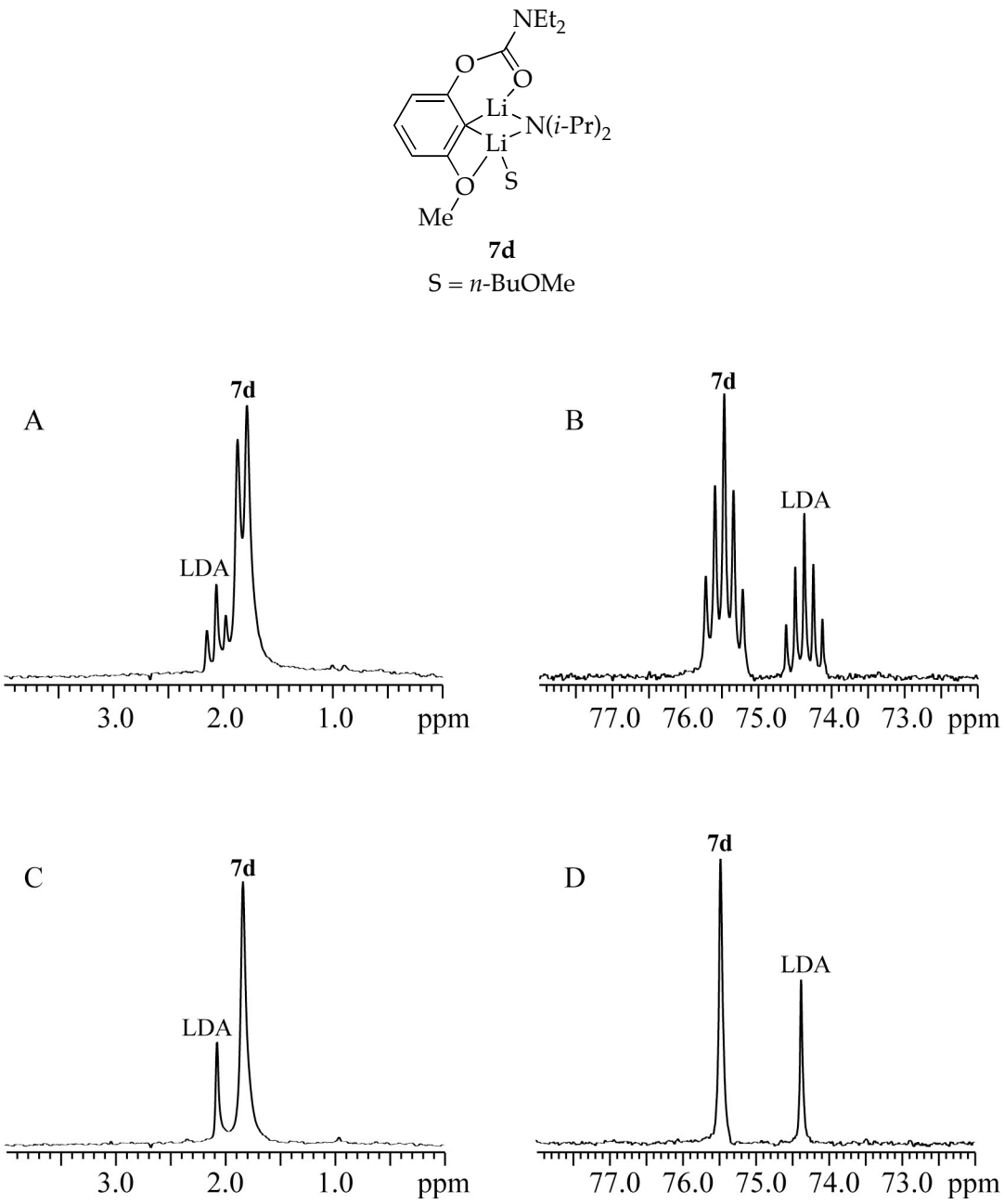


Figure 7. ^{6}Li and ^{15}N NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4b** in 4.0 M *n*-BuOMe/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

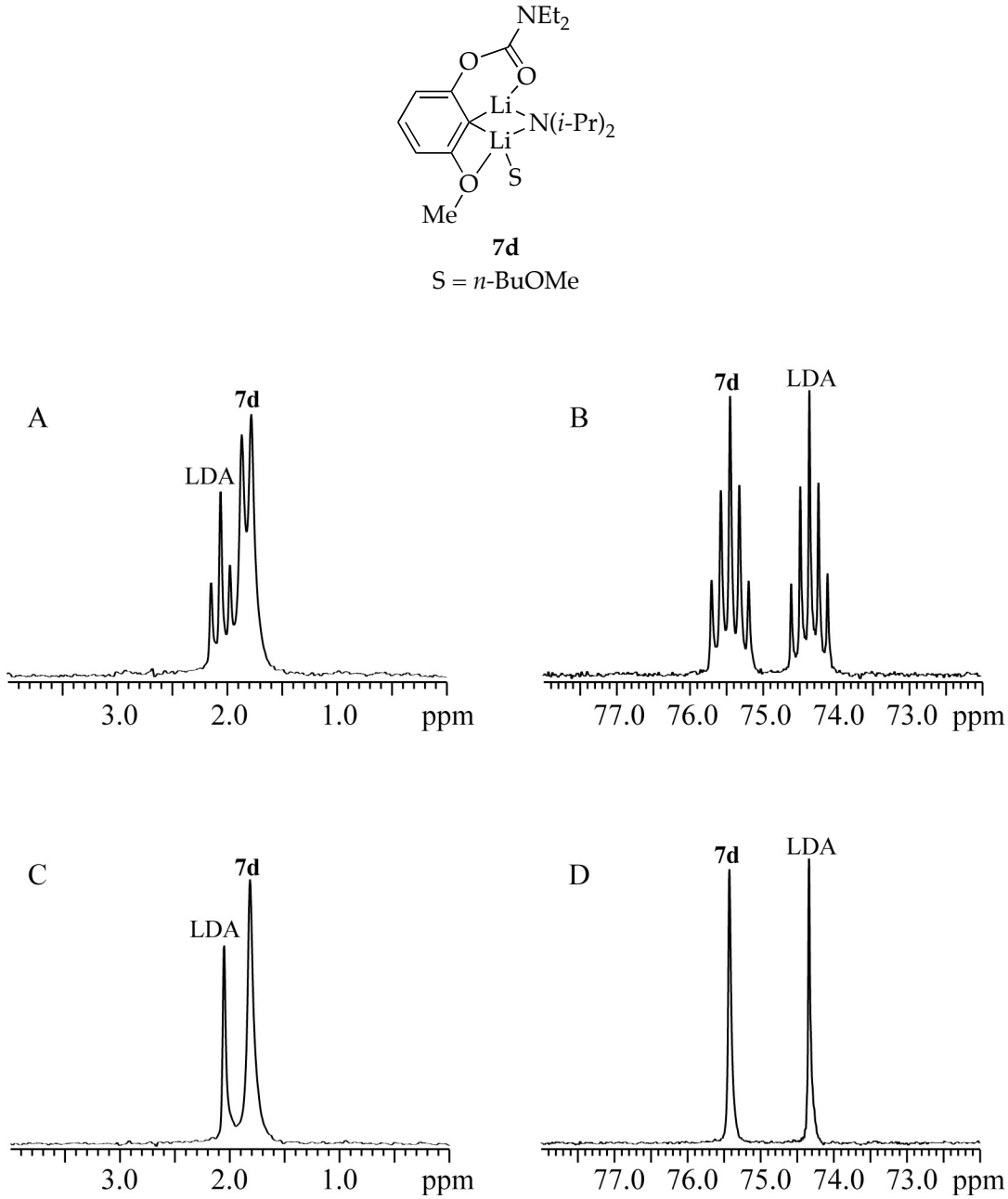


Figure 8. ^{6}Li and ^{15}N NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4b** in 7.0 M *n*-BuOMe/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

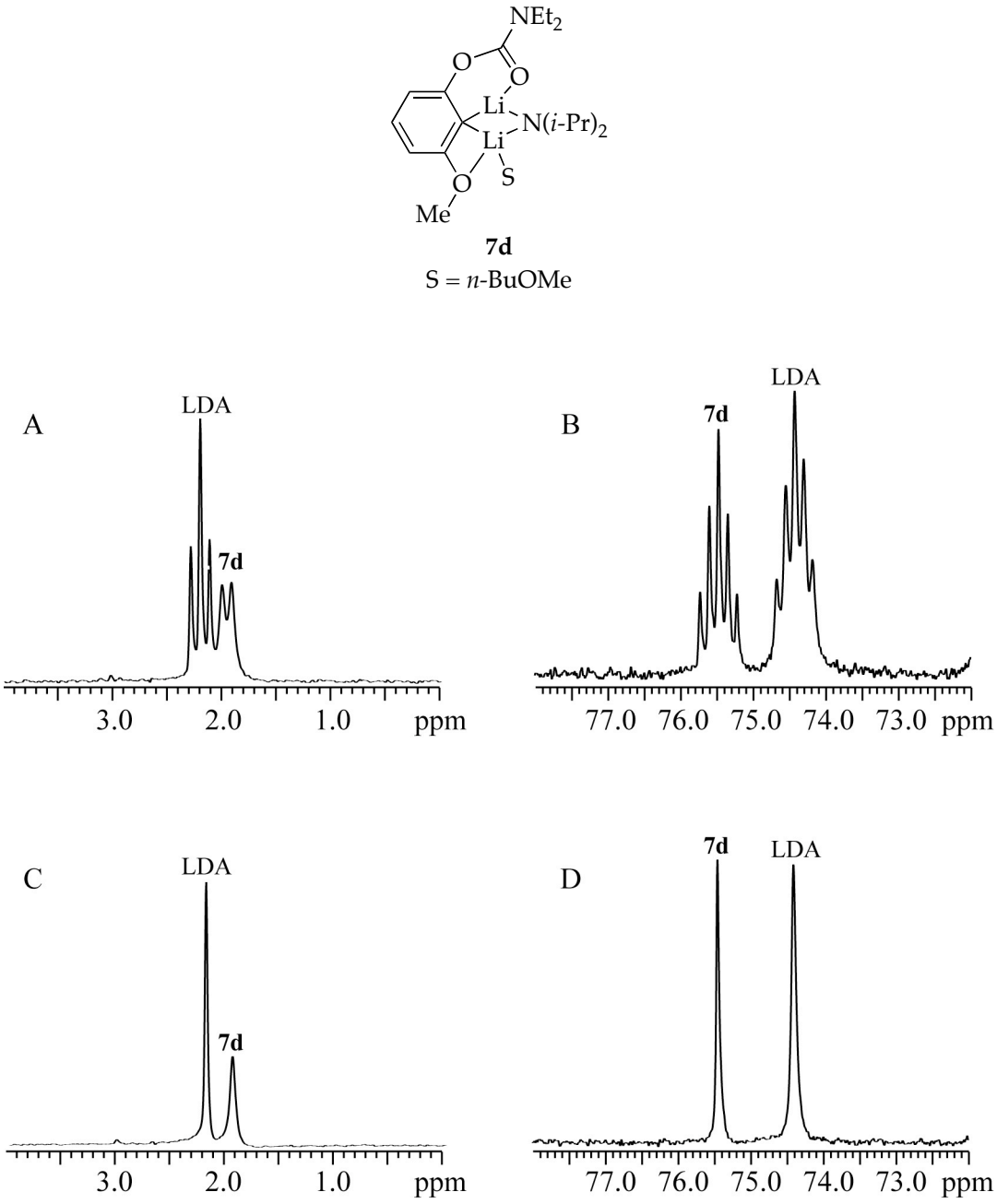
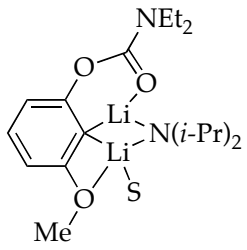


Figure 9. ^{6}Li and ^{15}N NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.20 equiv **4b** in 7.0 M *n*-BuOMe/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



7d

S = *n*-BuOMe

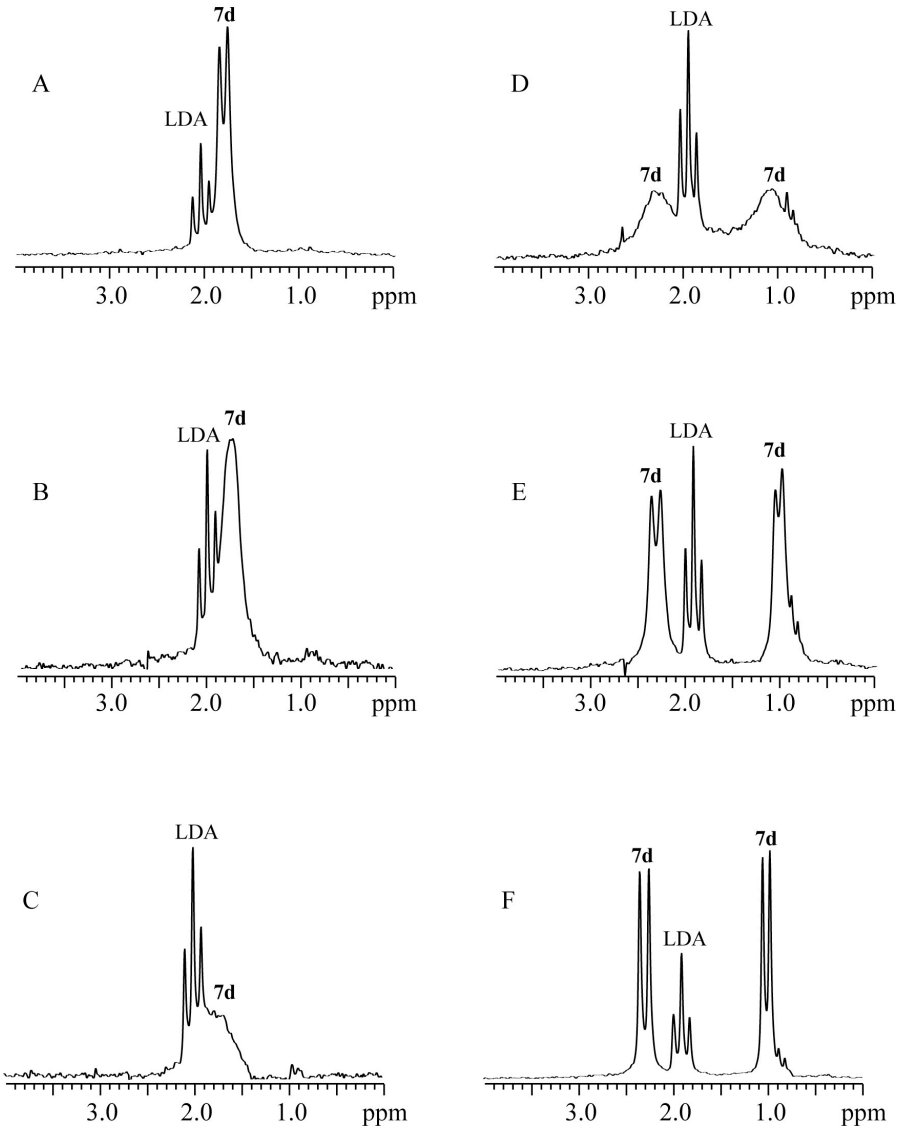


Figure 10. ^{6}Li NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4b** in 4.0 M *n*-BuOMe/pentane at various temperatures: (A) -70 °C; (B) -80 °C; (C) -90 °C; (D) -100 °C; (E) -110 °C; (F) -120 °C.

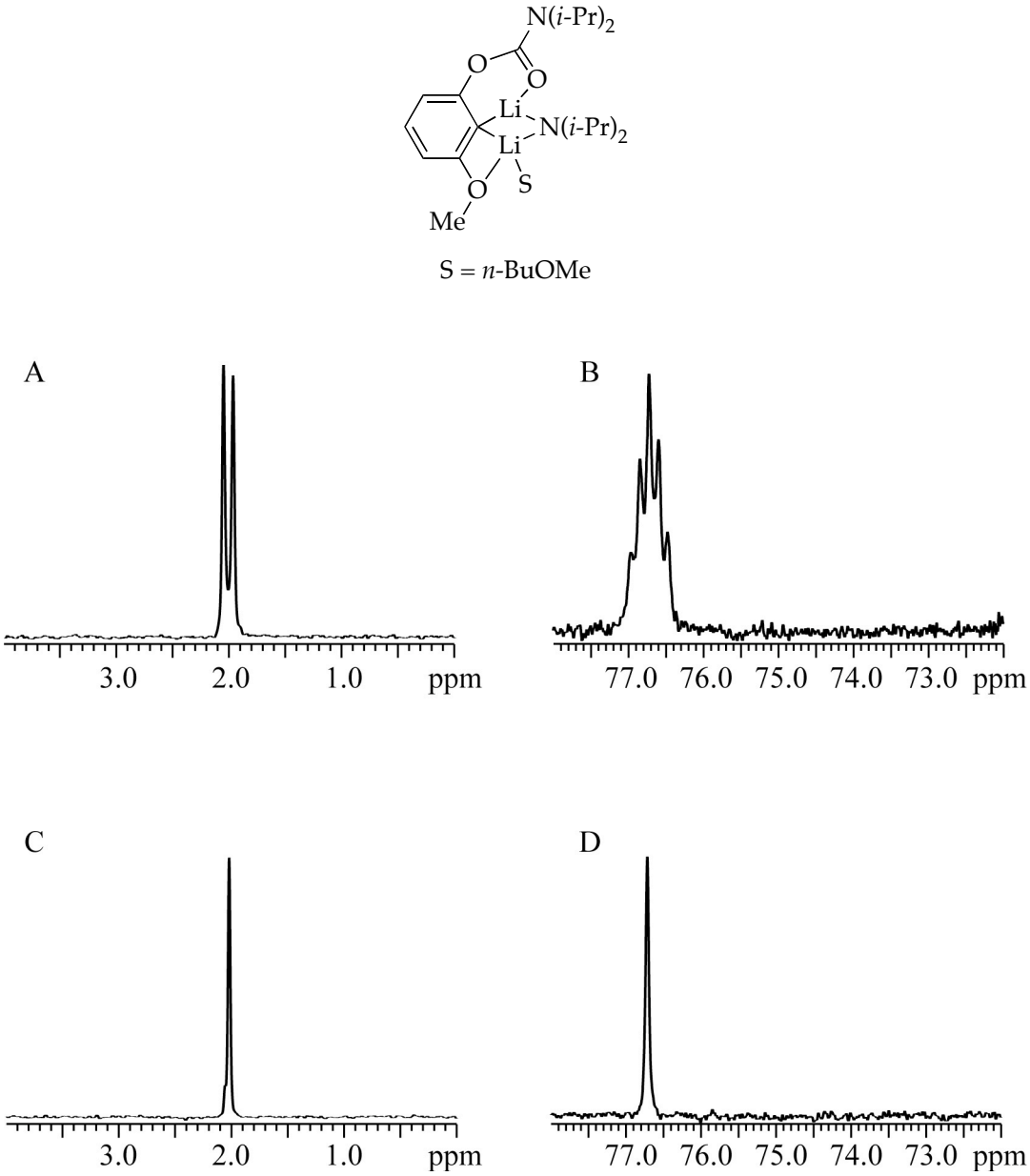


Figure 11. ^{6}Li and ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 1.0 equiv **4c** in 5.6 M *n*-BuOMe/pentane at -30 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

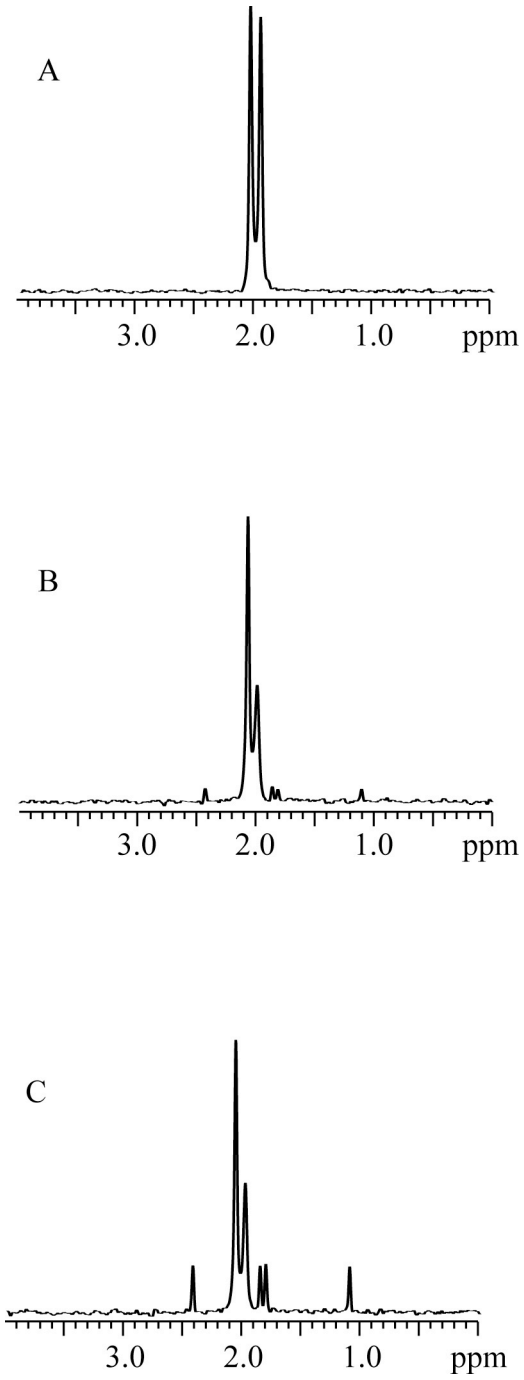


Figure 12. ^{6}Li spectra of 0.10 M [^{6}Li,^{15}N]LDA and with 1.0 equiv **4c** in 5.6 M *n*-BuOMe/pentane (A) at -30 °C; (B) at -30 °C after 1 minute of aging at -10 °C; (C) at -30 °C after 15 minutes of aging at -10 °C.

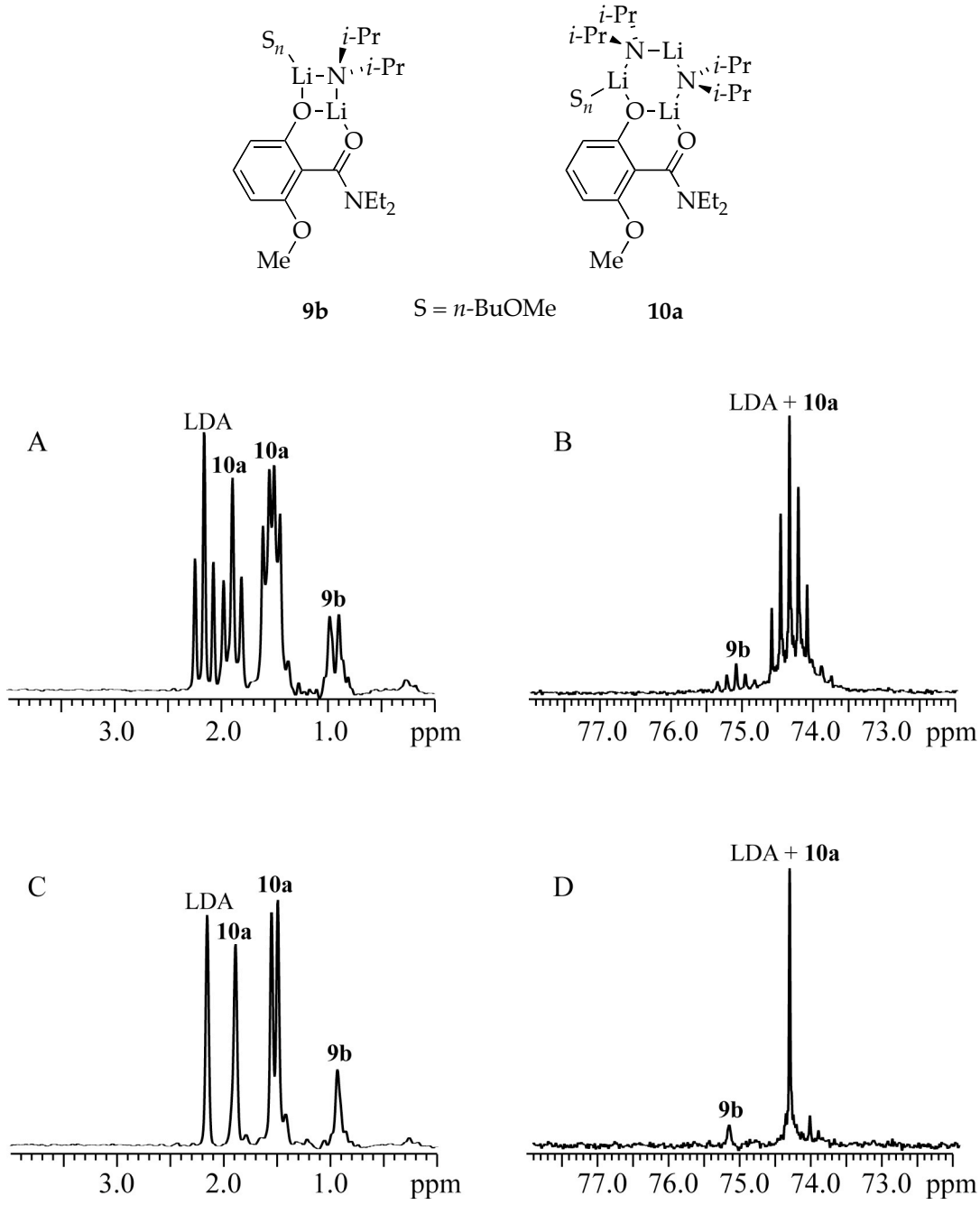


Figure 13. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4b** in 5.6 M *n*-BuOMe/pentane at -90 °C after aging at 0 °C for 2 hr: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

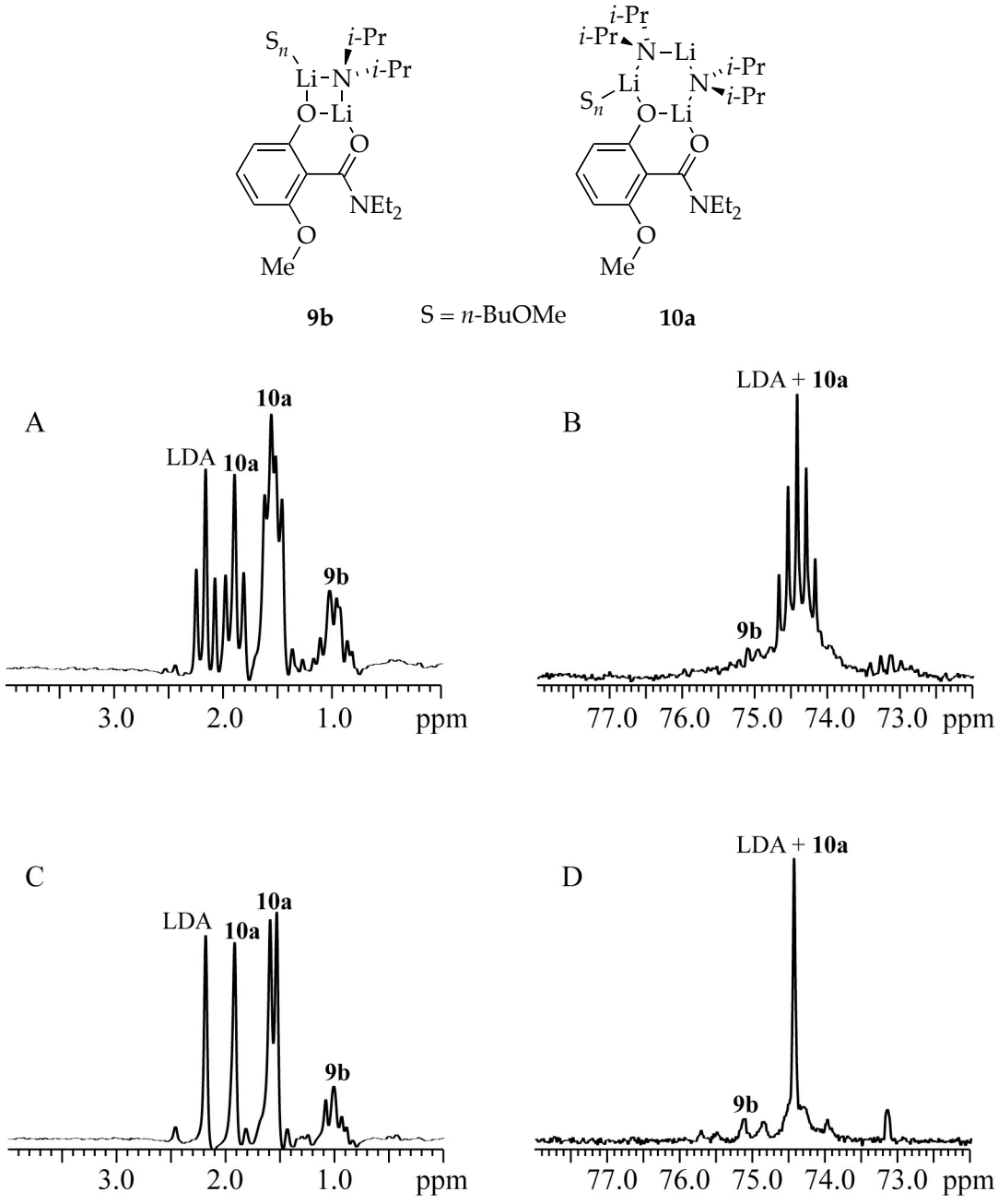


Figure 14. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **5b** in 5.6 M *n*-BuOMe/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

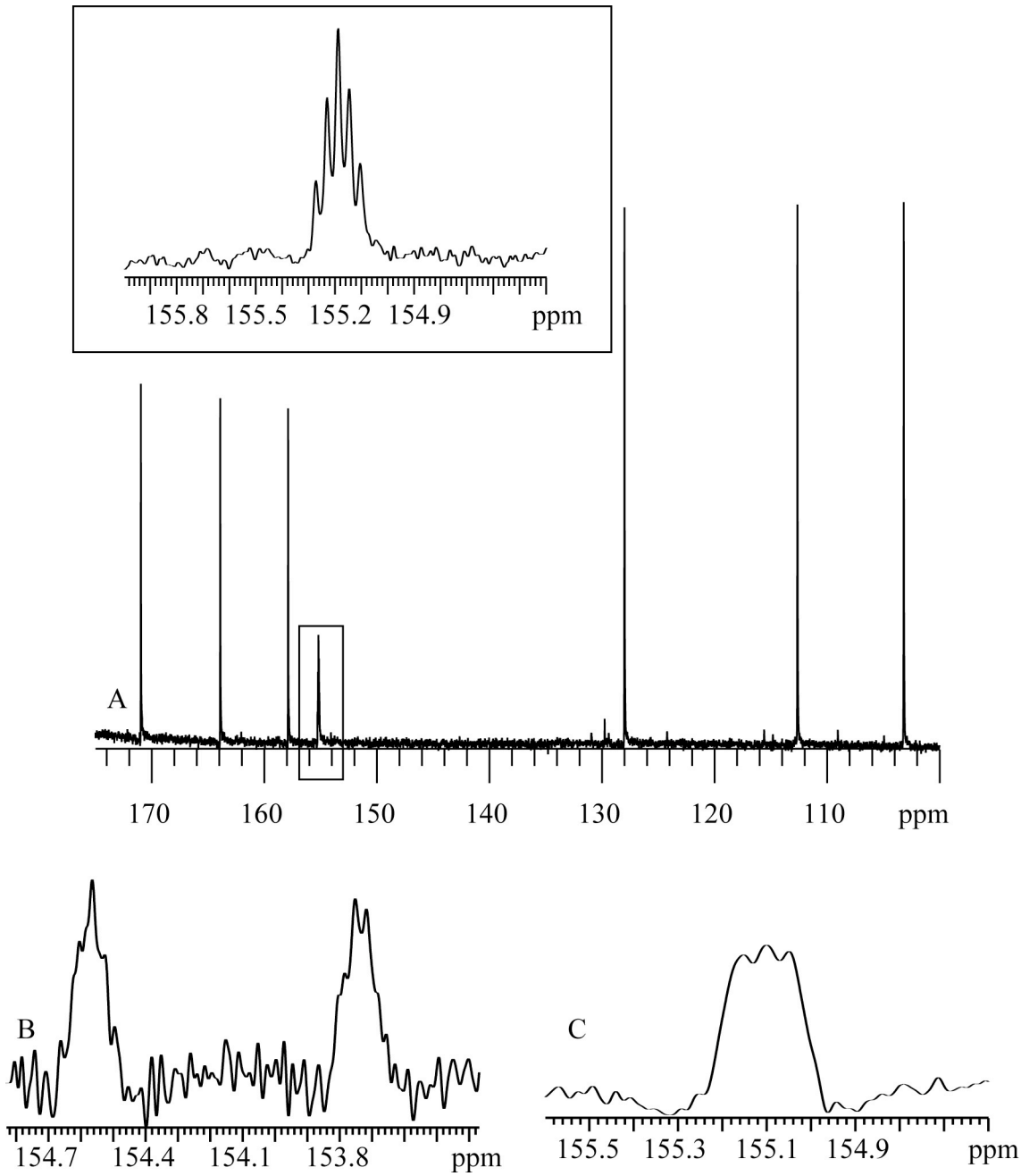


Figure 15. ^{13}C NMR spectra of: (A) 0.35 M [^{6}Li]LDA and with 0.30 equiv **4b** in 5.6 M *n*-BuOMe/pentane at -70 °C. Inset shows $^{1}J_{CLi} = 5.7$ Hz; (B) 0.80 M [^{6}Li,^{15}N]LDA and with 0.30 equiv **4e** in 2.0 M DME/pentane/toluene-d_8 at -90 °C. $^{2}J_{CF} = 123.1$ Hz, $^{1}J_{CLi} = 5.9$ Hz; (C) 0.80 M [^{6}Li,^{15}N]LDA and with 0.30 equiv **4b** in 0.5 M *R,R*-TMCDA/toluene-d_8 at -80 °C. $^{1}J_{CLi} = 7.7$ Hz.

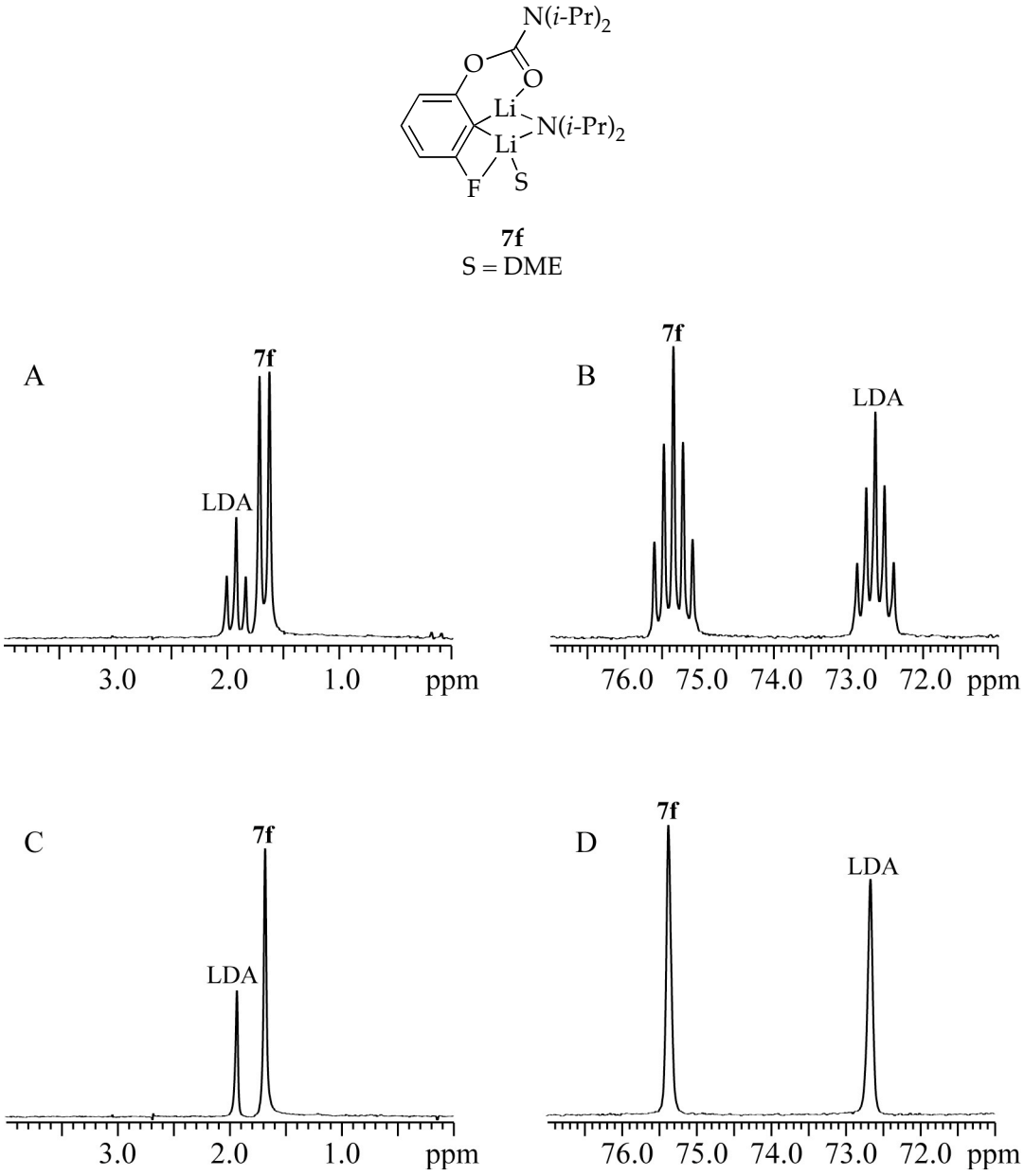
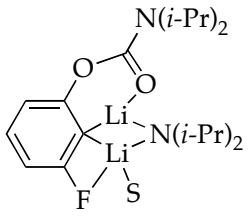


Figure 16. ^{6}Li and ^{15}N NMR spectra of 0.25 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4e** in 2.0 M DME/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



7f
S = DME

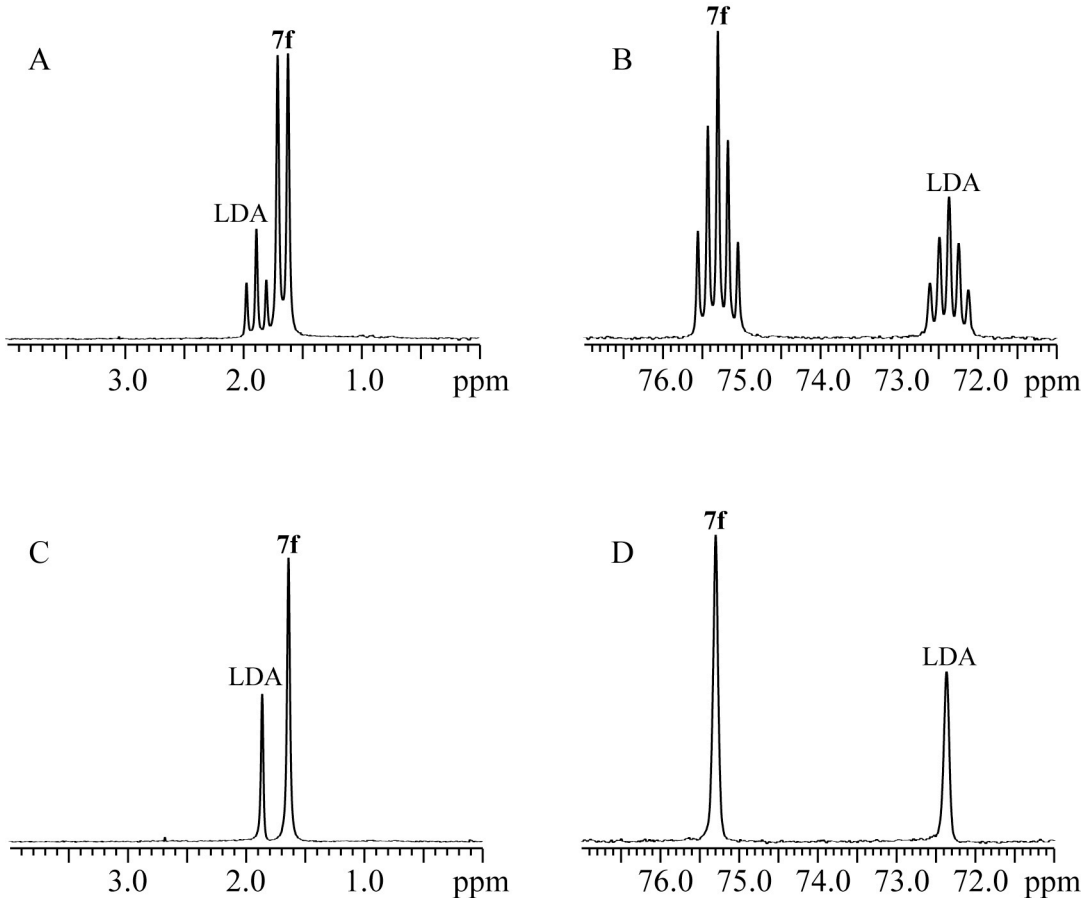
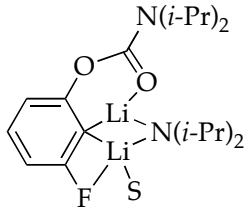


Figure 17. ^{6}Li and ^{15}N NMR spectra of 0.25 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4e** in 5.0 M DME/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



7f
S = DME

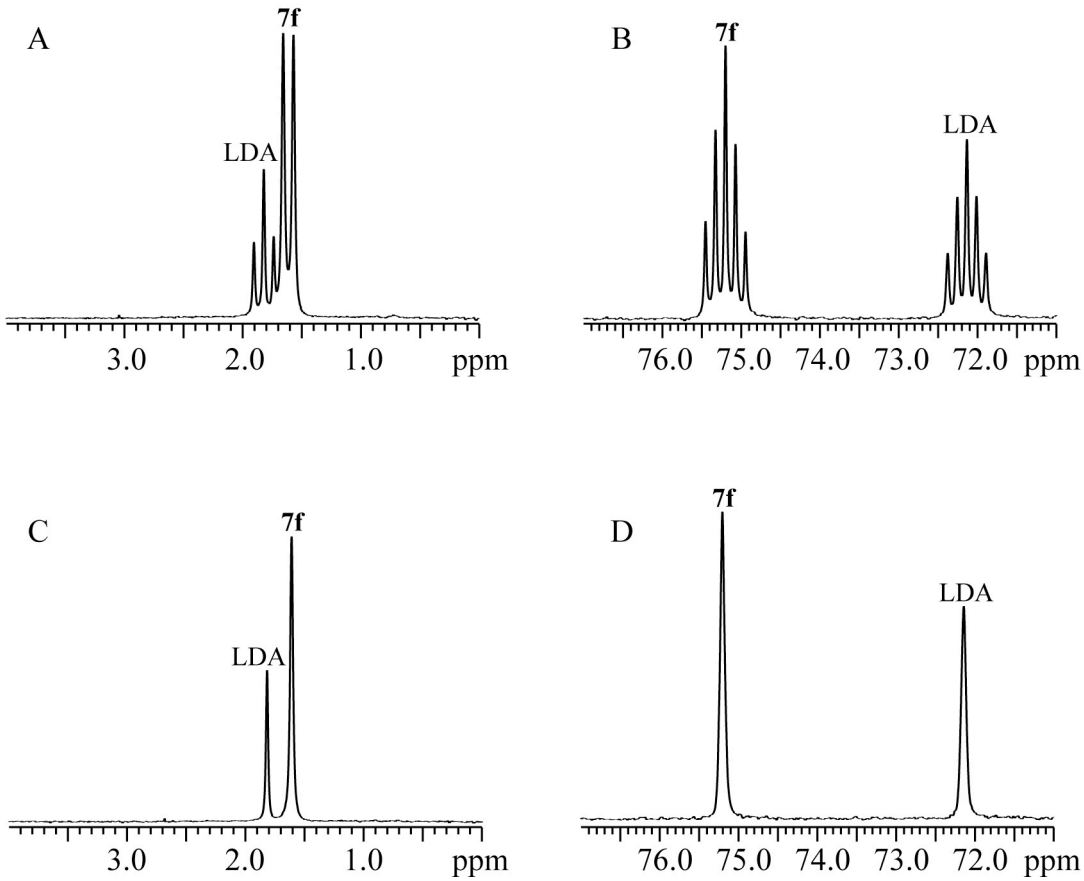
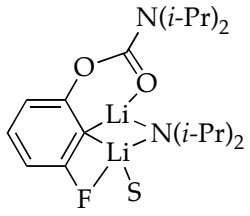


Figure 18. ^{6}Li and ^{15}N NMR spectra of 0.25 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4e** in 8.0 M DME/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



7f
S = DME

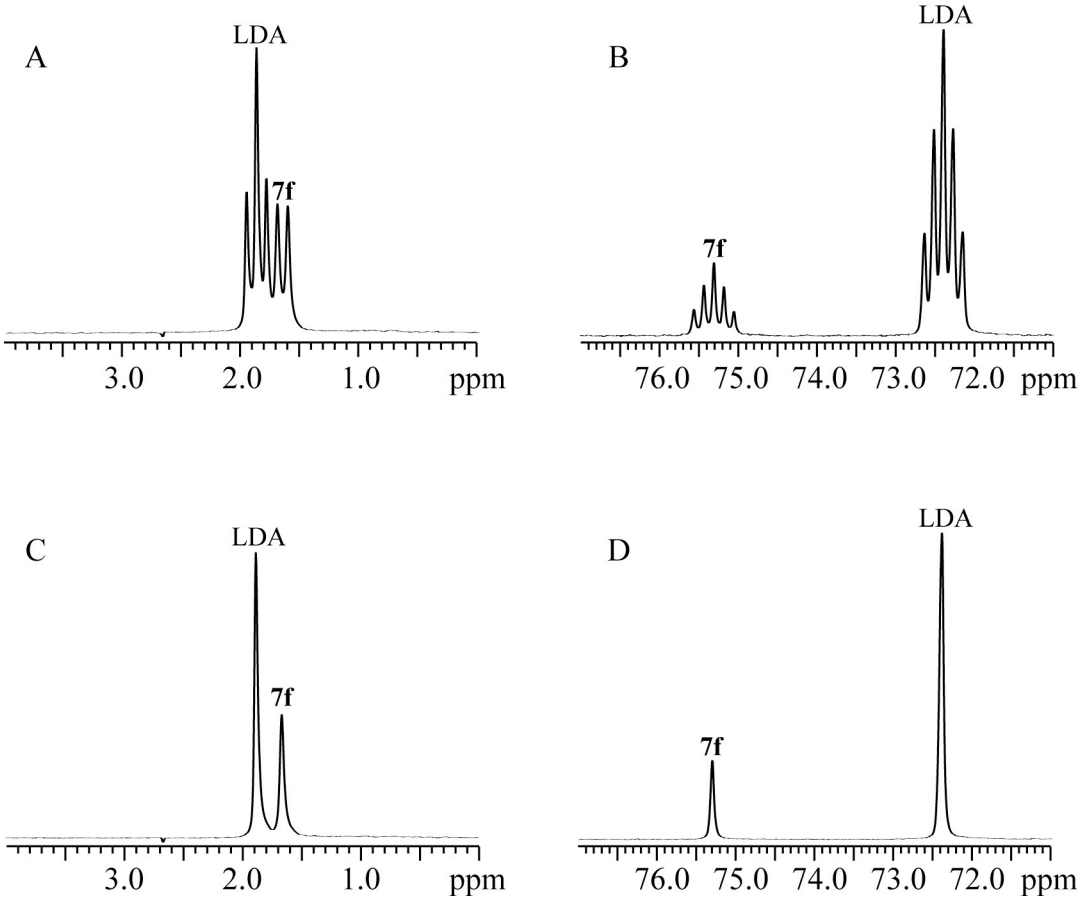
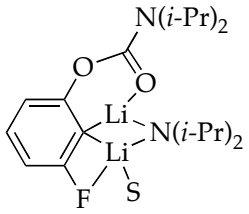


Figure 19. ^{6}Li and ^{15}N NMR spectra of 0.35 M [^{6}Li,^{15}N]LDA with 0.30 equiv **4e** in 5.0 M DME/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



7f
S = DME

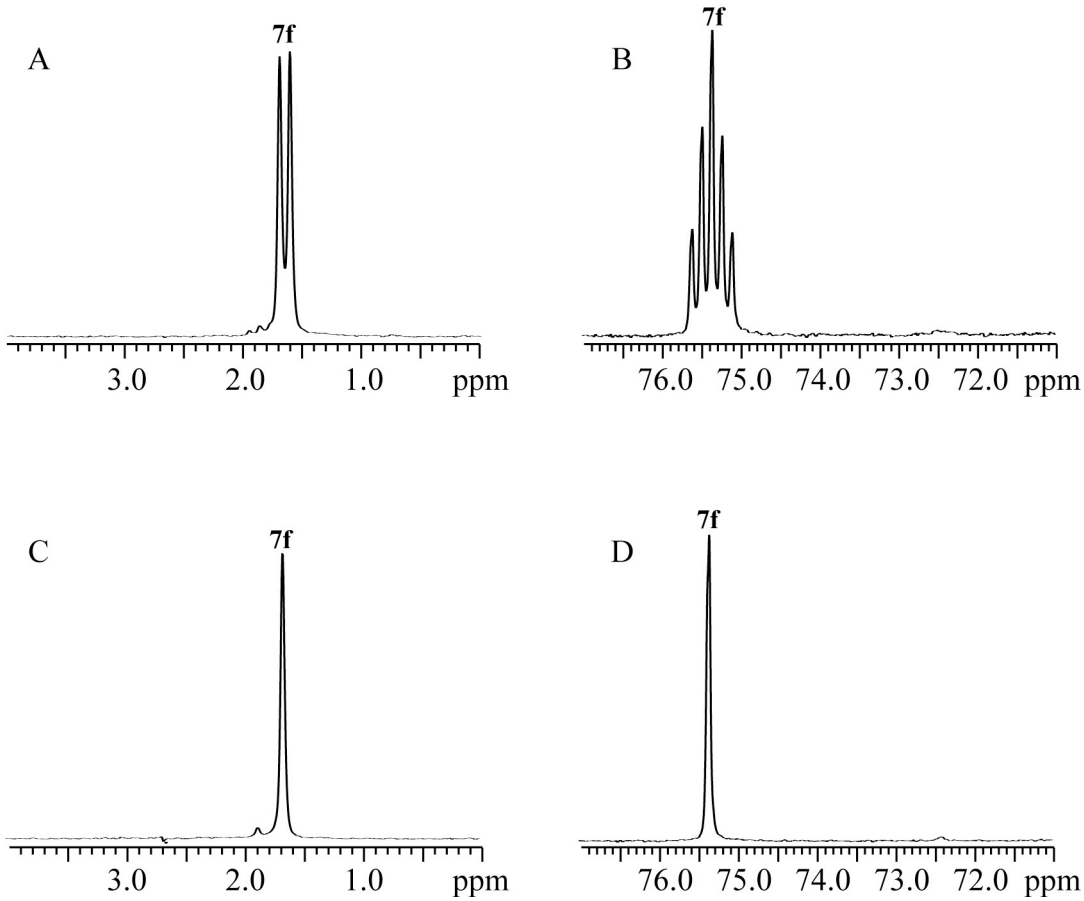
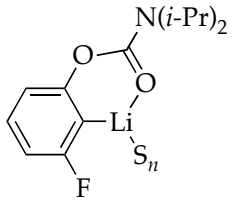


Figure 20. ^{6}Li and ^{15}N NMR spectra of 0.20 M [^{6}Li,^{15}N]LDA with 0.50 equiv **4e** in 5.0 M DME/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



6f
S = DME

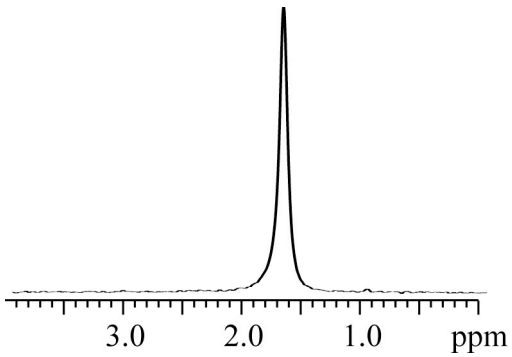


Figure 21. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]LDA with 1.0 equiv **4e** in 6.4 M DME/pentane at -90 °C.

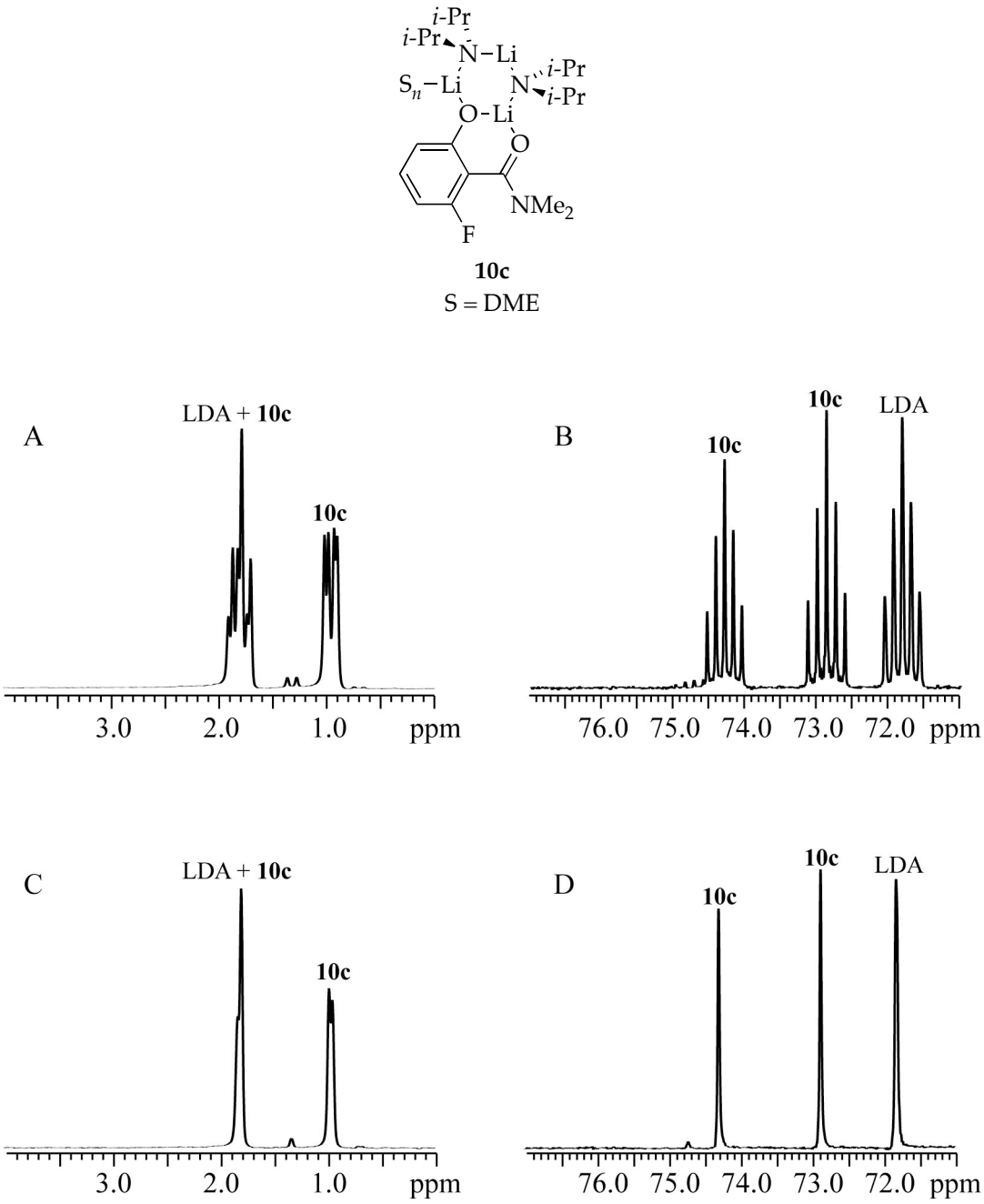
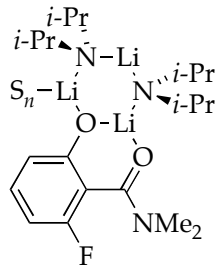


Figure 22. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4d** in 6.0 M DME/pentane at -85 °C after aging at -50 °C for 30 min: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



10c

S = DME

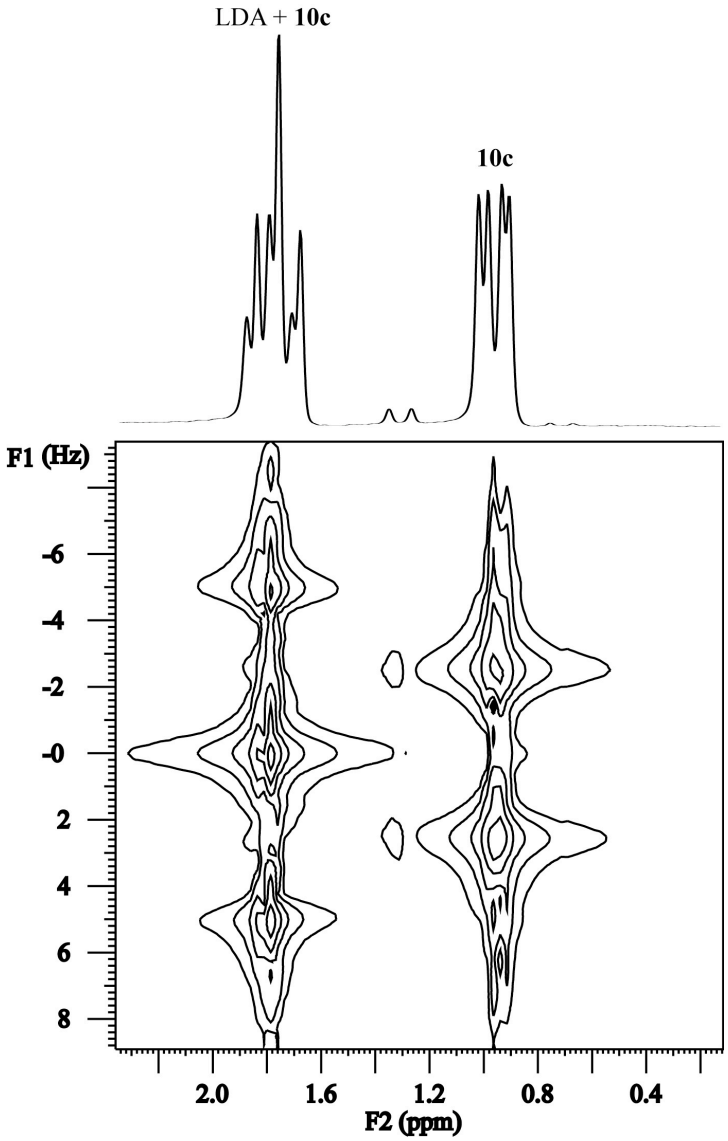


Figure 23. $^{1}J(^{6}Li,^{15}N)$-resolved NMR spectrum of 0.40 M [$^{6}Li,^{15}N$]LDA with 0.25 equiv of **4d** in 6.0 M DME/pentane at -85 °C after aging at -50 °C for 30 min.

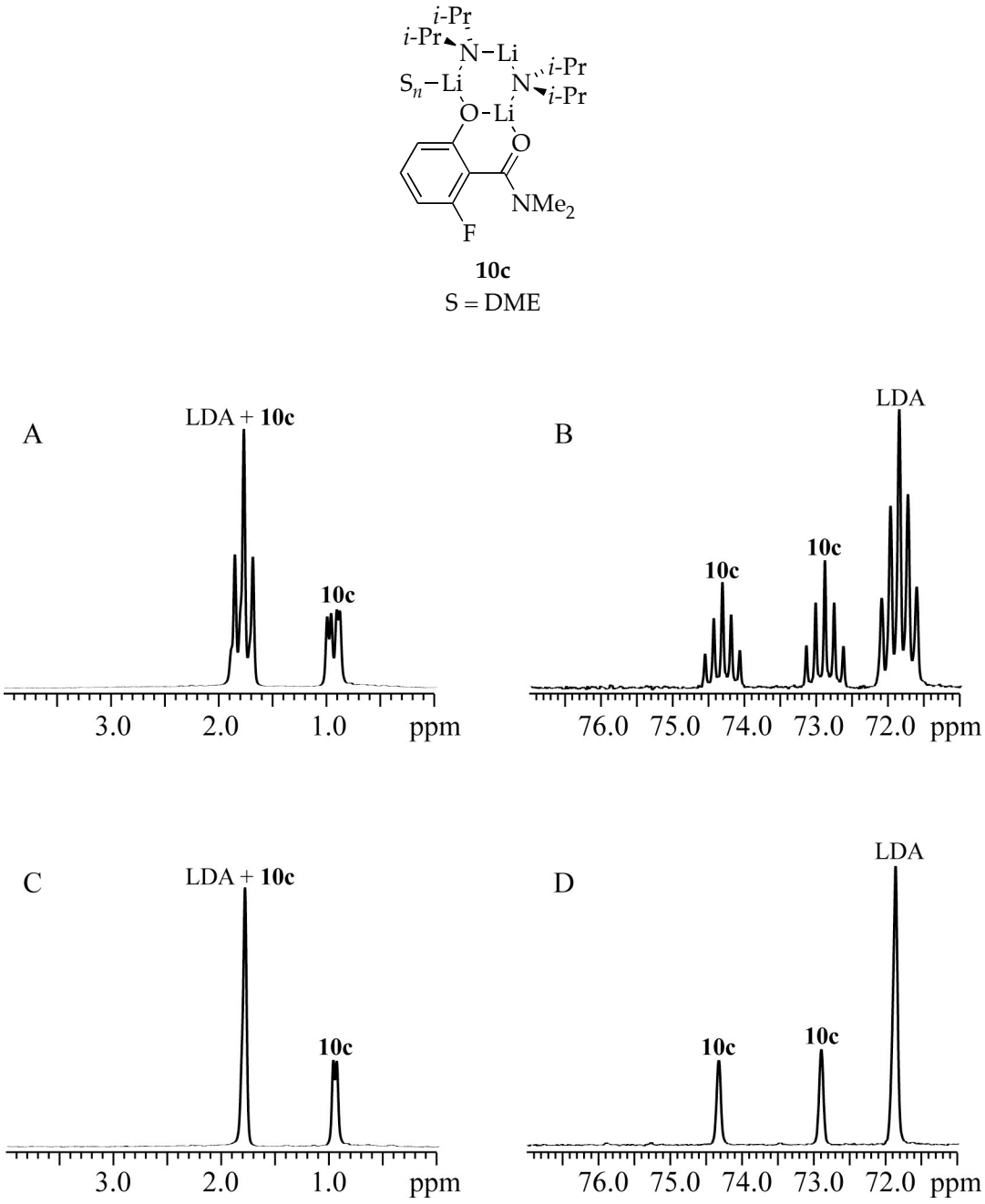
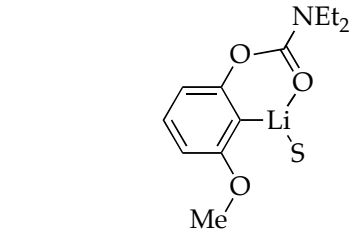


Figure 24. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **5c** in 6.0 M DME/pentane at -85 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



6g
S = TMCDA

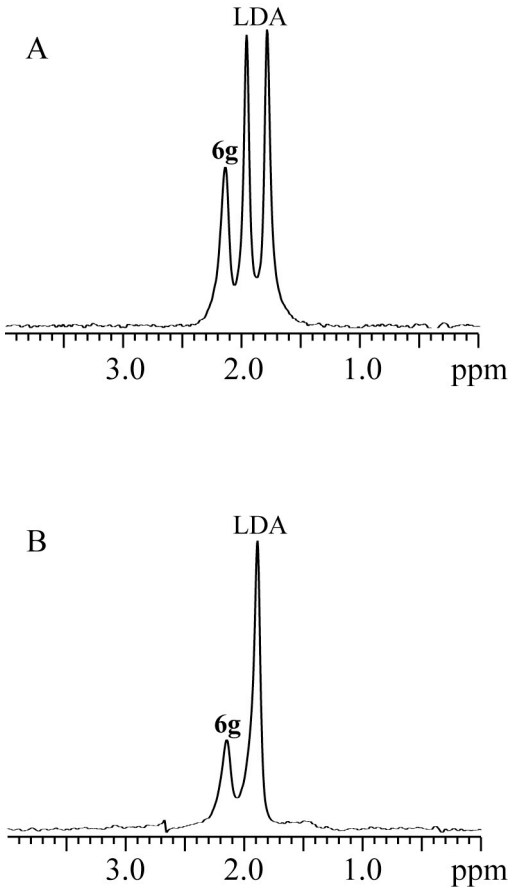
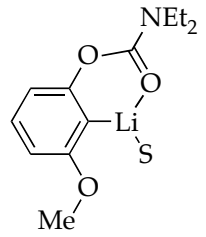
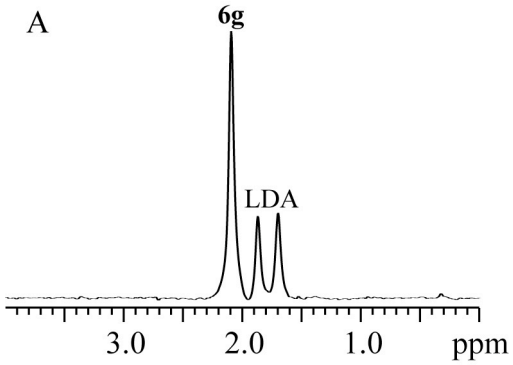


Figure 25. ^{6}Li NMR spectra of 0.25 M [^{6}Li,^{15}N]LDA with 0.40 equiv **4b** in 1.0 M *R,R*-TMCDA/toluene/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6g
S = TMCDA



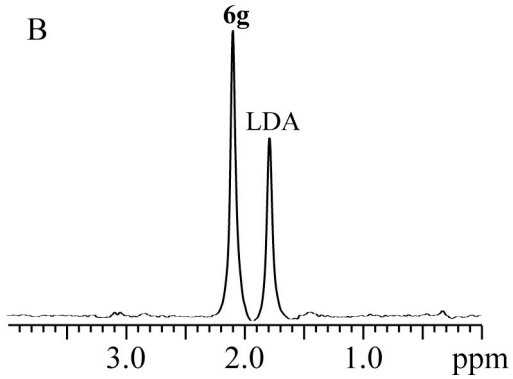
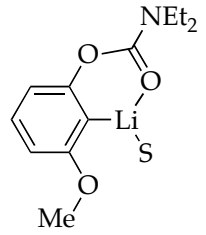
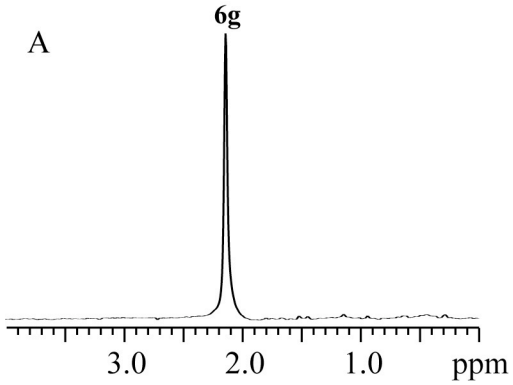


Figure 26. ^{6}Li NMR spectra of 0.15 M [^{6}Li,^{15}N]LDA with 0.60 equiv **4b** in 1.0 M *trans*-TMCDA/toluene/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6g
S = TMCDA



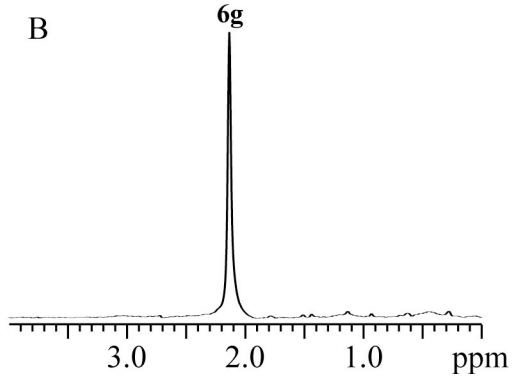
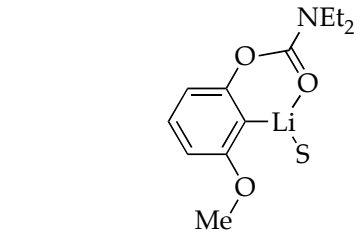
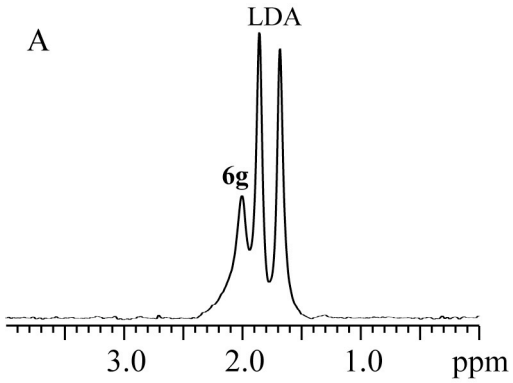


Figure 27. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 1.0 equiv **4b** in 1.0 M *trans*-TMCDA/toluene/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6g
S = TMCDA



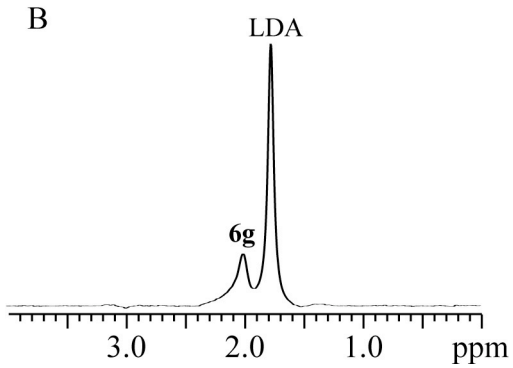
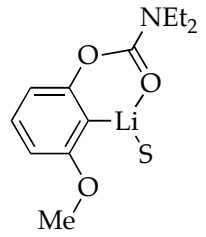


Figure 28. ^{6}Li NMR spectra of 0.30 M [^{6}Li,^{15}N]LDA with 0.30 equiv **4b** in 1.0 M *trans*-TMCDA/toluene/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6g
S = TMCDA

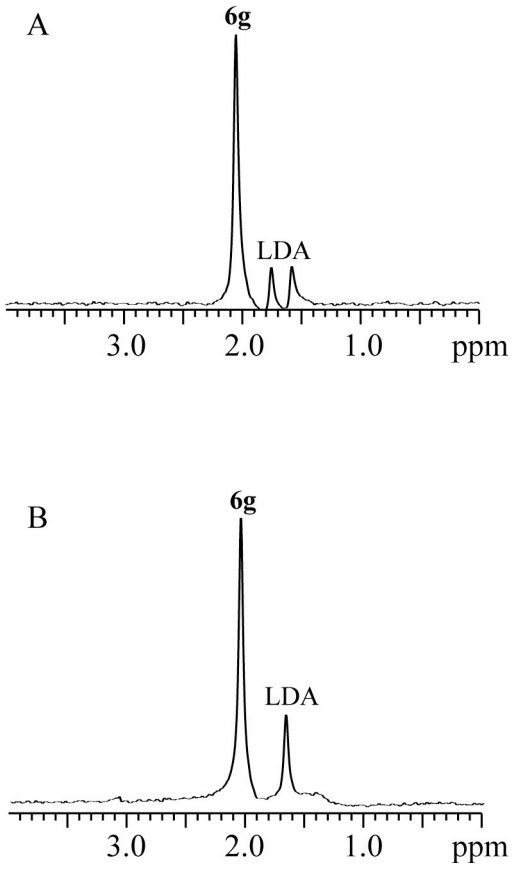


Figure 29. ^{6}Li NMR spectra of 0.15 M [^{6}Li,^{15}N]LDA with 0.60 equiv **4b** in 0.10 M *trans*-TMCDA/toluene/pentane at -70 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.

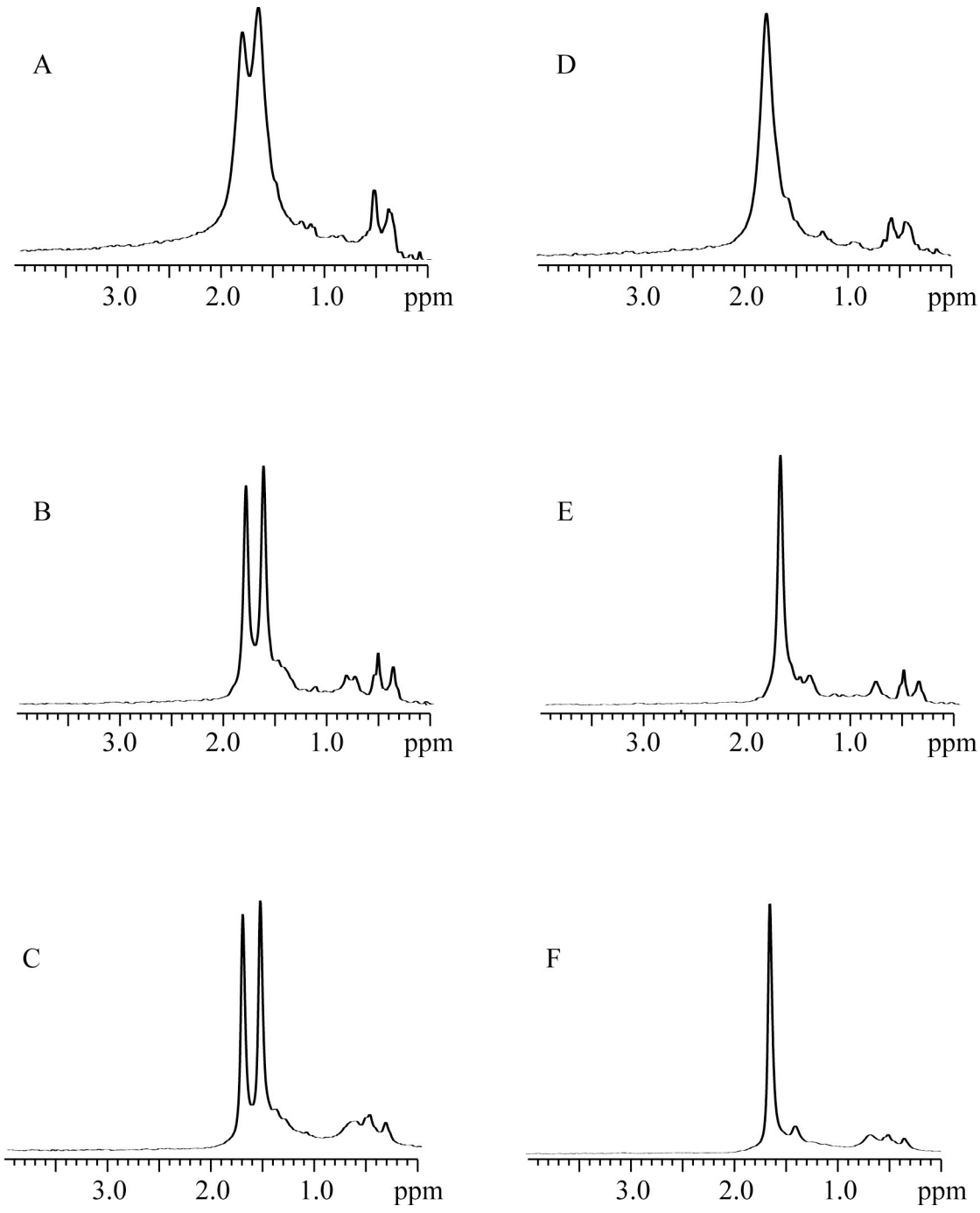


Figure 30. ^{6}Li and ^{6}Li{^{15}N} NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv of **4b** in 1.4 M *R,R*-TMCDA/toluene/pentane at various temperatures. ^{6}Li: (A) -50 °C; (B) -70 °C; (C) -90 °C. ^{6}Li{^{15}N}: (D) -50 °C; (E) -70 °C; (F) -90 °C.

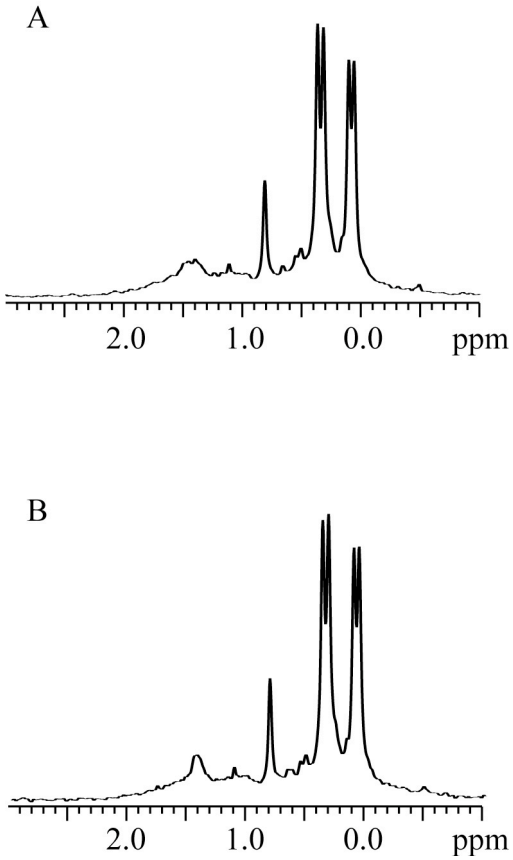
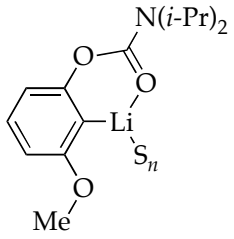


Figure 31. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA and with 1.0 equiv **5b** in 1.4 M *R,R*-TMCDA/toluene/pentane at -80 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6c
S = HMPA

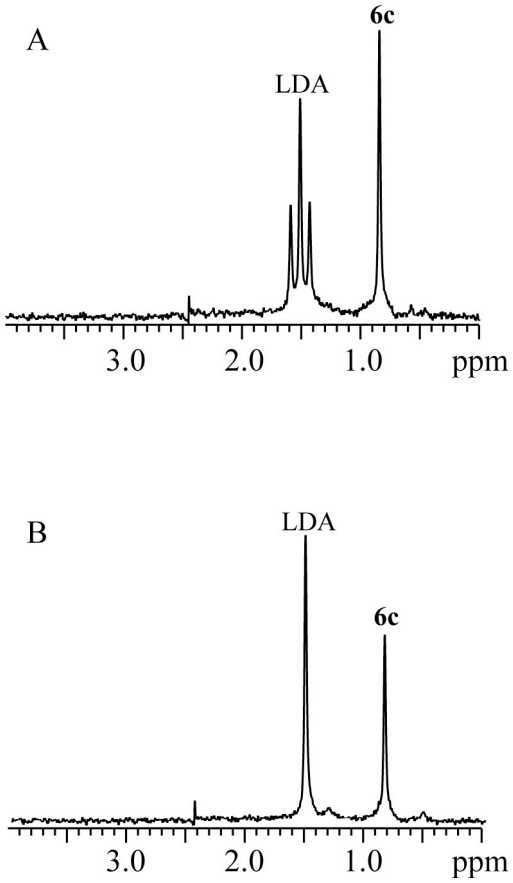
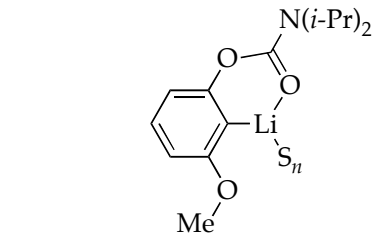
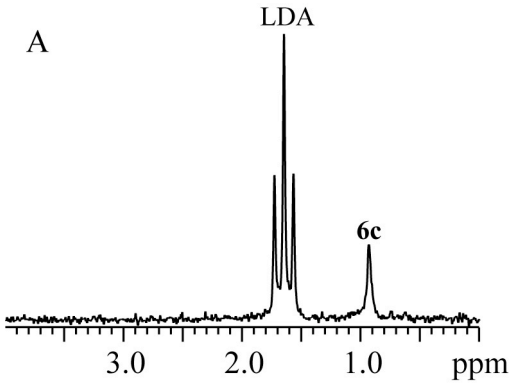


Figure 32. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4c** in 0.10 M HMPA/10.0 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6c
S = HMPA



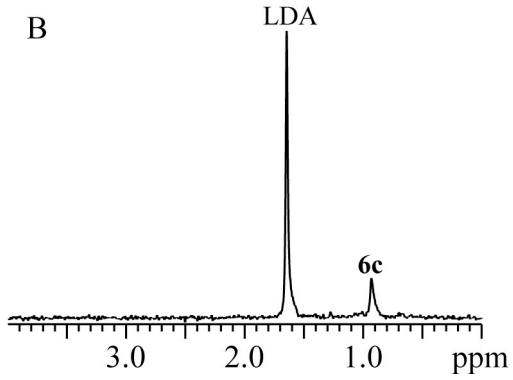


Figure 33. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4c** in 0.40 M HMPA/10.0 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.

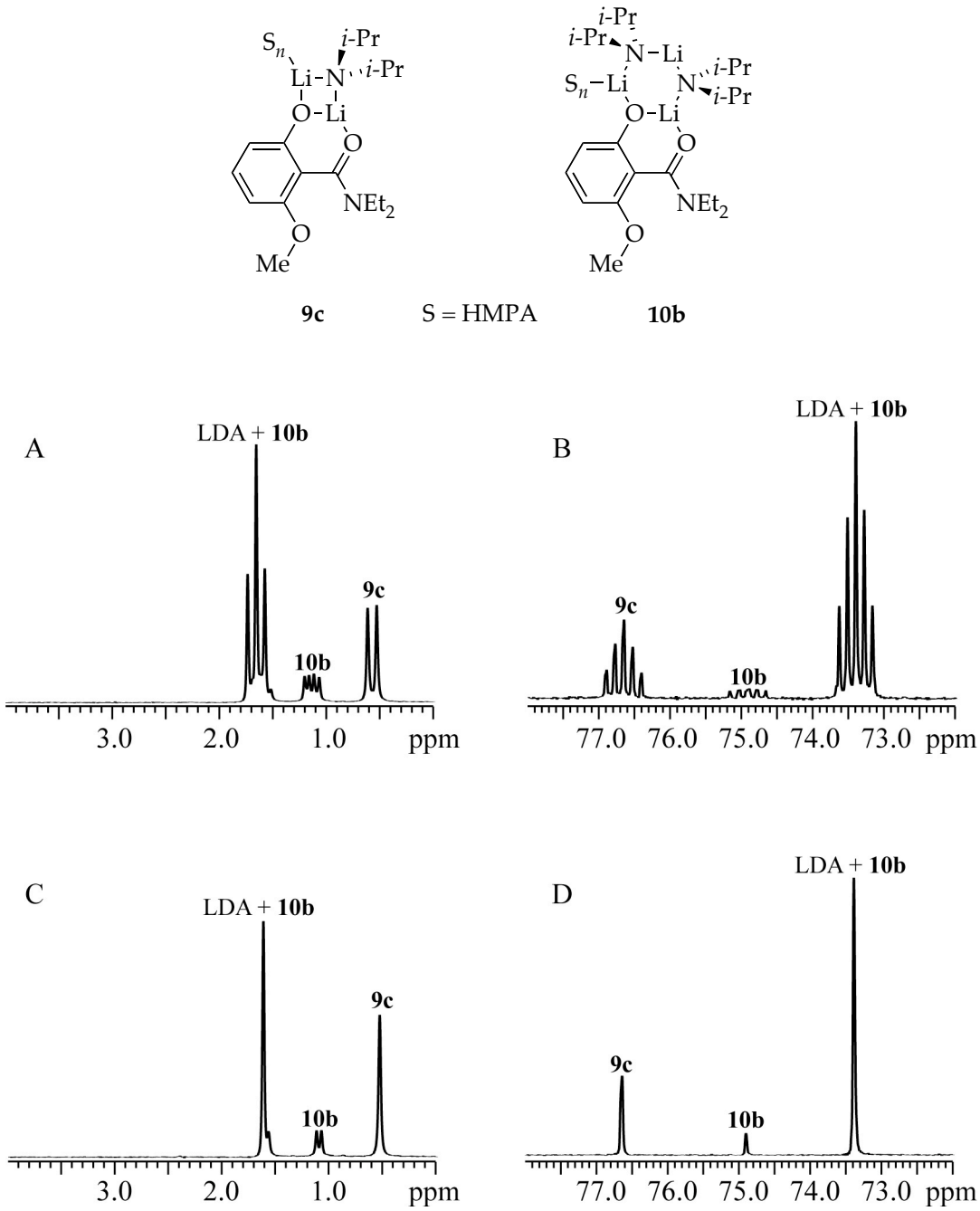
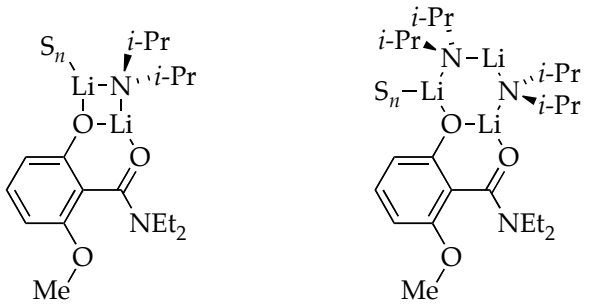


Figure 34. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4b** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



9c S = HMPA **10b**

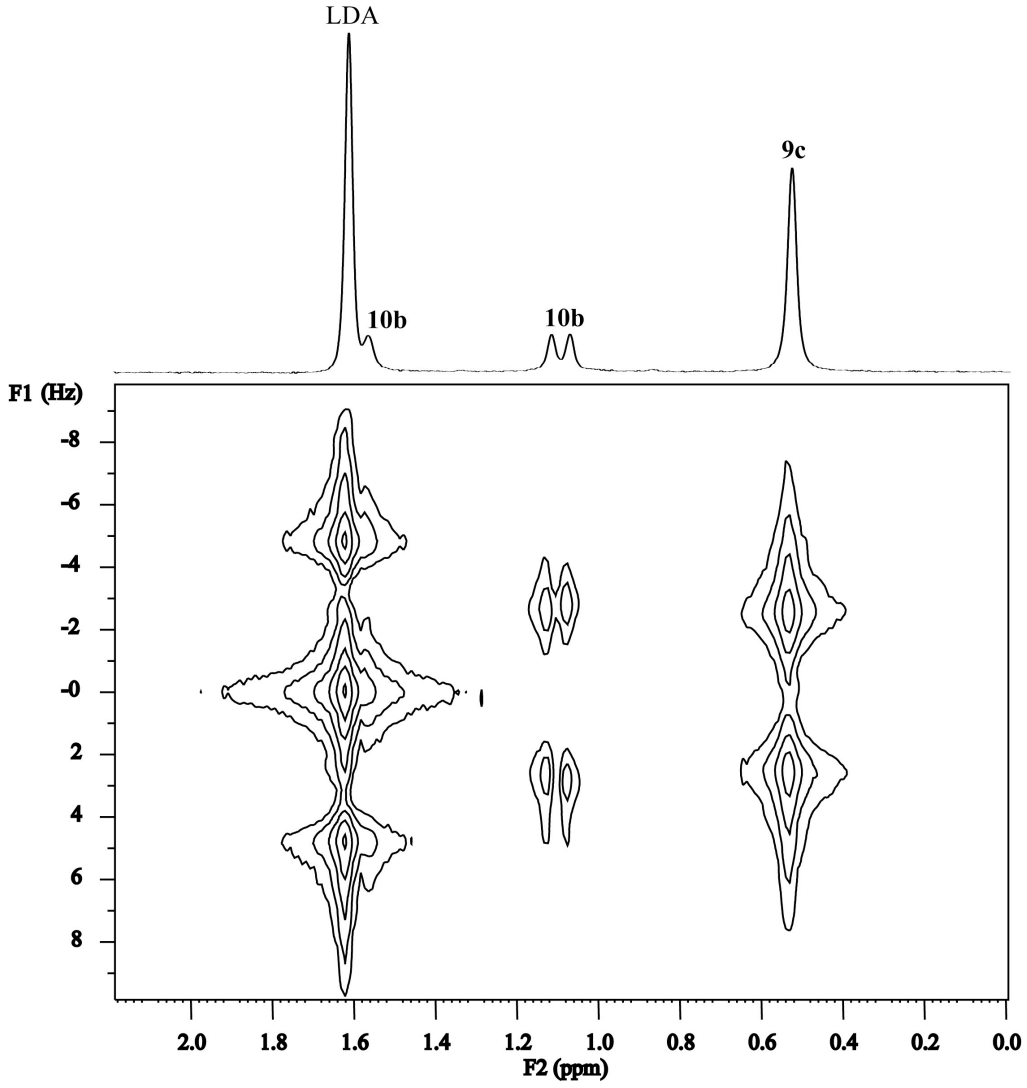


Figure 35. $^{1}J(^{6}Li,^{15}N)$-resolved NMR spectrum of 0.40 M [$^{6}Li,^{15}N$]LDA with 0.25 equiv of **4b** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C.

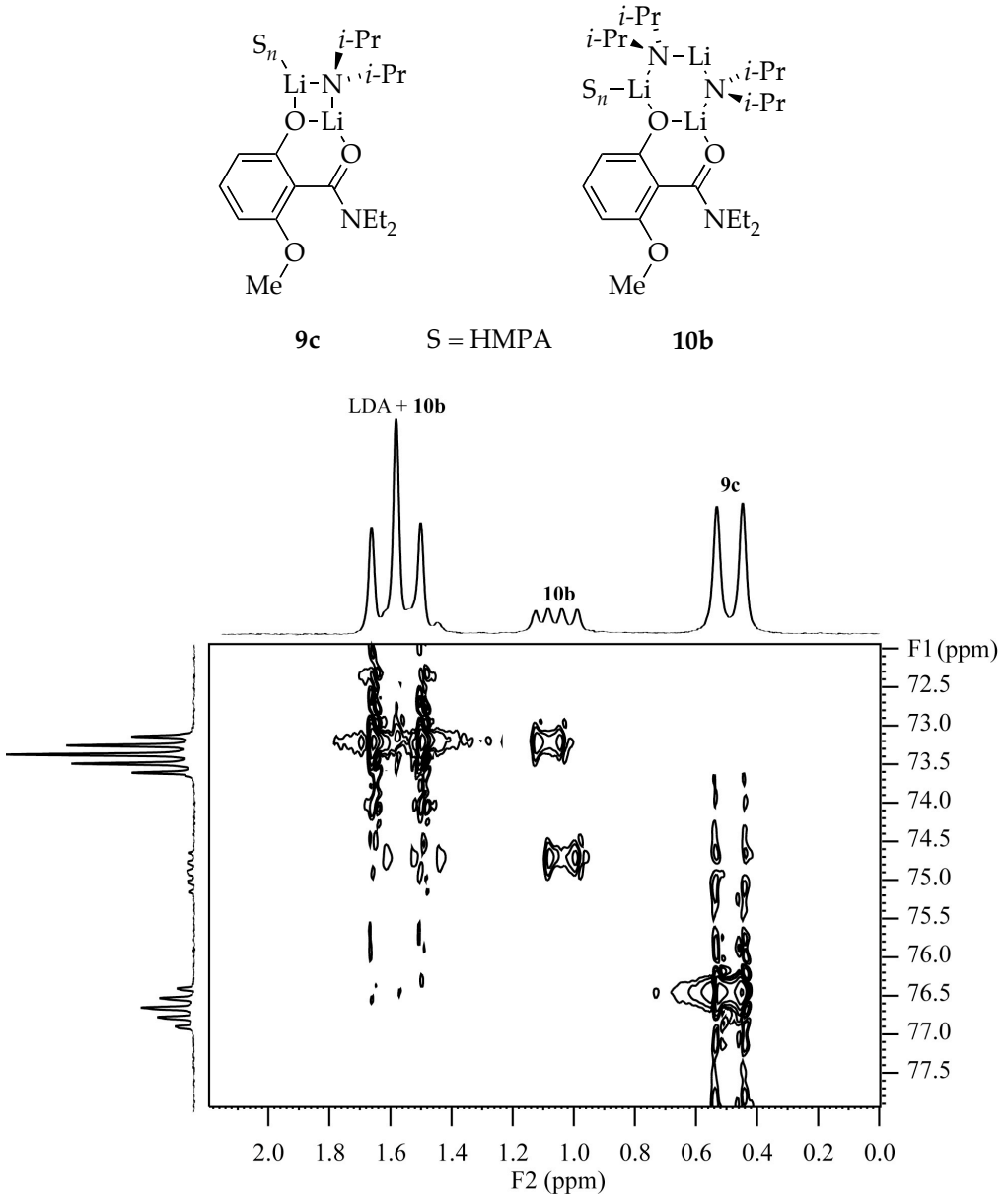


Figure 36. (^{6}Li,^{15}N)-HSQC NMR spectrum of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv of **4b** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C.

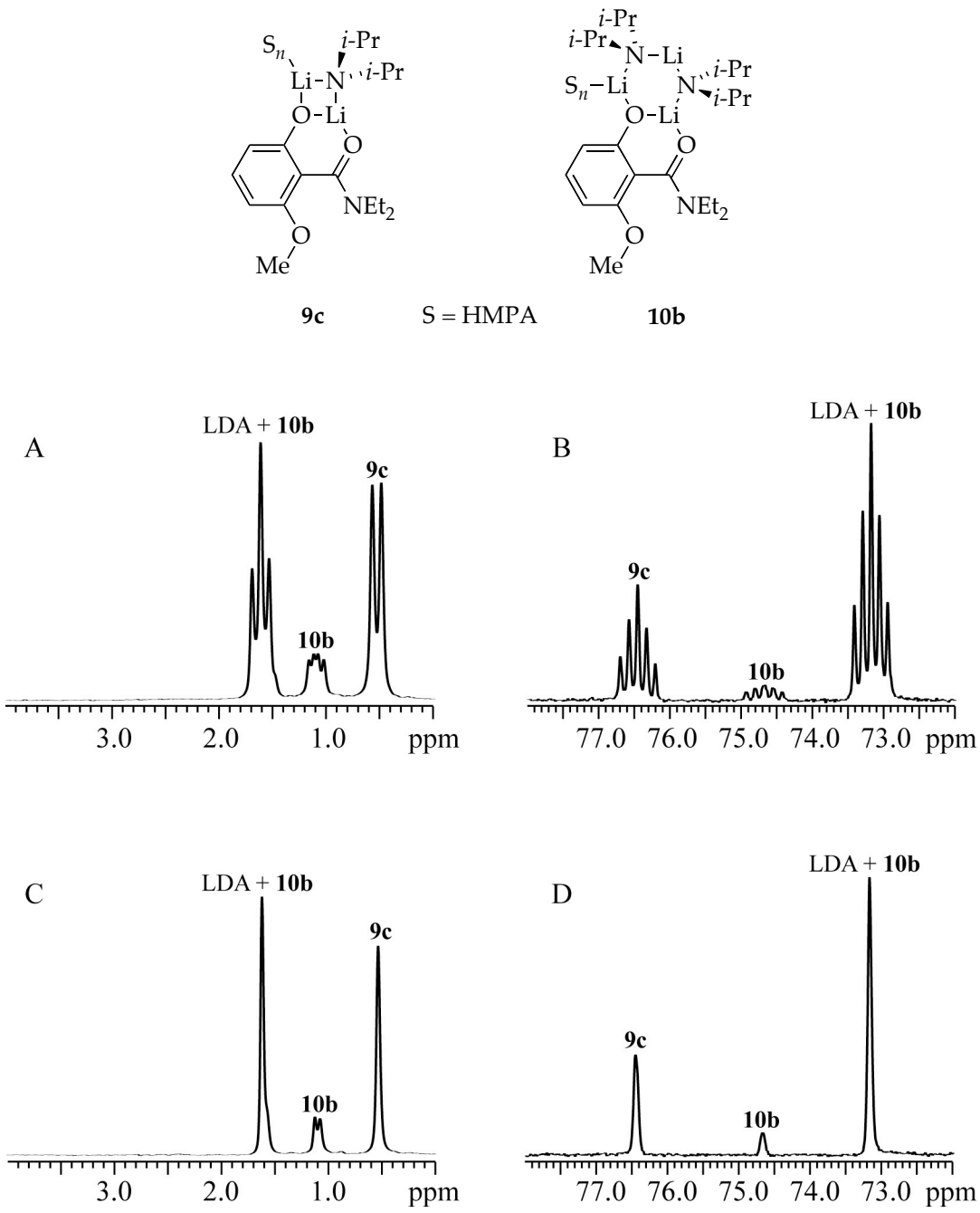
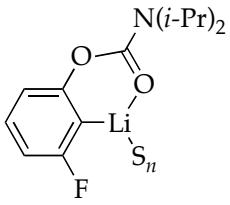
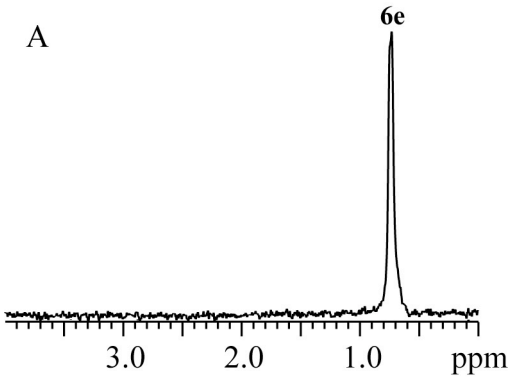


Figure 37. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **5b** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.



6e
S = HMPA



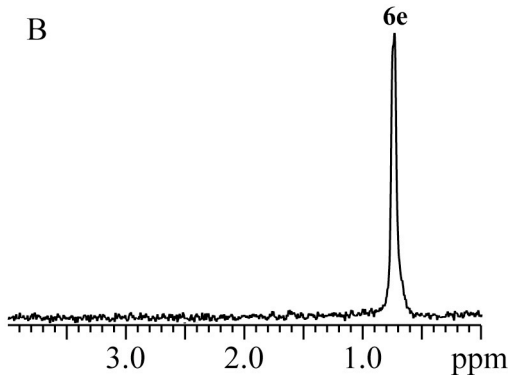
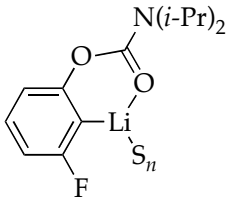
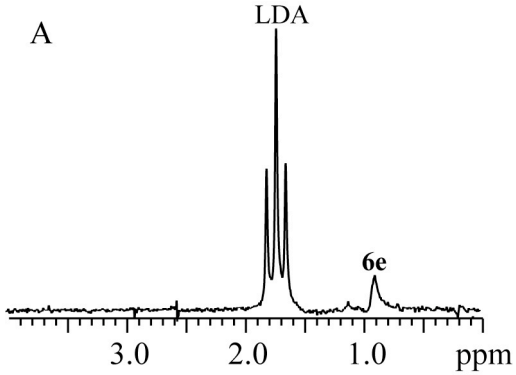


Figure 38. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 1.0 equiv **4e** in 0.40 M HMPA/10.0 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



6e
S = HMPA



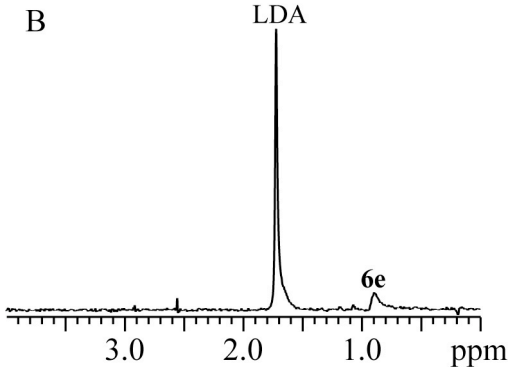
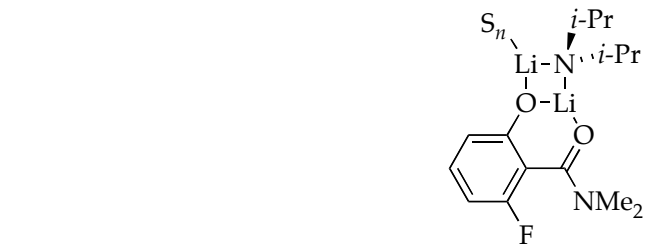


Figure 39. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4e** in 0.40 M HMPA/10.0 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{6}Li{^{15}N} spectrum.



9d
S = HMPA

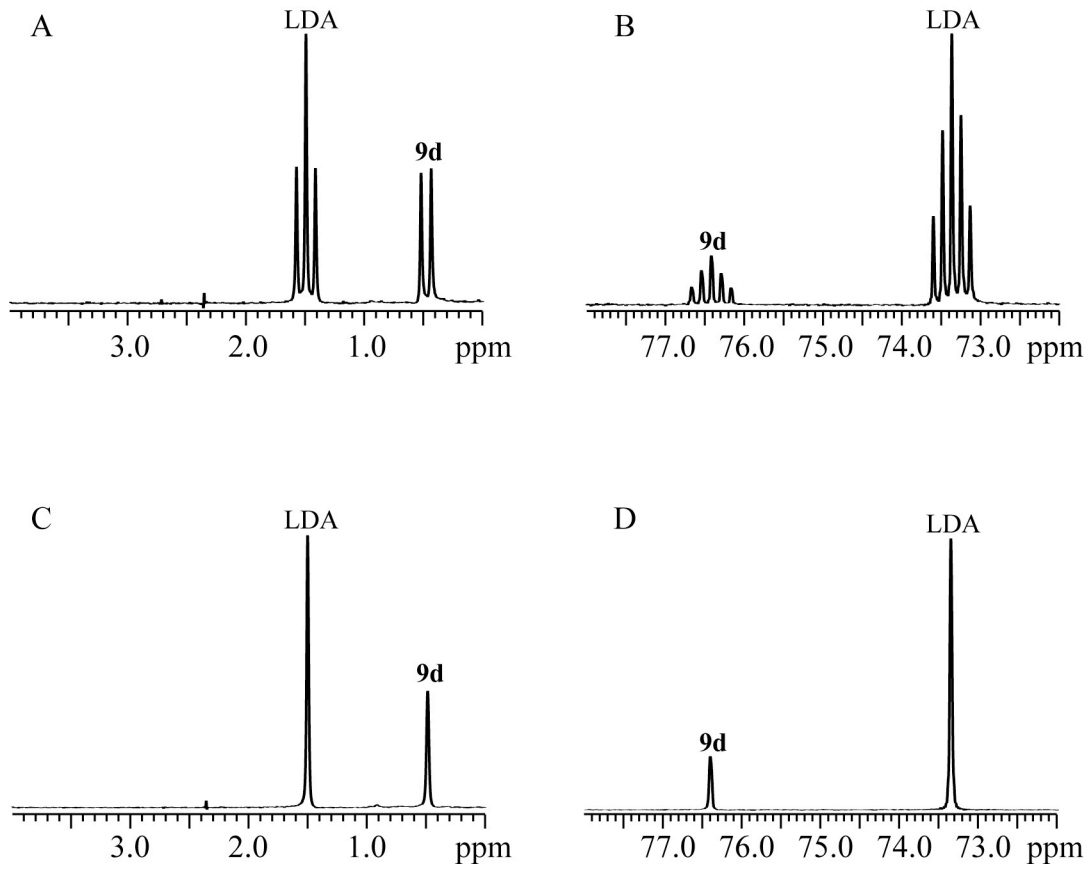


Figure 40. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4d** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

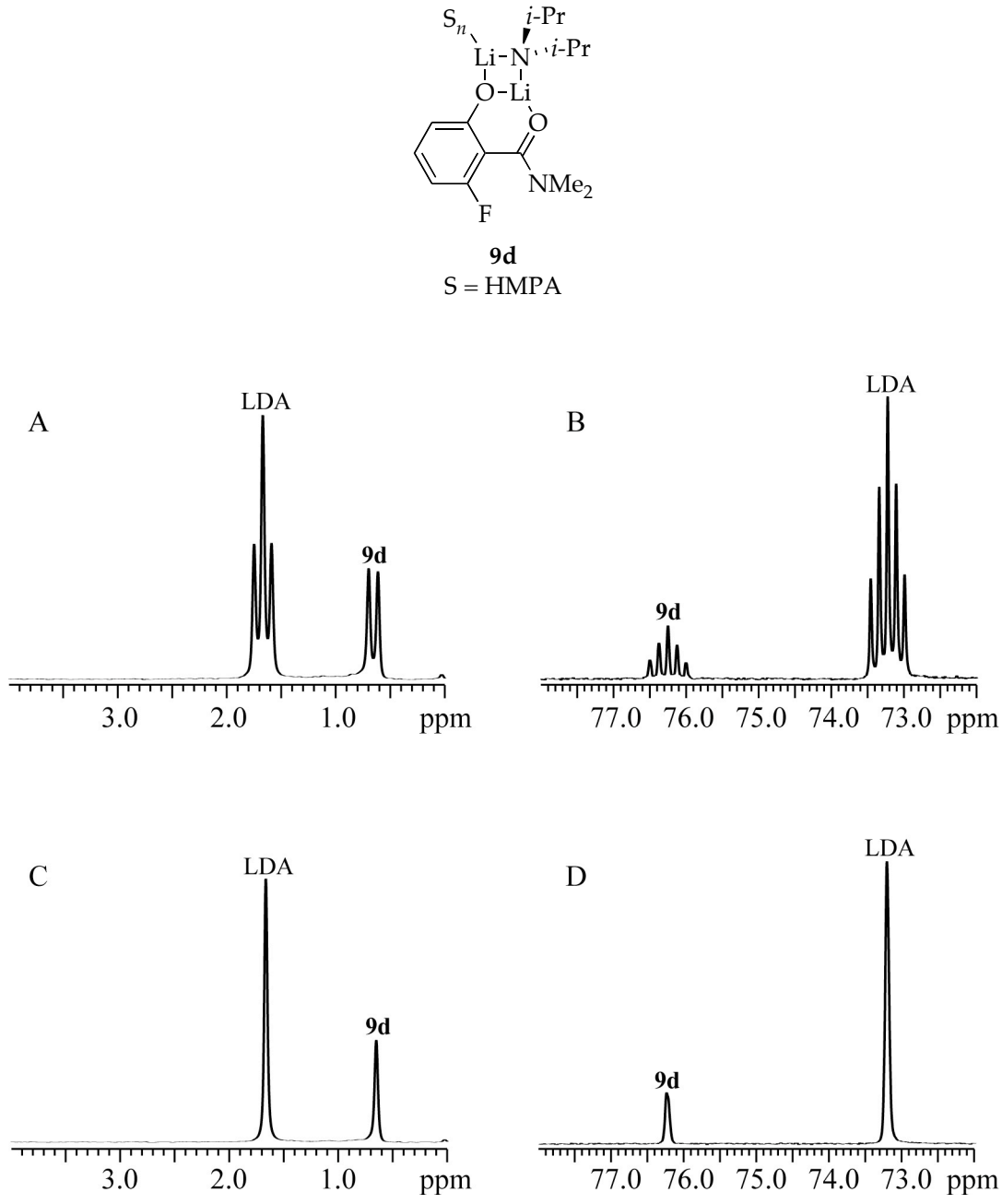


Figure 41. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **5c** in 1.0 M HMPA/8.2 M THF/pentane at -90 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum.

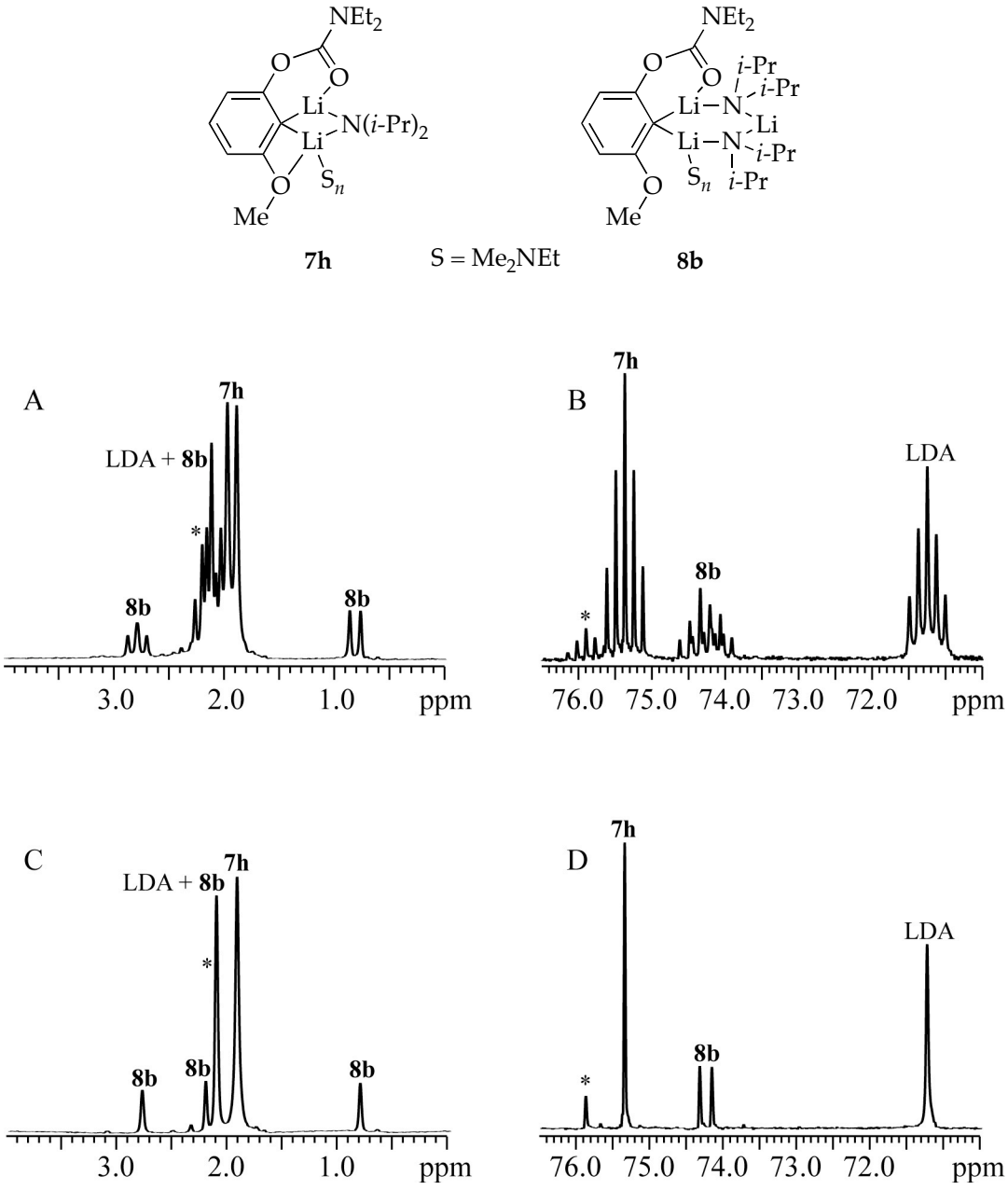


Figure 42. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4b** in 3.0 M Me_2NEt/toluene/pentane at -100 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum. *Unassigned ^{6}Li doublet and ^{15}N quintet.

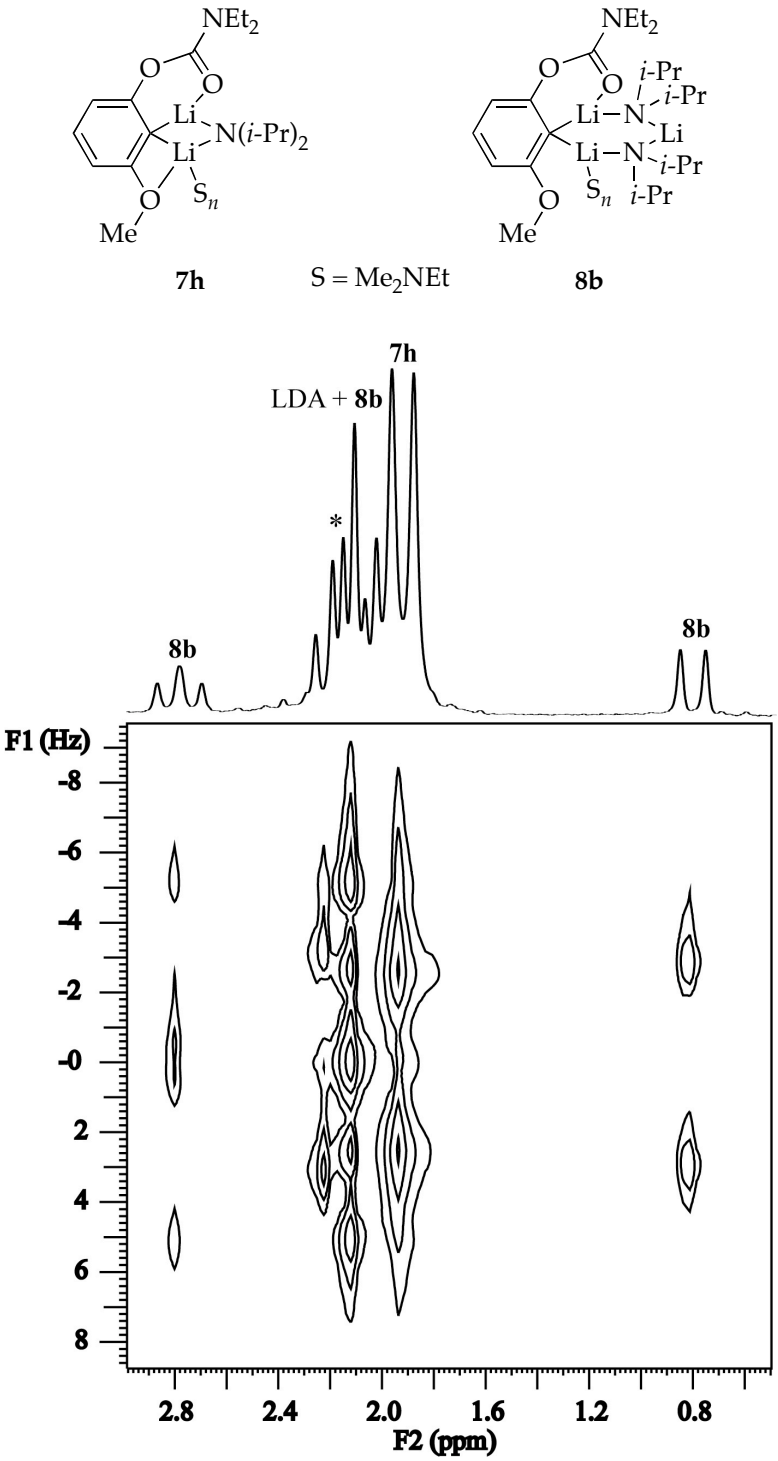


Figure 43. $^{1}J(^{6}Li,^{15}N)$-resolved NMR spectrum of 0.40 M [$^{6}Li,^{15}N$]LDA with 0.25 equiv of **4b** in 3.0 M Me_2NEt/toluene/pentane at -100 °C. * Unassigned ^{6}Li doublet and ^{15}N quintet.

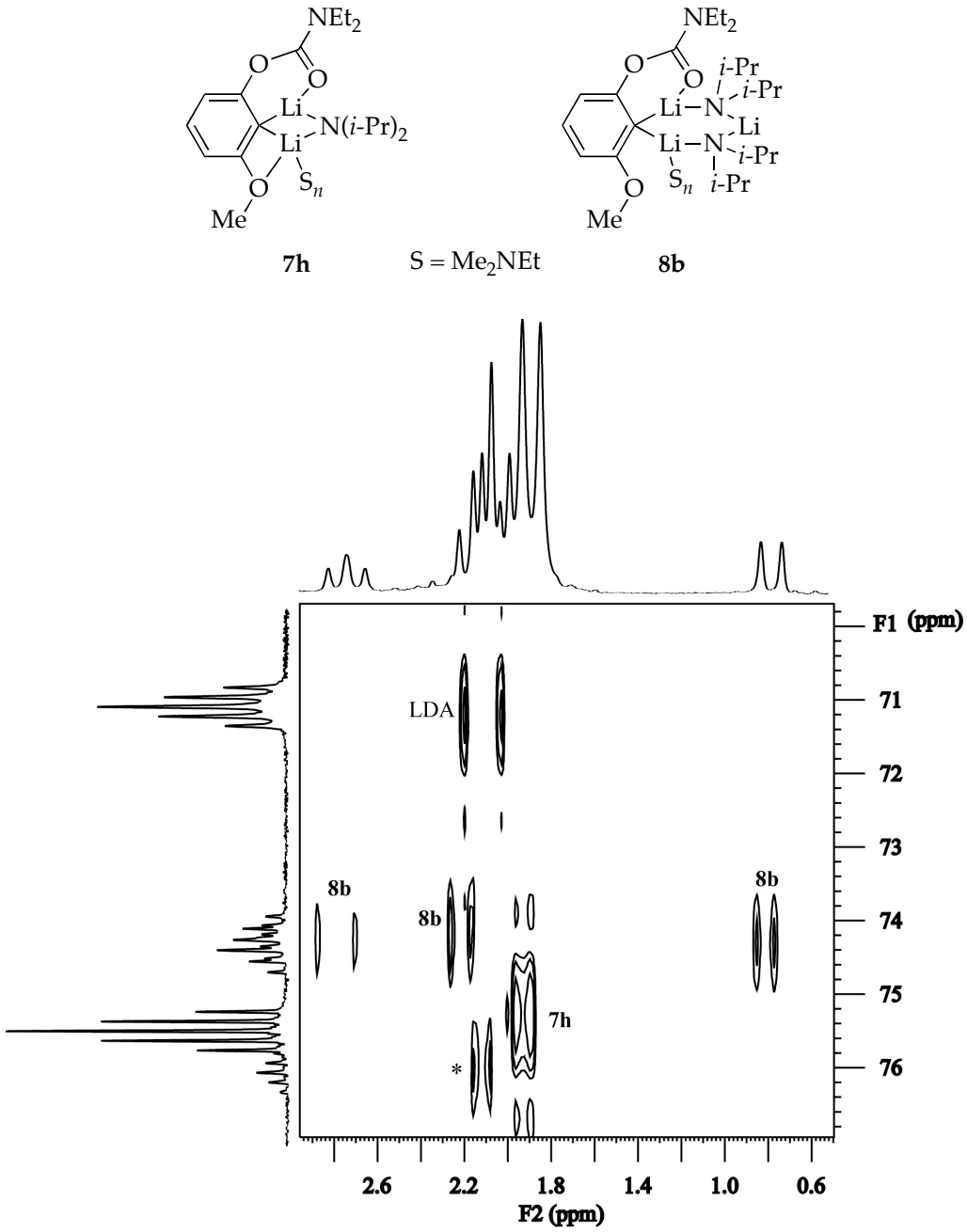
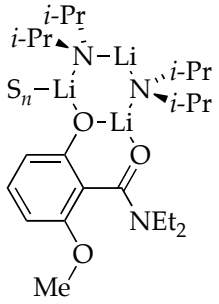


Figure 44. (^{6}Li,^{15}N)-HSQC NMR spectrum of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv of **4b** in 3.0 M Me_2NEt/toluene/pentane at -100 °C. *Unassigned ^{6}Li doublet and ^{15}N quintet.



10e

S = Me_2NEt

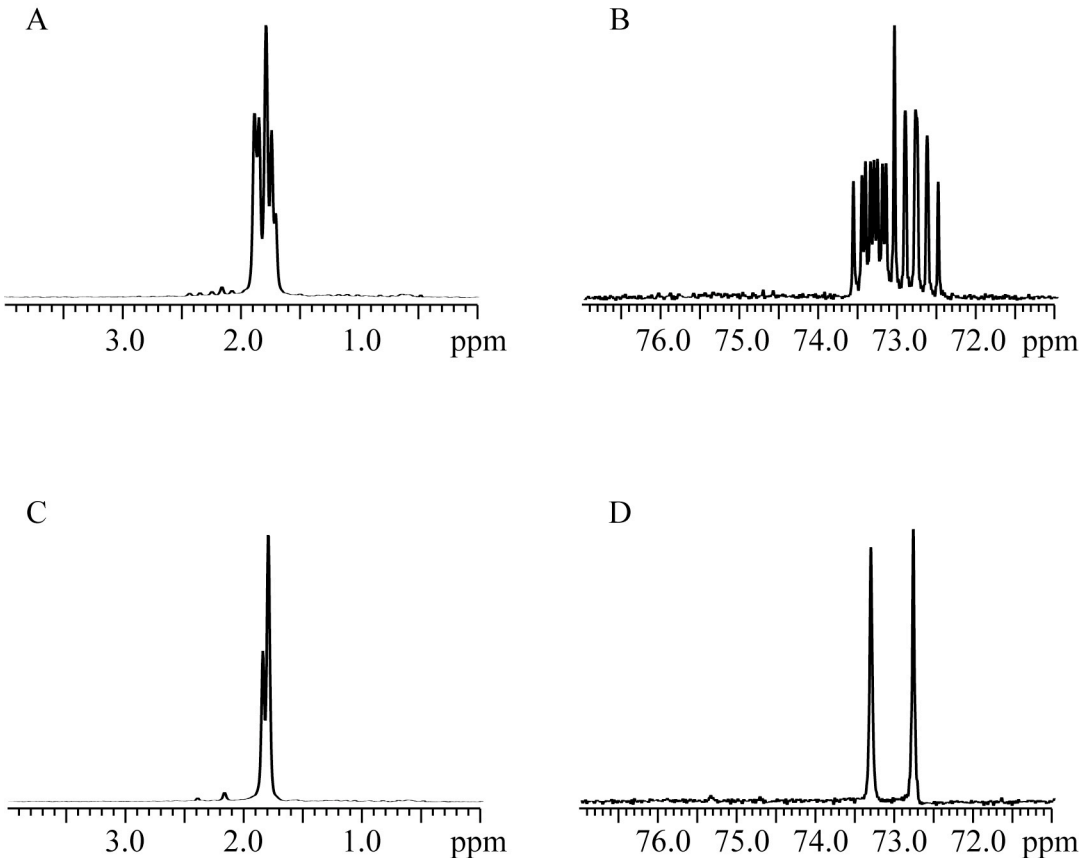
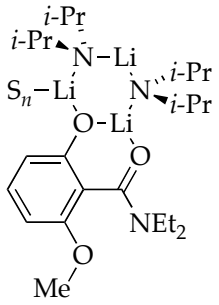


Figure 45. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **4b** in 3.0 M Me_2NEt/toluene/pentane at -100 °C after aging at 0 °C for 2 hr: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) $^{6}Li\{^{15}N\}$ spectrum; (D) $^{15}N\{^{6}Li\}$ spectrum.



10e

S = Me_2NEt

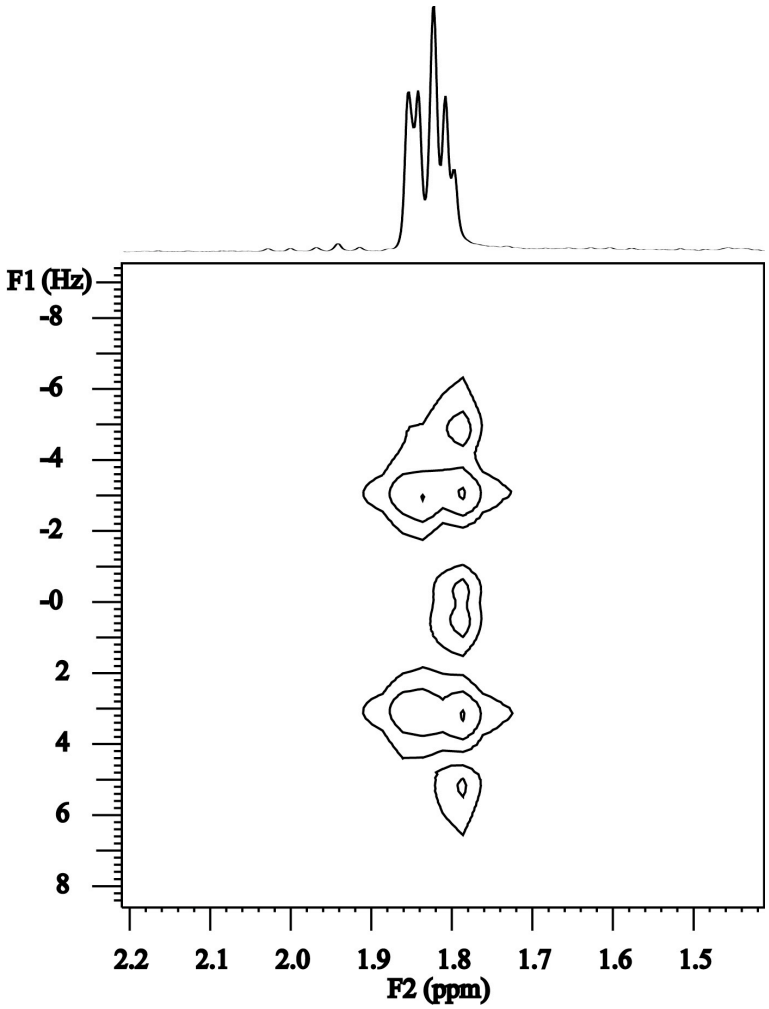
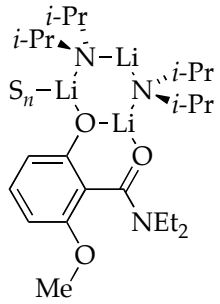


Figure 46. $^1J(^6Li,^{15}N)$-resolved NMR spectrum of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv of **4b** in 3.0 M Me_2NEt/toluene/pentane at -100 °C after aging at 0 °C for 2 hr.



10e

S = Me_2NEt

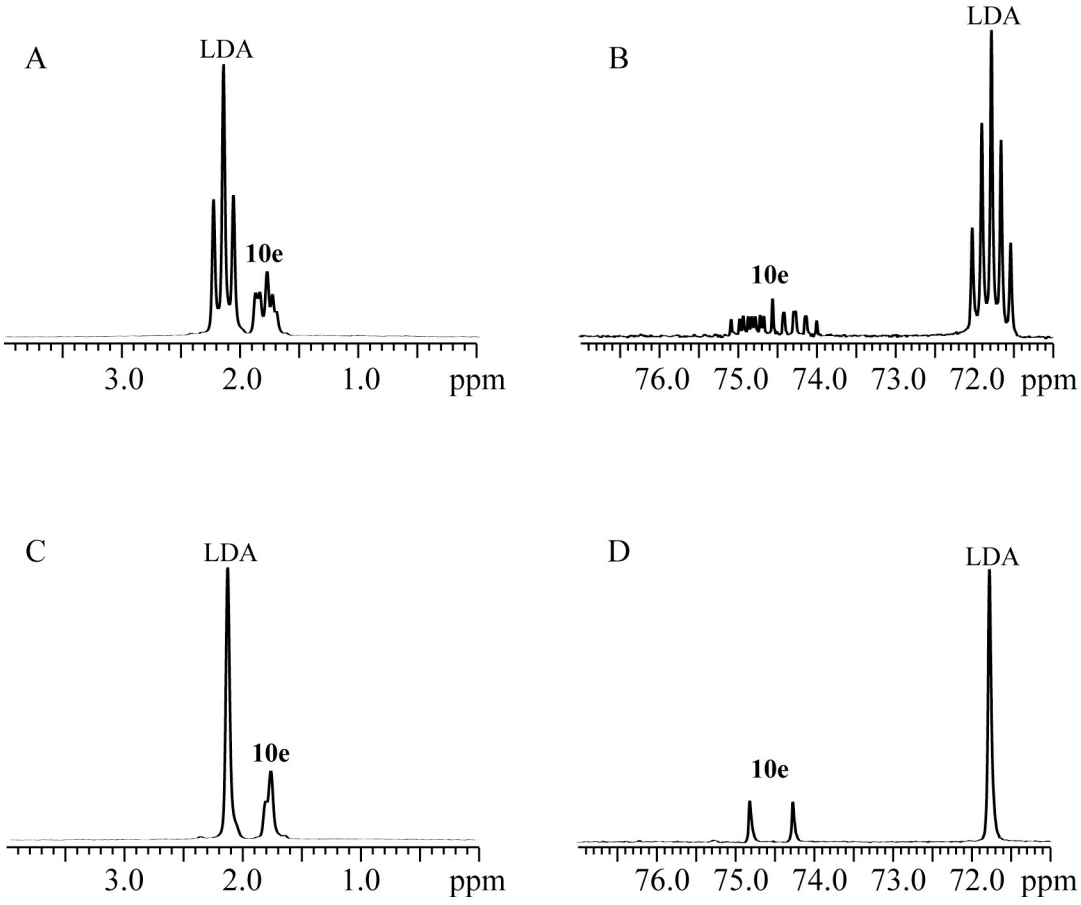


Figure 47. ^{6}Li and ^{15}N NMR spectra of 0.40 M [^{6}Li,^{15}N]LDA with 0.25 equiv **5b** in 7.7 M Me_2NEt/pentane at -100 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) $^{6}Li\{^{15}N\}$ spectrum; (D) $^{15}N\{^{6}Li\}$ spectrum.

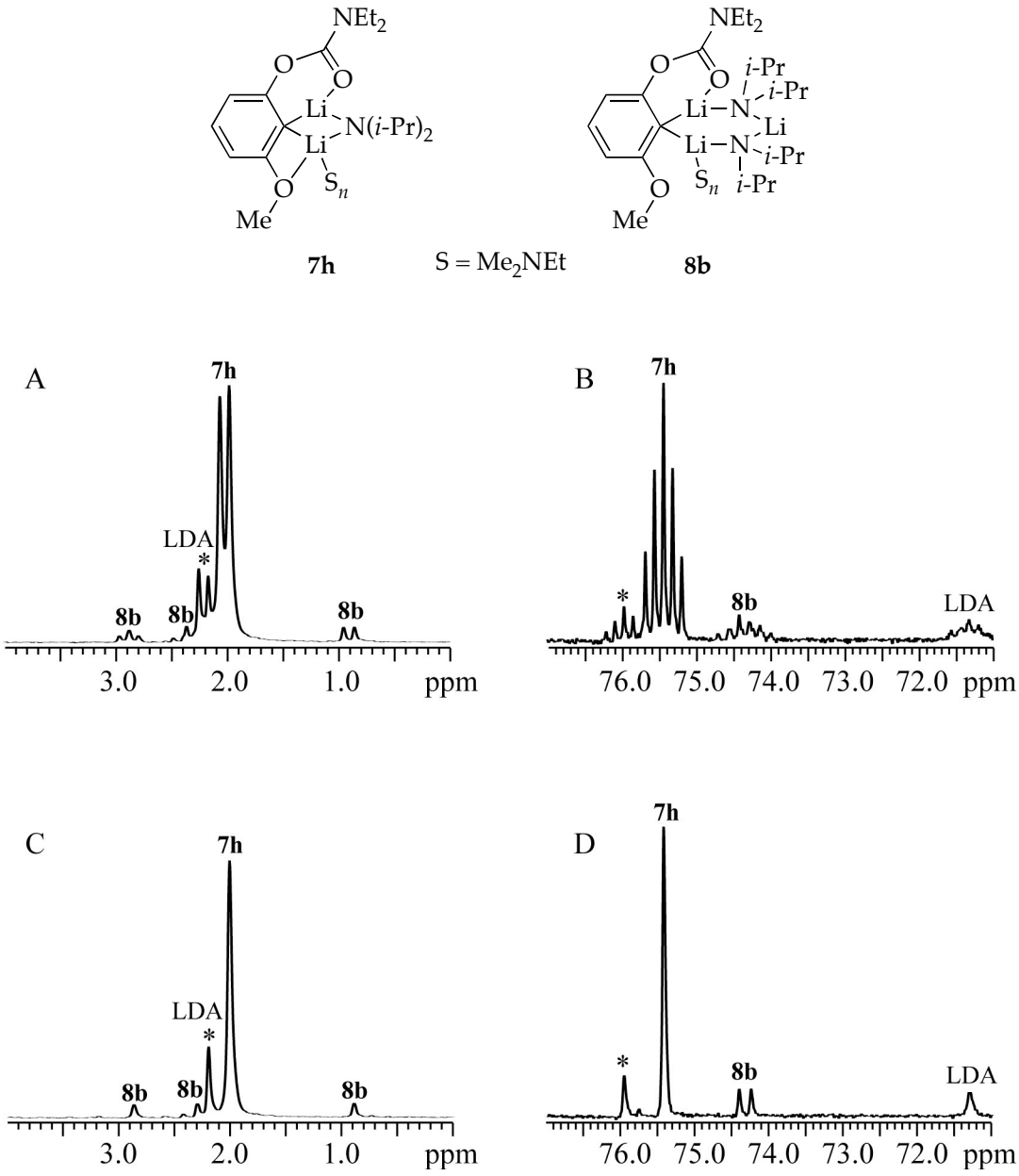


Figure 48. ^{6}Li and ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with 0.50 equiv **4b** in 7.7 M Me_2NEt/pentane at -100 °C: (A) ^{6}Li spectrum; (B) ^{15}N spectrum; (C) ^{6}Li{^{15}N} spectrum; (D) ^{15}N{^{6}Li} spectrum. * Unassigned ^{6}Li doublet and ^{15}N quintet.

Table 1. ^{6}Li and ^{15}N NMR spectroscopic data.[a,b]

ArLi	Solvent	R	X	^{6}Li, δ (mult, $^{1}J_{LiN}$)	^{15}N, δ(mult)
6a[c]	THF	*i*-Pr	F	1.23 (s)	--
6c[b]	HMPA	*i*-Pr	OMe	0.91 (s)	--
6e	HMPA	*i*-Pr	F	0.75 (s)	--
6f[c,b]	DME	*i*-Pr	F	1.65 (s)	--
6g[b]	TMCDA	Et	OMe	2.18 (s)	--
7b[b]	THF	*i*-Pr	F	1.71 (d, 5.3)	76.3 (q)
7d[b]	*n*-BuOMe	Et	OMe	1.85 (d, 5.8)	75.8 (q)
7f[b]	DME	*i*-Pr	F	1.60 (d, 5.4)	75.2 (q)
7g	TMEDA	*i*-Pr	OMe	2.01 (d, 4.9)	75.3 (q)
7h	Me_2NEt	Et	OMe	1.93 (d,5.2)	75.3 (q)
8a	TMEDA	*i*-Pr	OMe	0.78 (d, 5.7) 2.49 (t, 4.7) 2.50 (d, 5.7)	73.8 (tt) 75.3 (q)
8b	Me_2NEt	Et	OMe	0.81 (d, 6.3) 2.24 (d, 6.0) 2.80 (t, 4.9)	74.2 (tt) 74.3 (q)
9a	THF	Me	F	0.40 (d, 4.8)	79.1 (q)
9b	*n*-BuOMe	Et	OMe	0.93 (d, 4.9)	75.1 (q)
9c	HMPA	Et	OMe	0.54 (d, 5.3)	76.5 (q)
9d	HMPA	Me	F	0.66 (d, 4.6)	76.3 (q)
10a	*n*-BuOMe	Et	OMe	1.49 (d, 5.5) 1.55 (d, 6.2) 1.89 (t, 5.2)	74.4 (--)[d] 74.1 (--)[d]
10b	HMPA	Et	OMe	1.09 (d, 5.3) 1.12 (d, 5.3) 1.58 (t, 4.6)	73.2 (--)[d] 74.7 (tt)
10c	DME	Me	F	0.95 (d, 4.7) 0.98 (d, 5.1) 1.82 (t, 5.1)	72.9 (q) 74.3 (q)
10d	TMEDA	Me	OMe	1.21 (d, 5.0) 1.67 (t, 4.9)	74.9 (q) 75.1 (q)
10e	Me_2NEt	Et	OMe	1.79 (d, 6.2) 1.79 (t, 5.1) 1.84 (d, 6.1)	73.8 (tt) 74.3 (tt)

[a]Multiplicities are denoted as follows: s, singlet; d, doublet; t, triplet; q, quintet. The chemical shifts are reported relative to 0.30 M ^{6}LiCl/MeOH (δ 0.0 ppm) and neat Me_2NEt (δ 25.7 ppm) at -90 °C. ^{13}C NMR spectra are referenced to toluene-d_8 (δ 137.9 ppm), pentane (δ 14.1 ppm), or THF (δ 67.6 ppm). Chemical shifts are reported in ppm, and *J* values are reported in Hz. [b]Carbon-13 resonances of the carbanionic carbons: **6c**, δ 158.7 (br s); **6f**, δ 150.1 (br d, J_{FC}=120.7); **6g**, δ 155.1 (t, J_{CLi}=7.7); **7b**, δ 150.5 (br d, J_{FC}=123); **7d**, δ 155.2 (q, J_{CLi}=5.7); **7f**, δ 154.6 (dq, J_{FC}=123, J_{CLi}=5.9). [c]1.0 equiv [^{6}Li,^{15}N]LDA. [d]Obscured by another resonance.

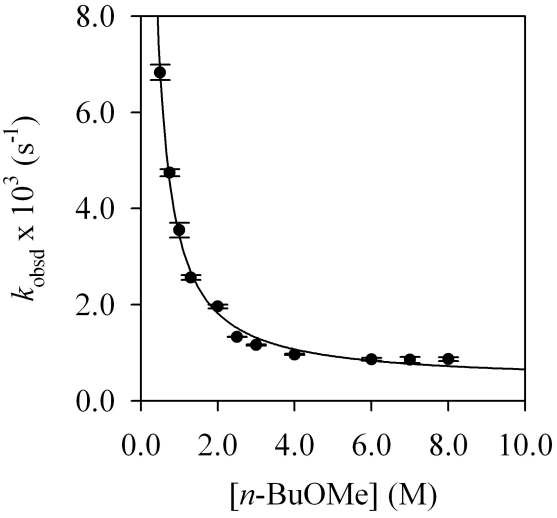


Figure 49. Plot of k_{obsd} versus [*n*-BuOMe] in pentane cosolvent for the Fries rearrangement of **7d** (0.004 M) by LDA (0.075 M) at 15 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[n\text{-BuOMe}]^n + k'$ (k = (3.0 ± 0.1) x 10^{-3}, n = -1.10 ± 0.05, k' = (4.1 ± 0.1) x 10^{-4}).

[*n*-BuOMe] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.50	6.94 ± 0.05	6.71 ± 0.05	6.8 ± 0.2
0.75	4.79 ± 0.04	4.67 ± 0.04	4.74 ± 0.08
1.0	3.5 ± 0.1	3.65 ± 0.08	3.5 ± 0.2
1.3	2.53 ± 0.06	2.60 ± 0.06	2.56 ± 0.05
2.0	1.99 ± 0.04	1.93 ± 0.03	1.96 ± 0.04
2.5	1.33 ± 0.02	1.33 ± 0.02	1.33 ± 0.01
3.0	1.15 ± 0.02	1.17 ± 0.02	1.16 ± 0.02
4.0	0.97 ± 0.01	0.95 ± 0.01	0.96 ± 0.01
6.0	0.89 ± 0.02	0.84 ± 0.01	0.86 ± 0.03
7.0	0.80 ± 0.02	0.90 ± 0.01	0.85 ± 0.07
8.0	0.89 ± 0.02	0.84 ± 0.01	0.87 ± 0.04

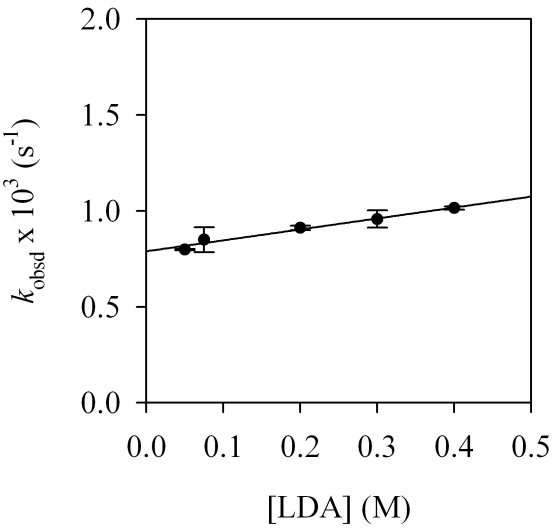


Figure 50. Plot of k_{obsd} versus [LDA] in 7.0 M *n*-BuOMe/pentane for the Fries rearrangement of **7d** (0.004 M) at 15 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{LDA}] + k'$ ($k = (5.7 \pm 0.8) \times 10^{-4}$, $k' = (7.9 \pm 0.2) \times 10^{-4}$).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.050	0.80 ± 0.01	0.80 ± 0.01	0.80 ± 0.01
0.075	0.80 ± 0.02	0.90 ± 0.01	0.85 ± 0.07
0.20	0.92 ± 0.01	0.90 ± 0.01	0.91 ± 0.01
0.30	0.93 ± 0.01	0.99 ± 0.02	0.96 ± 0.05
0.40	1.01 ± 0.01	1.02 ± 0.02	1.01 ± 0.01

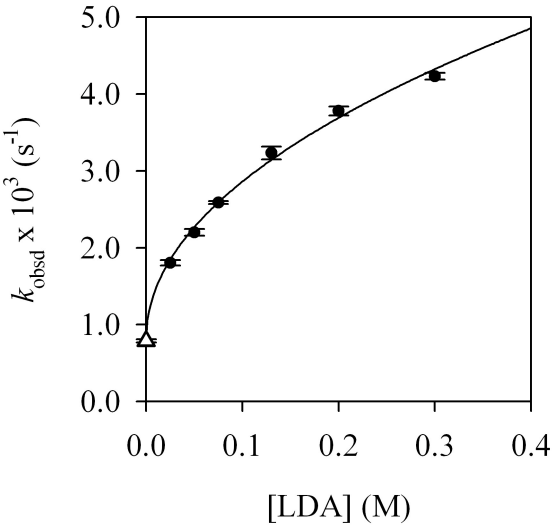


Figure 51. Plot of k_{obsd} versus [LDA] in 1.3 M *n*-BuOMe/pentane for the Fries rearrangement of **7d** (0.004 M) at 15 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{LDA}]^n + k'$ (k = (6.3 ± 0.2) x 10^{-3}, n = 0.49 ± 0.09, k' = (7.9 ± 0.2) x 10^{-4}). k' (see Δ) was set to equal k' in Figure 50.

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.025	1.83 ± 0.06	1.78 ± 0.04	1.80 ± 0.04
0.050	2.23 ± 0.07	2.17 ± 0.05	2.20 ± 0.04
0.075	2.53 ± 0.06	2.60 ± 0.06	2.56 ± 0.05
0.13	3.29 ± 0.03	3.17 ± 0.02	3.23 ± 0.08
0.20	3.82 ± 0.04	3.74 ± 0.03	3.78 ± 0.06
0.30	4.26 ± 0.04	4.20 ± 0.03	4.23 ± 0.05

Table 2. Data from Figures 49, 50, and 51 fit to $[\mathbf{7d}] = \{(\alpha\text{-}1)k_{obsd}t + [\mathbf{7d}]_0^{-(1-\alpha)}\}^{-1/(\alpha-1)}$ to determine the order of the decay. The adjustable parameter α corresponds to the reaction order in **7d**.[1]

[*n*-BuOMe] (M)	[LDA] (M)	α 1	α 2
0.50	0.075	1.15 ± 0.01	1.01 ± 0.02
0.75	0.075	0.99 ± 0.03	0.99 ± 0.01
1.0	0.075	0.99 ± 0.12	1.05 ± 0.03
1.3	0.075	0.98 ± 0.08	0.96 ± 0.06
2.0	0.075	1.07 ± 0.03	0.99 ± 0.03
2.5	0.075	1.00 ± 0.05	1.06 ± 0.02
3.0	0.075	0.99 ± 0.07	0.91 ± 0.02
4.0	0.075	0.98 ± 0.06	0.98 ± 0.03
6.0	0.075	1.09 ± 0.02	1.01 ± 0.01
7.0	0.075	1.01 ± 0.02	0.94 ± 0.09
8.0	0.075	1.01 ± 0.03	1.02 ± 0.01
7.0	0.050	0.97 ± 0.06	1.04 ± 0.01
7.0	0.20	1.00 ± 0.03	0.97 ± 0.06
7.0	0.30	0.91 ± 0.02	1.01 ± 0.06
7.0	0.40	0.99 ± 0.01	0.96 ± 0.07
1.3	0.025	0.95 ± 0.09	0.95 ± 0.09
1.3	0.050	0.94 ± 0.09	1.040± 0.04
1.3	0.13	1.03 ± 0.01	1.00 ± 0.01
1.3	0.20	1.04 ± 0.01	1.02 ± 0.01
1.3	0.30	1.00 ± 0.04	1.1 ± 0.1

Average $\alpha = 1.00 \pm 0.05$

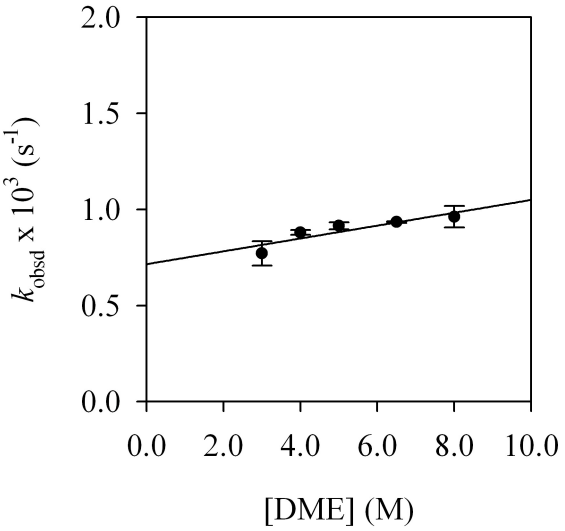


Figure 52. Plot of k_{obsd} versus [DME] in pentane cosolvent for the Fries rearrangement of **7e** (0.004 M) by LDA (0.40 M) at -60 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[DME] + k' (k = (3.3 ± 0.1) x 10^{-5}, k' = (7.1 ± 0.5) x 10^{-4}).

[DME] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
3.0	0.73 ± 0.01	0.82 ± 0.01	0.77 ± 0.03
4.0	0.87 ± 0.01	0.89 ± 0.07	0.88 ± 0.01
5.0	0.90 ± 0.01	0.93 ± 0.01	0.93 ± 0.02
6.5	0.94 ± 0.01	0.93 ± 0.01	0.93 ± 0.01
8.0	0.96 ± 0.01	0.97 ± 0.01	0.96 ± 0.06

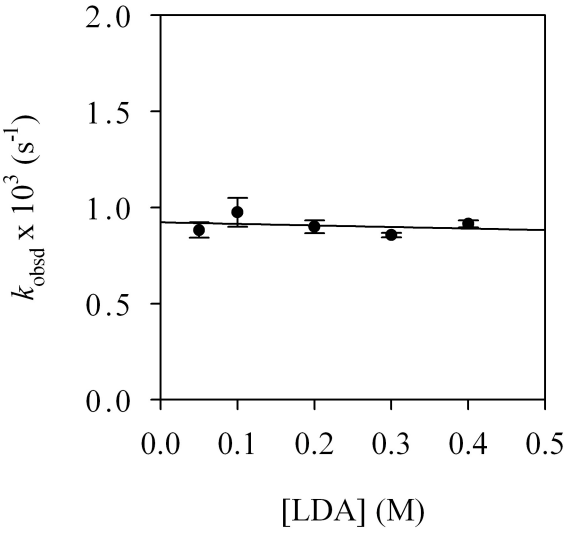


Figure 53. Plot of k_{obsd} versus [LDA] in 5.0 M DME/pentane for the Fries rearrangement of **7e** (0.004 M) at -60 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{LDA}] + k'$ (k = (-8.1 ± 17.2) x 10^{-5}, k' = (9.2 ± 0.4) x 10^{-4}).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.05	0.85 ± 0.01	0.91 ± 0.01	0.88 ± 0.04
0.10	0.92 ± 0.01	1.03 ± 0.01	0.97 ± 0.08
0.20	0.88 ± 0.01	0.92 ± 0.01	0.90 ± 0.03
0.30	0.86 ± 0.01	0.85 ± 0.01	0.86 ± 0.01
0.40	0.90 ± 0.01	0.93 ± 0.01	0.93 ± 0.02

Table 3. Data from Figures 52 and 53 fit to $[\mathbf{7e}] = \{(\alpha\text{-}1)k_{obsd}\,t + [\mathbf{7e}]_0^{-(1-\alpha)}\}^{-1/(\alpha-1)}$ to determine the order of the decay. The adjustable parameter α corresponds to the reaction order in **7e**.[1]

[DME] (M)	[LDA] (M)	α 1	α 2
3.0	0.40	1.00 ± 0.04	1.1 ± 0.1
4.0	0.40	1.01 ± 0.03	1.00 ± 0.02
5.0	0.40	1.00 ± 0.04	1.04 ± 0.01
6.5	0.40	0.96 ± 0.08	1.00 ± 0.02
8.0	0.40	1.01 ± 0.02	0.95 ± 0.09
5.0	0.05	0.99 ± 0.03	1.00 ± 0.02
5.0	0.10	1.02 ± 0.05	1.03 ± 0.04
5.0	0.20	1.01 ± 0.03	0.97 ± 0.06
5.0	0.30	1.02 ± 0.05	1.02 ± 0.03

Average α = 1.01 ± 0.03

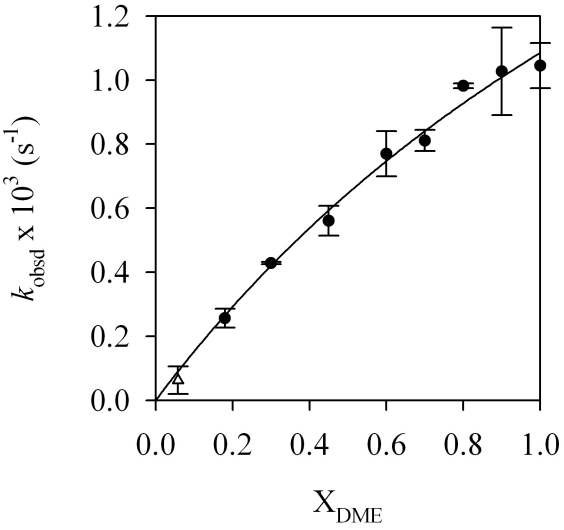


Figure 54. Plot of k_{obsd} versus mole fraction of DME (X_{DME}) for the rearrangement of **7e** (0.004 M) by LDA (0.05 M) at -60 °C. The donor solvent concentration is held constant ([DME]+[*n*-BuOMe]=5.0 M) using pentane as cosolvent. The curve depicts an unweighted least-squares fit to $k_{obsd} = (a + bx)/(1 + cx)$ ($a = (0.0 \pm 0.1) \times 10^{-3}$, $b = 1.6 \pm 0.5$, $c = 0.5 \pm 0.4$) such that $1 + c = K_{eq}$.[2] At low DME concentrations the lithium phenolate precipitated during the reaction; the value of k_{obsd} (shown as Δ) was not included in the fit.

X_{DME}	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.06	0.09 ± 0.01	0.03 ± 0.01	0.06 ± 0.04
0.18	0.28 ± 0.01	0.24 ± 0.01	0.26 ± 0.03
0.30	0.43 ± 0.01	0.42 ± 0.01	0.43 ± 0.01
0.45	0.53 ± 0.01	0.59 ± 0.01	0.56 ± 0.04
0.60	0.72 ± 0.01	0.82 ± 0.01	0.77 ± 0.07
0.70	0.83 ± 0.02	0.79 ± 0.01	0.81 ± 0.03
0.80	0.98 ± 0.01	0.99 ± 0.01	0.99 ± 0.01
0.90	1.12 ± 0.01	0.93 ± 0.01	1.03 ± 0.13
1.0	1.10 ± 0.01	0.99 ± 0.01	1.05 ± 0.08

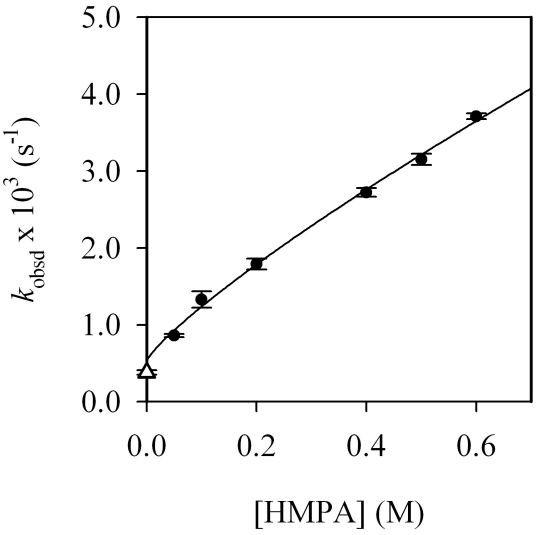


Figure 55. Plot of k_{obsd} versus [HMPA] in 10.0 M THF/hexanes cosolvent for the Fries rearrangement of **6b** (0.004 M) by LDA (0.10 M) at -65 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{HMPA}]^n + k'$ (k = (4.8 ± 0.2) x 10^{-3}, n = 0.8 ± 0.1, k' = (0.5 ± 0.2) x 10^{-3}). Pseudo-first-order conditions not maintained at 0.05 M HMPA (Δ); data was omitted from the fit.

[HMPA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.0	0.40 ± 0.03	0.36 ± 0.02	0.38 ± 0.03
0.05	0.87 ± 0.03	0.84 ± 0.02	0.86 ± 0.02
0.10	1.25 ± 0.02	1.40 ± 0.04	1.3 ± 0.1
0.20	1.74 ± 0.01	1.84 ± 0.02	1.79 ± 0.07
0.40	2.76 ± 0.01	2.68 ± 0.02	2.72 ± 0.06
0.50	3.10 ± 0.02	3.20 ± 0.05	3.15 ± 0.07
0.60	3.68 ± 0.05	3.73 ± 0.01	3.71 ± 0.04

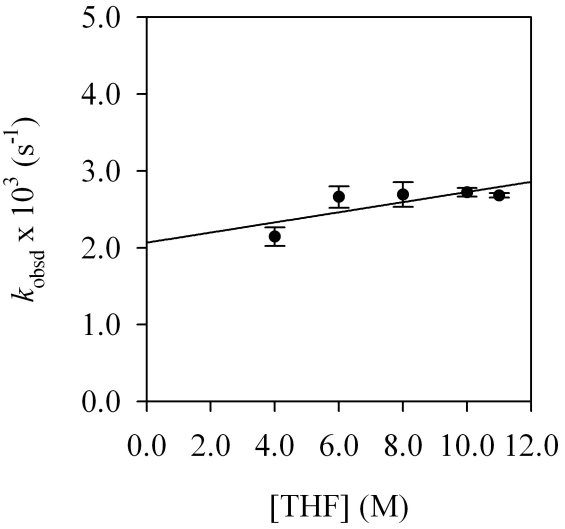


Figure 56. Plot of k_{obsd} versus [THF] in 0.40 M HMPA/hexanes cosolvent for the Fries rearrangement of **6b** (0.004 M) by LDA (0.10 M) at -65 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[HMPA] + k' (k = (7 ± 3) x 10^{-5}, k' = (2.1 ± 0.3) x 10^{-3}).

[THF] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
4.0	2.06 ± 0.02	2.23 ± 0.04	2.1 ± 0.1
6.0	2.76 ± 0.01	2.56 ± 0.01	2.7 ± 0.1
8.0	2.80 ± 0.01	2.58 ± 0.01	2.7 ± 0.2
10.0	2.76 ± 0.02	2.68 ± 0.01	2.72 ± 0.06
11.0	2.66 ± 0.02	2.70 ± 0.02	2.68 ± 0.03

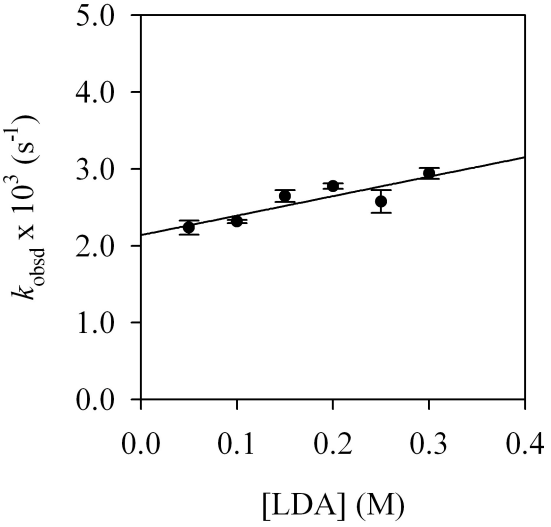


Figure 57. Plot of k_{obsd} versus [LDA] in 0.40 M HMPA/10.0 M THF/hexanes for the Fries rearrangement of **6b** (0.004 M) at -65 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[LDA] + k' (k = (2.5 ± 0.7) x 10^{-3}, k' = (2.1 ± 0.1) x 10^{-3}).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.05	2.17 ± 0.01	2.33 ± 0.02	2.24 ± 0.09
0.10	2.33 ± 0.04	2.30 ± 0.02	2.32 ± 0.02
0.15	2.59 ± 0.01	2.71 ± 0.01	2.65 ± 0.08
0.20	2.75 ± 0.01	2.80 ± 0.03	2.78 ± 0.04
0.25	2.47 ± 0.01	2.68 ± 0.05	2.6 ± 0.1
0.30	2.89 ± 0.02	2.99 ± 0.01	2.94 ± 0.07

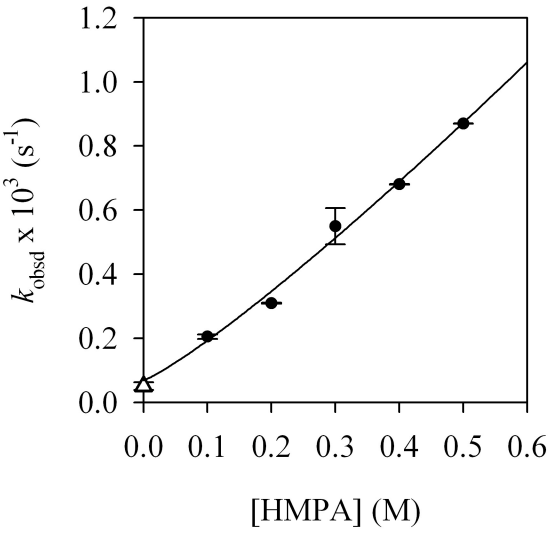


Figure 58. Plot of k_{obsd} versus [HMPA] in 10.0 M THF/hexanes cosolvent for the Fries rearrangement of **6d** (0.004 M) by LDA (0.10 M) at -78 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{HMPA}]^n + k'$ ($k = (1.8 \pm 0.3) \times 10^{-3}$, $n = 1.2 \pm 0.3$, $k' = (0.7 \pm 10) \times 10^{-4}$). Pseudo-first-order conditions not maintained at 0.05 M HMPA (Δ); data was omitted from the fit.

[HMPA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.0	0.04 ± 0.01	0.06 ± 0.01	0.05 ± 0.01
0.10	0.21 ± 0.01	0.21 ± 0.01	0.21 ± 0.01
0.20	0.31 ± 0.01	0.31 ± 0.01	0.31 ± 0.01
0.30	0.51 ± 0.01	0.59 ± 0.01	0.55 ± 0.06
0.40	0.68 ± 0.01	0.68 ± 0.01	0.68 ± 0.01
0.50	0.87 ± 0.01	0.87 ± 0.01	0.87 ± 0.01

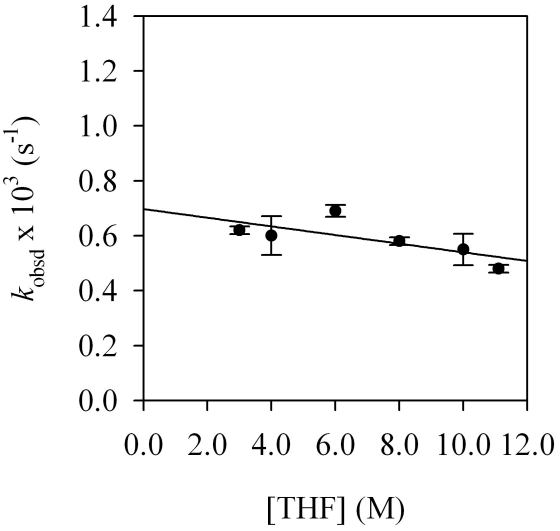


Figure 59. Plot of k_{obsd} versus [THF] in 0.40 M HMPA/hexanes cosolvent for the Fries rearrangement of **6d** (0.004 M) by LDA (0.10 M) at -78 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[HMPA] + k' (k = (-1.6 ± 0.7) x 10^{-5}, k' = (0.70 ± 0.06) x 10^{-3}).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
3.0	0.61 ± 0.01	0.63 ± 0.01	0.62 ± 0.01
4.0	0.55 ± 0.02	0.65 ± 0.01	0.60 ± 0.07
6.0	0.70 ± 0.01	0.67 ± 0.01	0.69 ± 0.02
8.0	0.59 ± 0.01	0.57 ± 0.01	0.58 ± 0.01
10.0	0.51 ± 0.01	0.59 ± 0.01	0.55 ± 0.06
11.1	0.47 ± 0.02	0.49 ± 0.01	0.48 ± 0.01

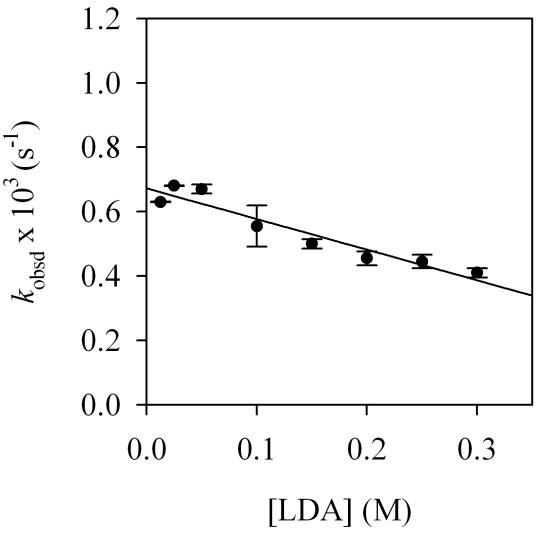


Figure 60. Plot of k_{obsd} versus [LDA] in 0.40 M HMPA/10.0 M THF/hexanes for the Fries rearrangement of **6d** (0.004 M) at -78 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[LDA] + k' (k = (-0.9 ± 0.1) x 10^{-3}, k' = (0.67 ± 0.02) x 10^{-3}).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.013	0.63 ± 0.01	0.63 ± 0.01	0.63 ± 0.01
0.025	0.68 ± 0.01	0.68 ± 0.01	0.68 ± 0.01
0.050	0.66 ± 0.01	0.68 ± 0.01	0.67 ± 0.01
0.10	0.60 ± 0.01	0.51 ± 0.01	0.56 ± 0.06
0.15	0.49 ± 0.01	0.51 ± 0.01	0.50 ± 0.01
0.20	0.47 ± 0.01	0.44 ± 0.01	0.46 ± 0.02
0.25	0.43 ± 0.01	0.46 ± 0.01	0.45 ± 0.02
0.30	0.40 ± 0.01	0.42 ± 0.01	0.41 ± 0.01

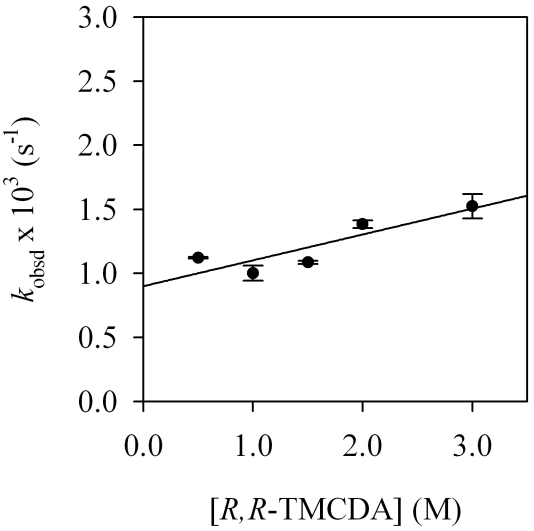


Figure 61. Plot of k_{obsd} versus [*R,R*-TMCDA] in toluene cosolvent for the Fries rearrangement of **6g** (0.004 M) by LDA (0.10 M) at -25 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k$[*R,R*-TMCDA] + k' (k = (2.0 ± 0.4) x 10^{-4}, k' = (9.0 ± 0.8) x 10^{-4}).

[*R,R*-TMCDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.5	1.12 ± 0.02	1.13 ± 0.02	1.13 ± 0.01
1.0	1.04 ± 0.01	0.96 ± 0.01	1.00 ± 0.06
1.5	1.08 ± 0.01	1.09 ± 0.01	1.09 ± 0.01
2.0	1.41 ± 0.01	1.36 ± 0.02	1.39 ± 0.04
3.0	1.59 ± 0.02	1.46 ± 0.02	1.53 ± 0.09

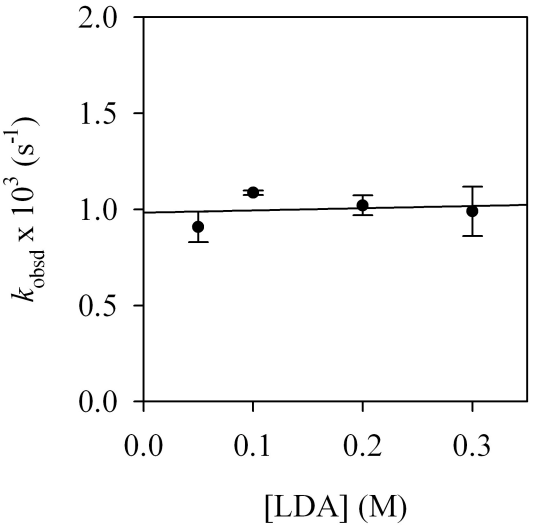


Figure 62. Plot of k_{obsd} versus [LDA] in 1.5 M *R,R*-TMCDA/toluene for the Fries rearrangement of **6g** (0.004 M) at -25 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[\text{LDA}] + k'$ ($k = (1 \pm 4) \times 10^{-4}$, $k' = (9.8 \pm 0.7) \times 10^{-4}$).

[LDA] (M)	k_{obsd} 1 x 10^3 (s^{-1})	k_{obsd} 2 x 10^3 (s^{-1})	k_{obsd} avg x 10^3 (s^{-1})
0.05	0.96 ± 0.01	0.85 ± 0.01	0.91 ± 0.08
0.10	1.08 ± 0.01	1.09 ± 0.01	1.09 ± 0.01
0.20	1.06 ± 0.01	0.98 ± 0.01	1.02 ± 0.06
0.30	1.08 ± 0.01	0.90 ± 0.01	0.99 ± 0.12

Table 4. Data from Figures 61 and 62 fit to $[\mathbf{6g}] = \{(\alpha\text{-}1)k_{obsd}t + [\mathbf{6g}]_0^{-(1-\alpha)}\}^{-1/(\alpha-1)}$ to determine the order of the decay. The adjustable parameter α corresponds to the reaction order in **6g**.[1]

[*R,R*-TMCDA] (M)	[LDA] (M)	α 1	α 2
0.5	0.10	1.09 ± 0.02	1.00 ± 0.02
1.0	0.10	1.01 ± 0.01	0.87 ± 0.01
1.5	0.10	1.02 ± 0.01	1.05 ± 0.01
2.0	0.10	1.06 ± 0.01	1.24 ± 0.01
3.0	0.10	0.91 ± 0.01	0.93 ± 0.01
1.5	0.05	0.93 ± 0.01	1.00 ± 0.01
1.5	0.20	0.95 ± 0.01	0.95 ± 0.01
1.5	0.30	1.10 ± 0.02	0.96 ± 0.01

Average $\alpha = 1.01 \pm 0.10$

Computational Studies. Calculations based on density functional theory (DFT) were performed at the B3LYP/6-31G(d) level of theory using Gaussian 03 and visualized with GaussView 3.09.[3,4] Gibbs free energies (ΔG^{o}, kcal/mol) include thermal corrections at 298 K. Calculated transition structures were shown to be legitimate saddle points by the existence of a single imaginary frequency. The alkyl groups on the carbamate were modeled as methyl groups and LDA was modeled as lithium dimethylamide. THF and *n*-BuOMe were modeled as dimethylether. TMCDA was modeled as TMEDA. The following equilibrium equations have been balanced, so the energies can be compared.

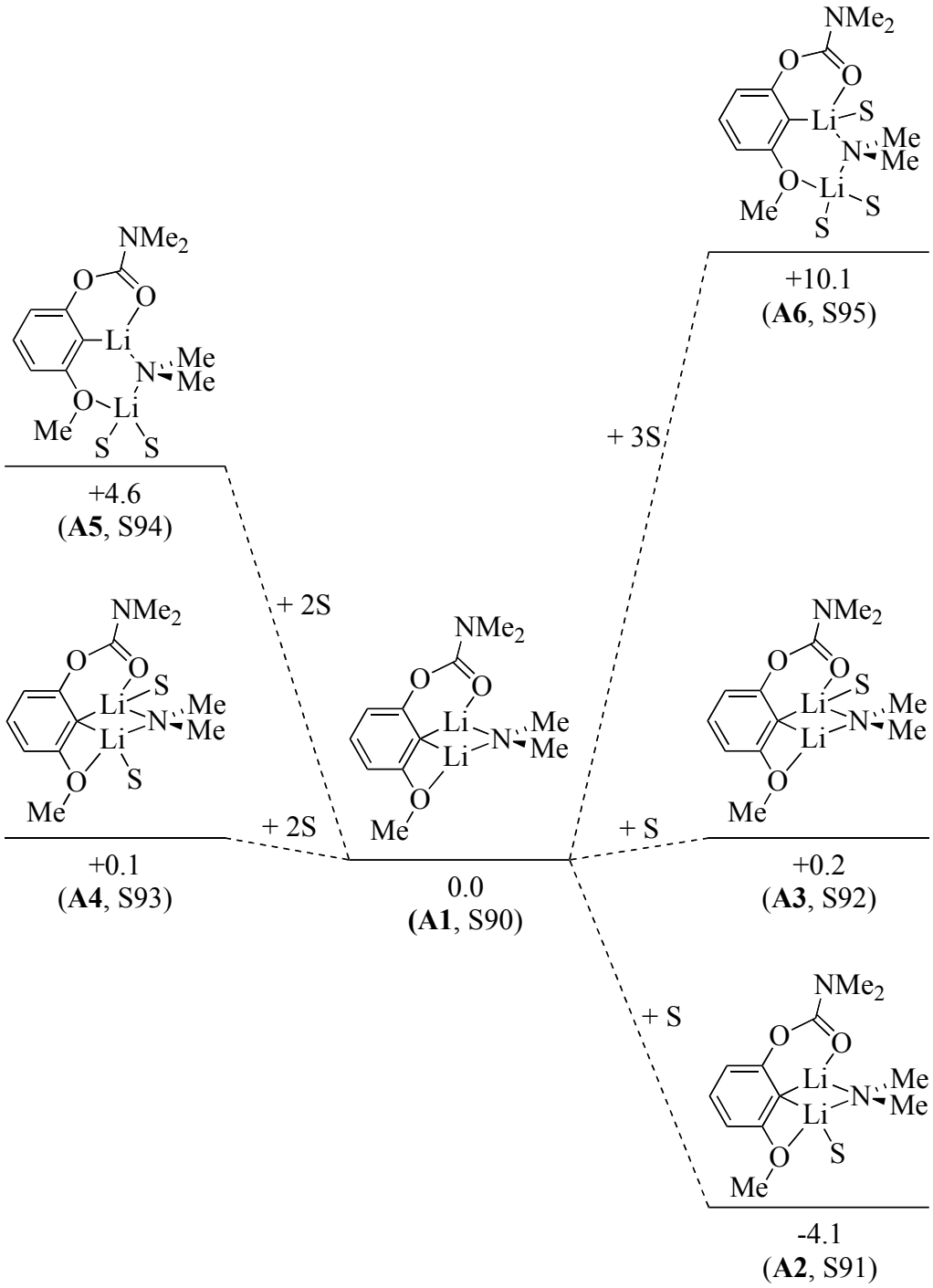


Figure 63. Relative free energies (ΔG°, kcal/mol). S = Me_2O

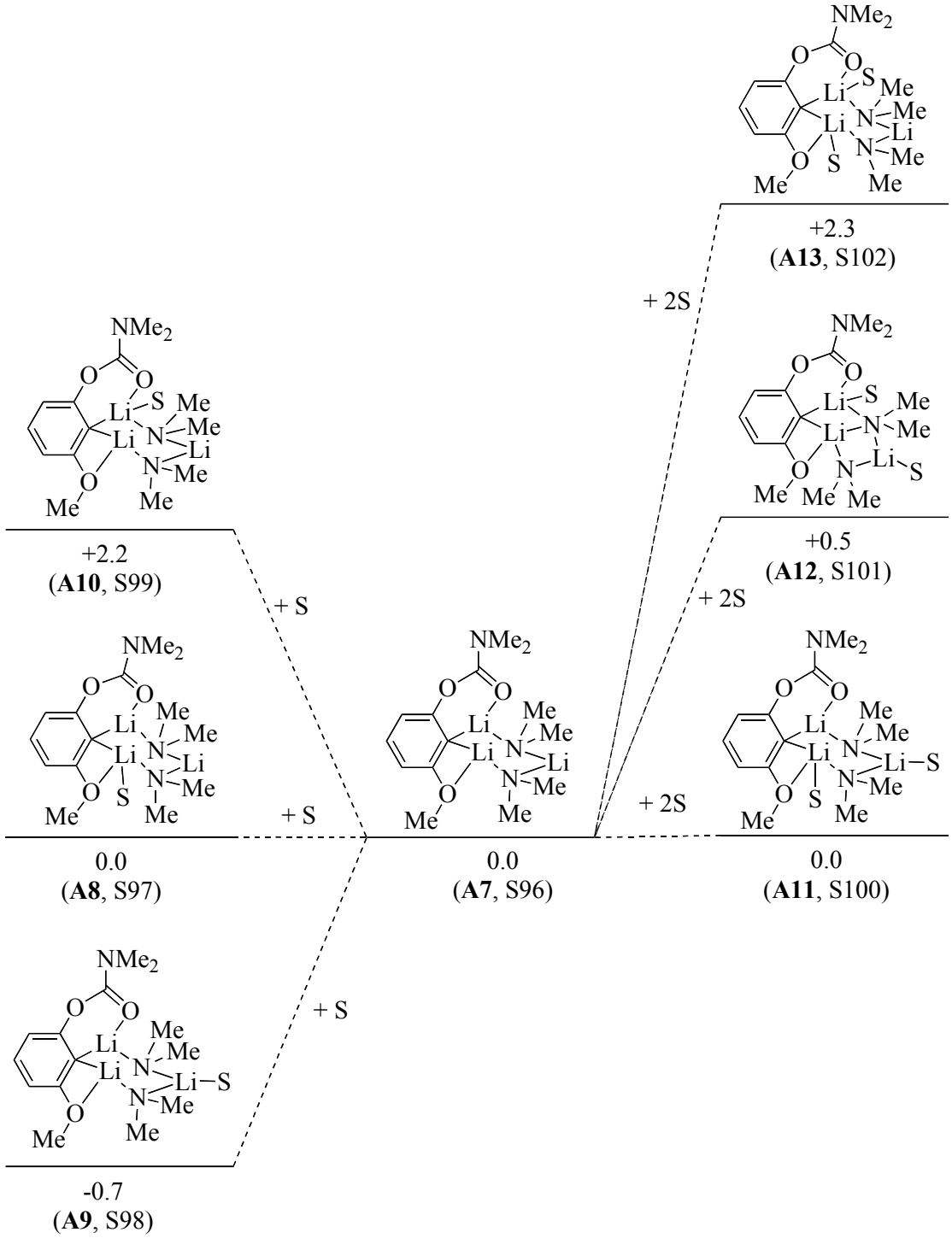


Figure 64. Relative free energies (ΔG°, kcal/mol). S = Me_2O

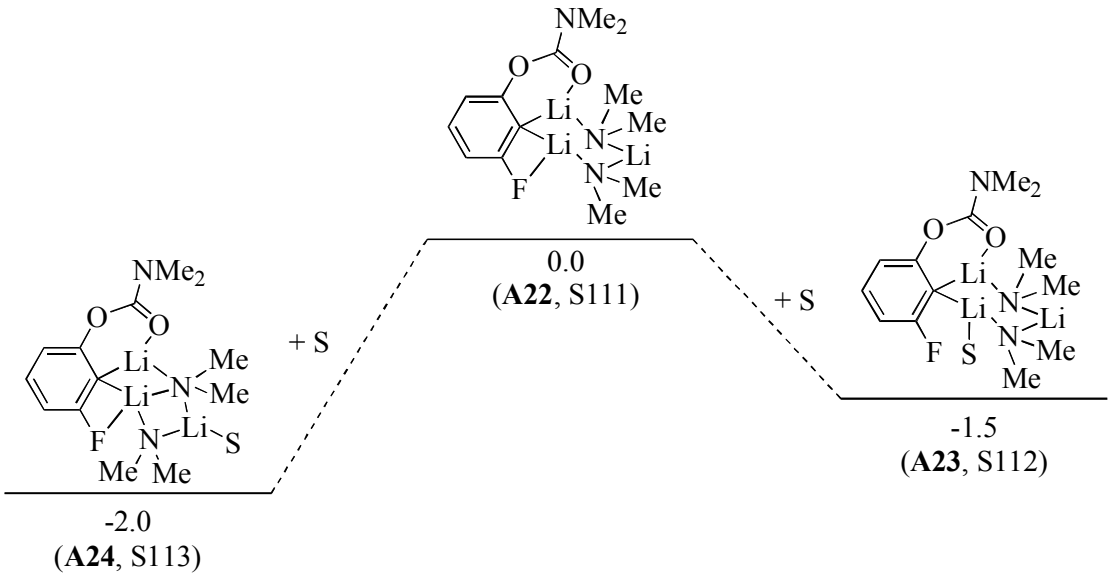


Figure 65. Relative free energies ($\Delta G°$, kcal/mol). S = Me_2O

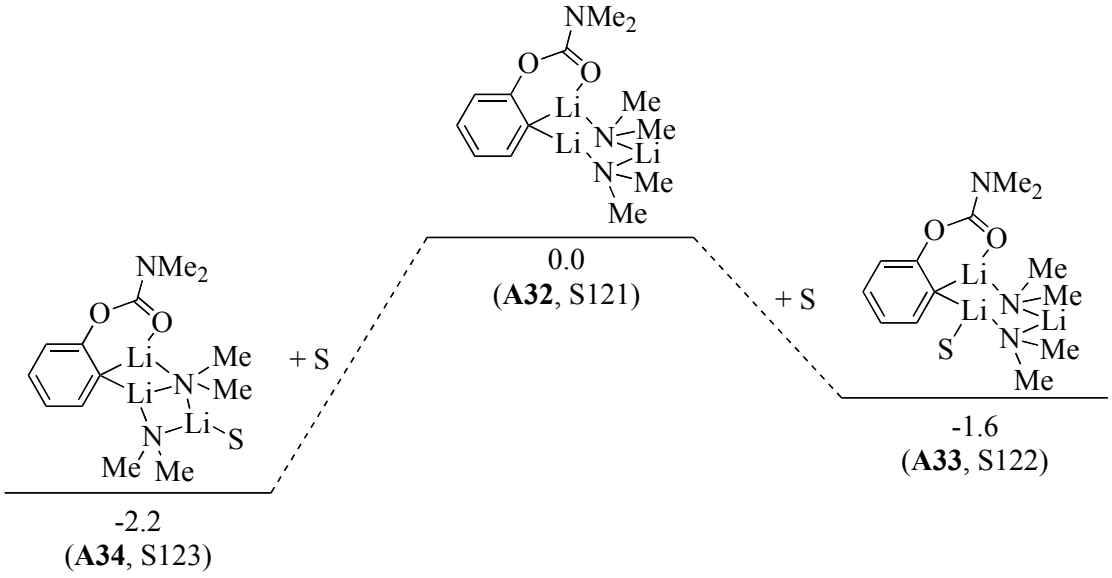


Figure 66. Relative free energies ($\Delta G°$, kcal/mol). S = Me_2O

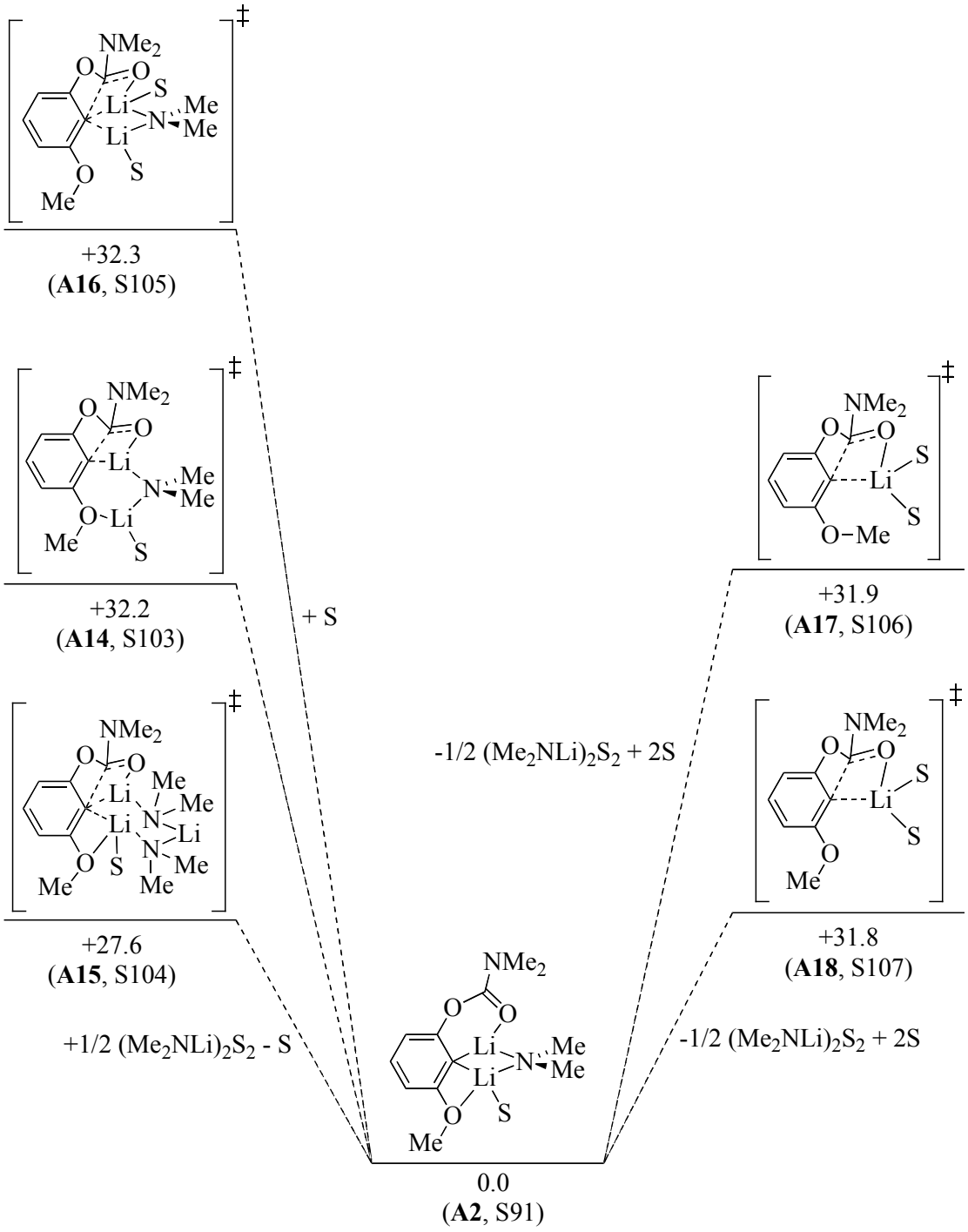


Figure 67. Relative free energies (ΔG°, kcal/mol). S = Me_2O.

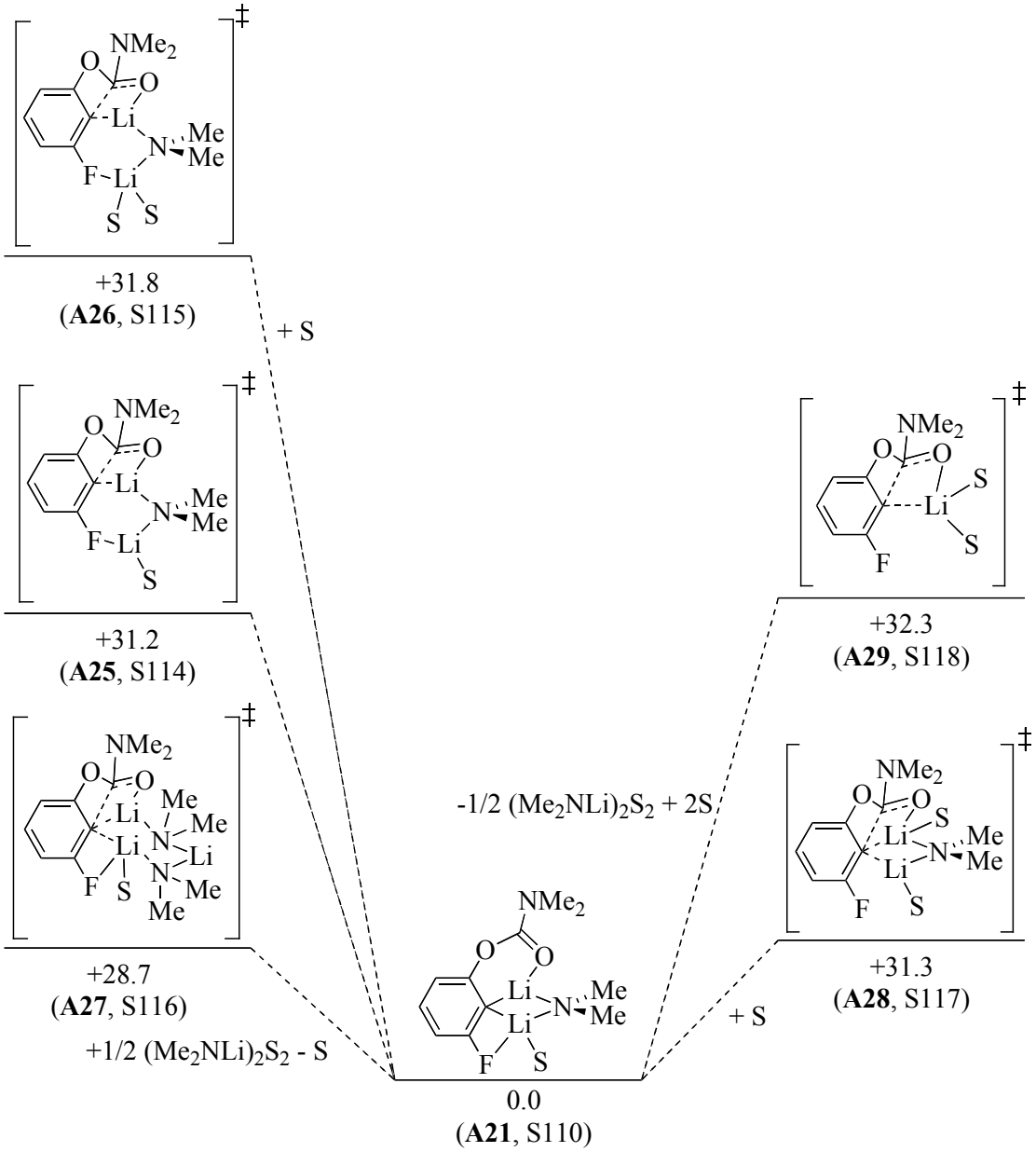


Figure 68. Relative free energies (ΔG°, kcal/mol). S = Me_2O.

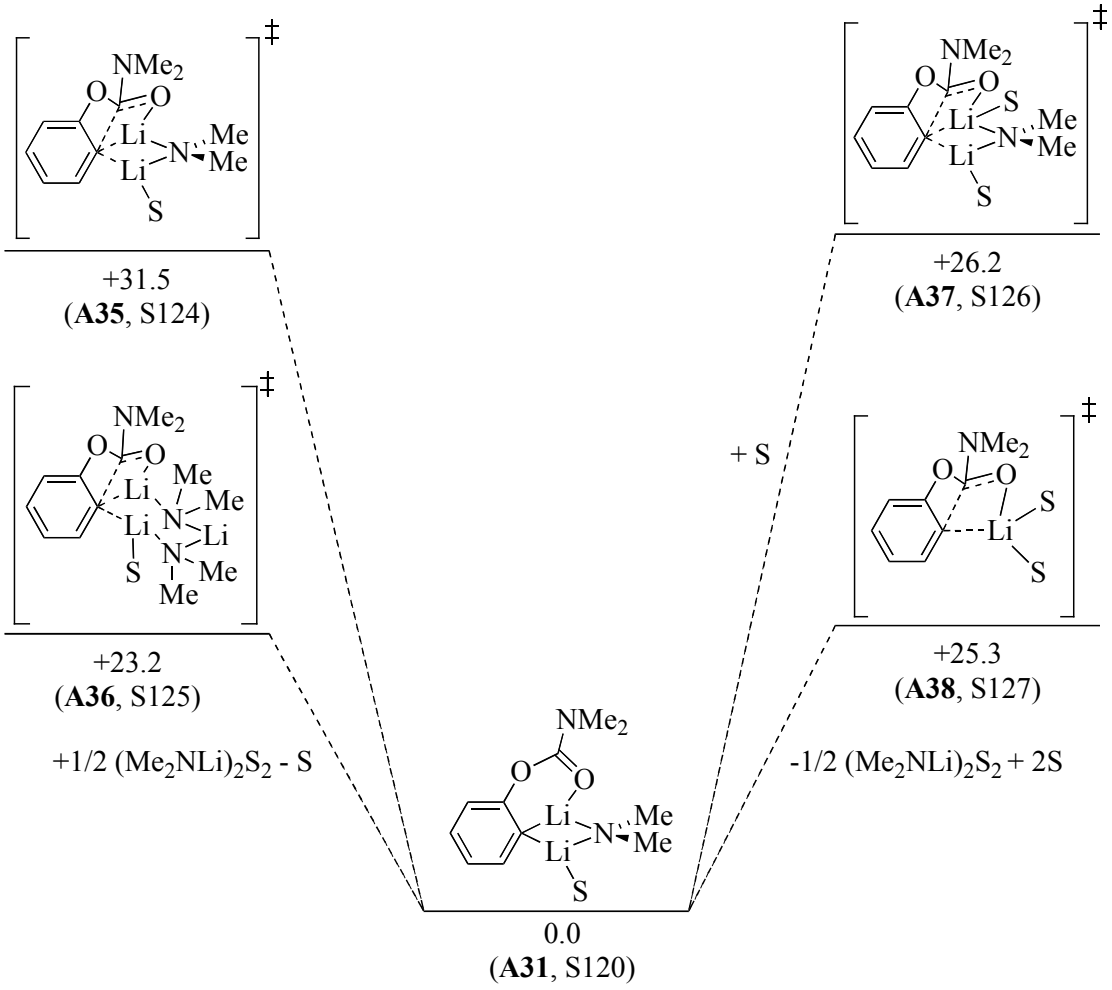


Figure 69. Relative free energies (ΔG°, kcal/mol). S = Me_2O.

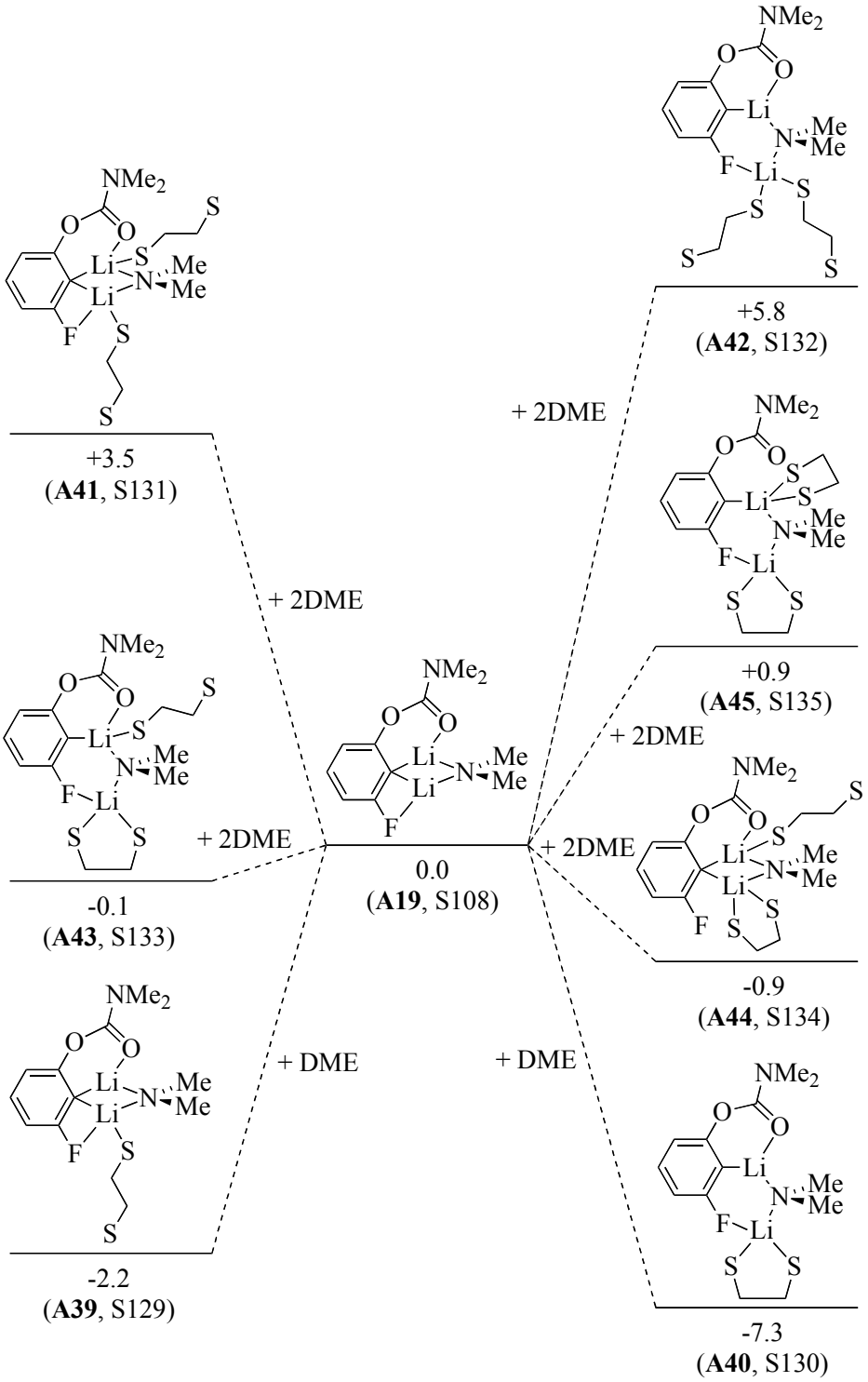


Figure 70. Relative free energies (ΔG°, kcal/mol). S = OMe.

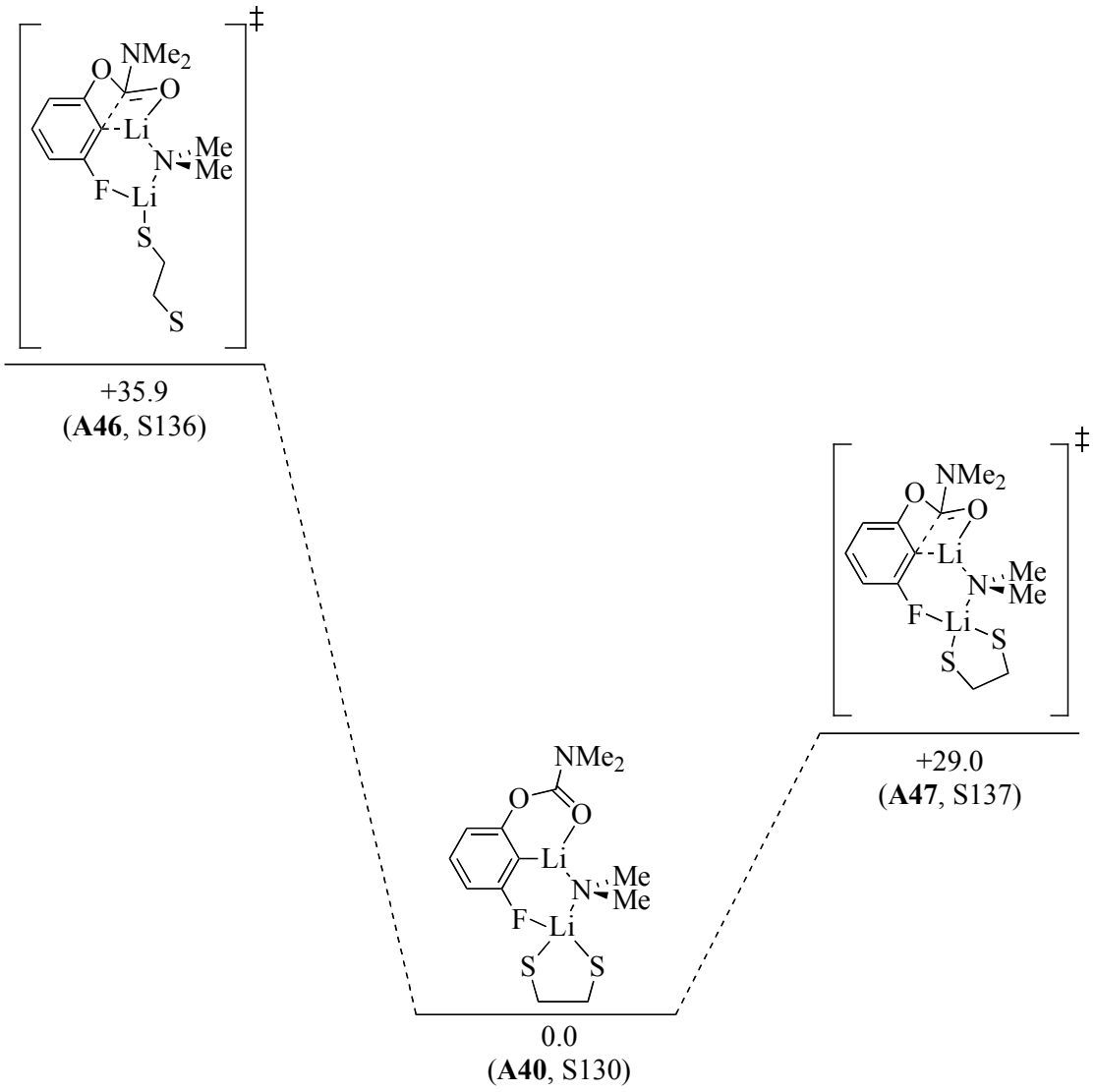


Figure 71. Relative free energies (ΔG°, kcal/mol). S = OMe.

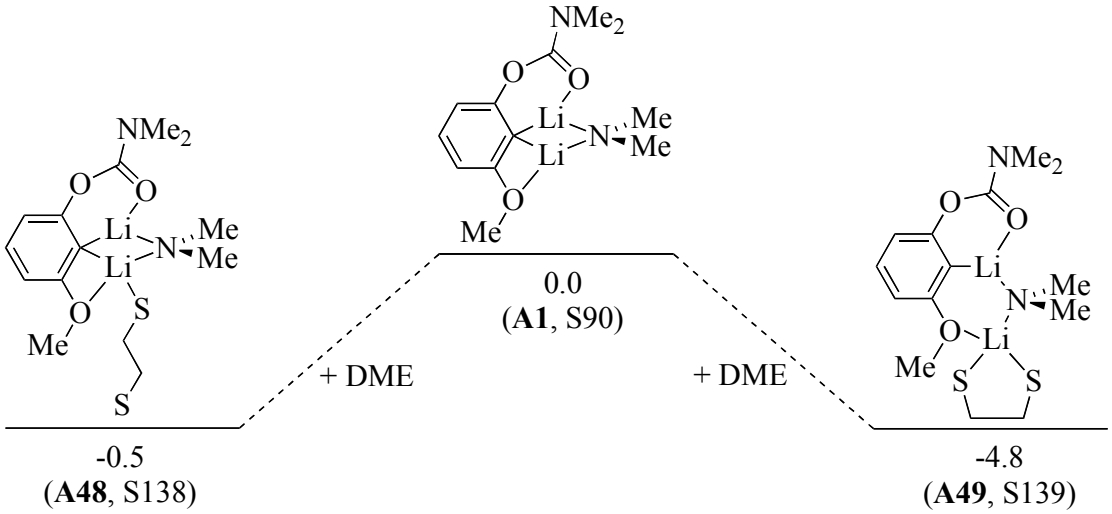


Figure 72. Relative free energies (ΔG°, kcal/mol). S = OMe.

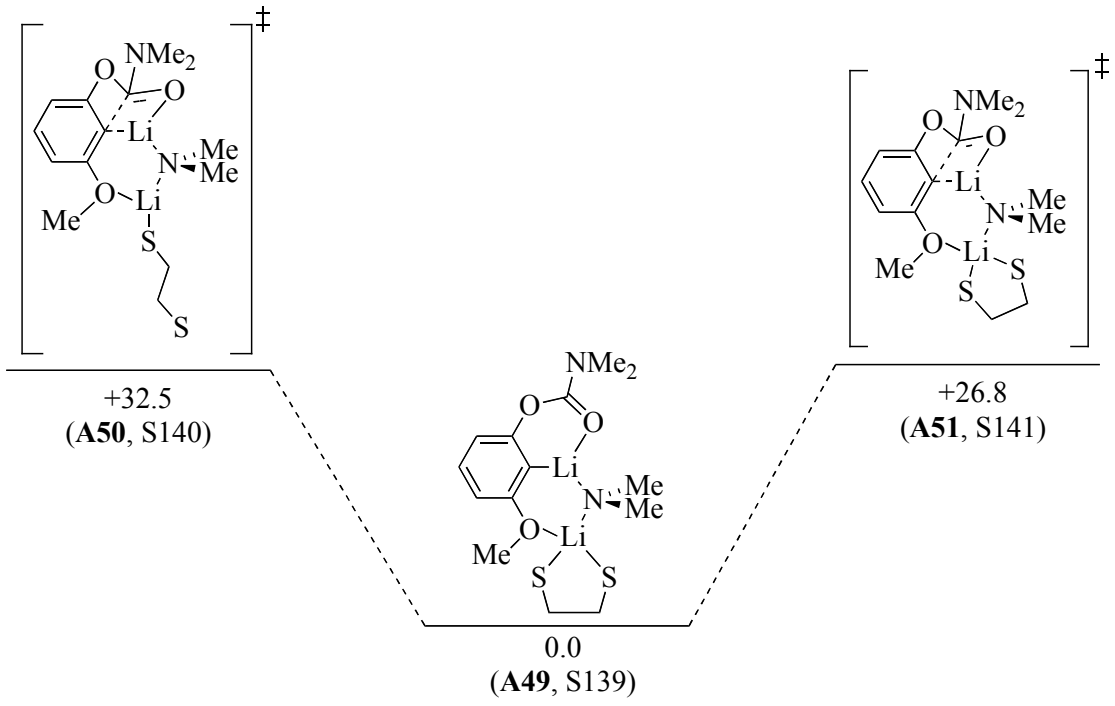


Figure 73. Relative free energies (ΔG°, kcal/mol). S = OMe.

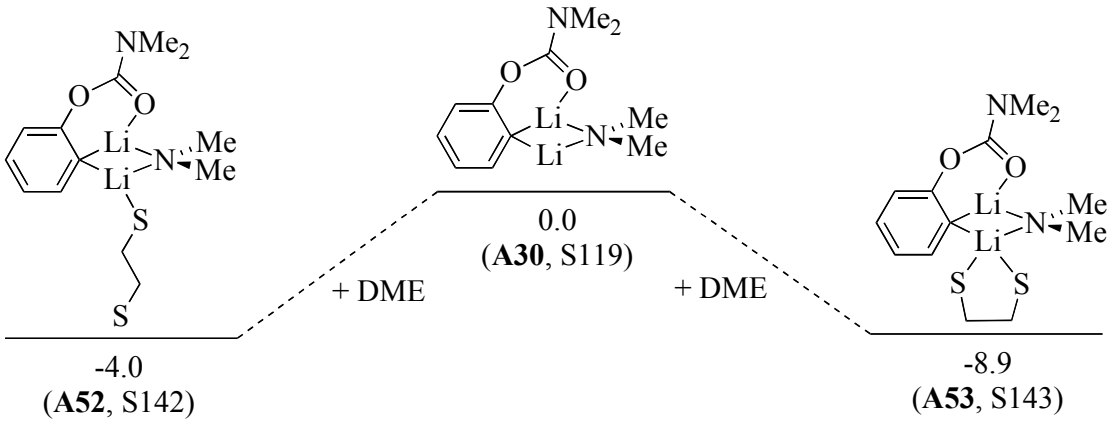


Figure 74. Relative free energies (Δ*G*°, kcal/mol). S = OMe.

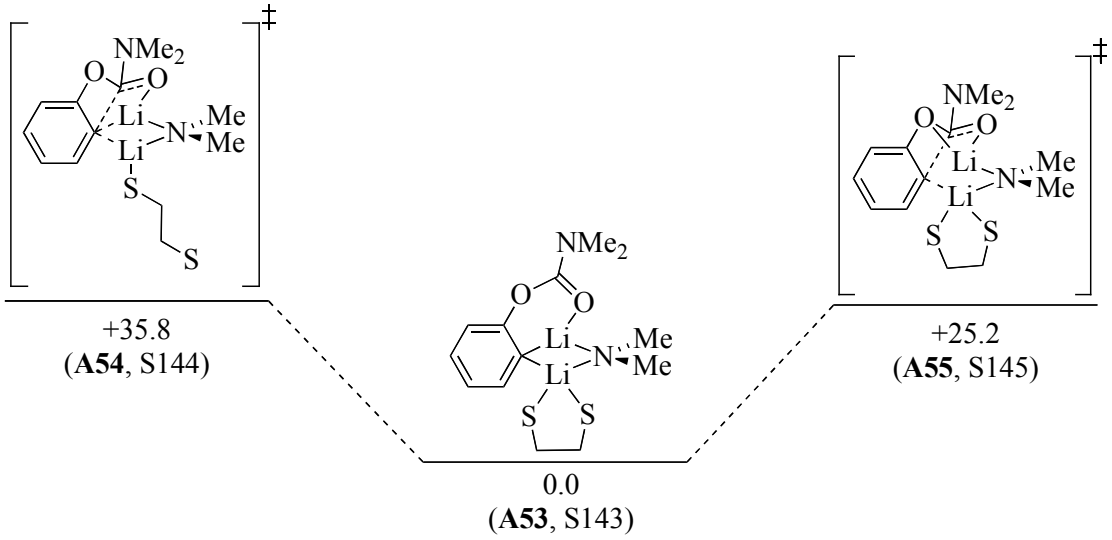


Figure 75. Relative free energies (Δ*G*°, kcal/mol). S = OMe.

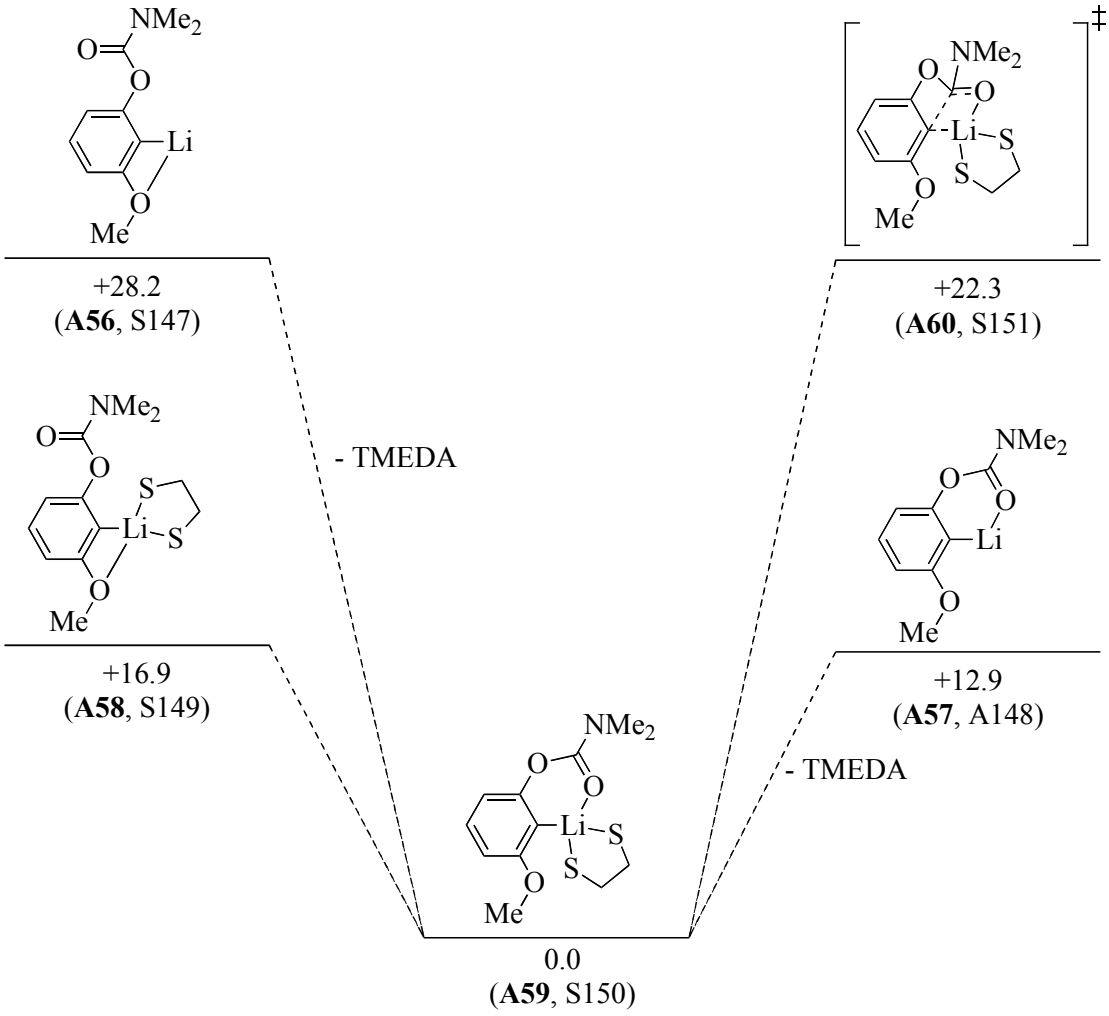


Figure 76. Relative free energies (ΔG°, kcal/mol). S = NMe_2

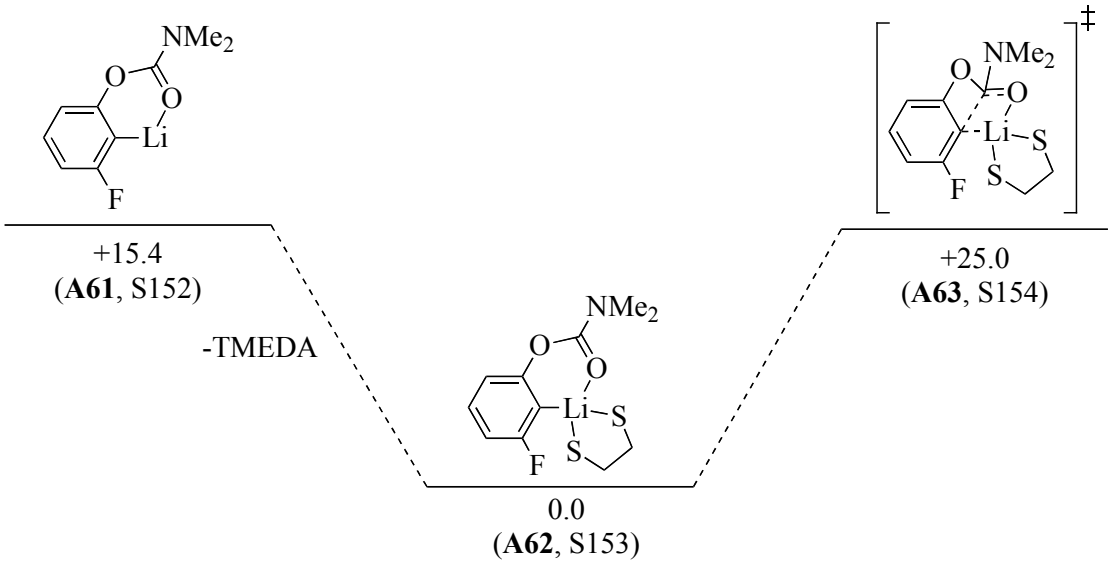


Figure 77. Relative free energies ($\Delta G°$, kcal/mol). S = NMe_2

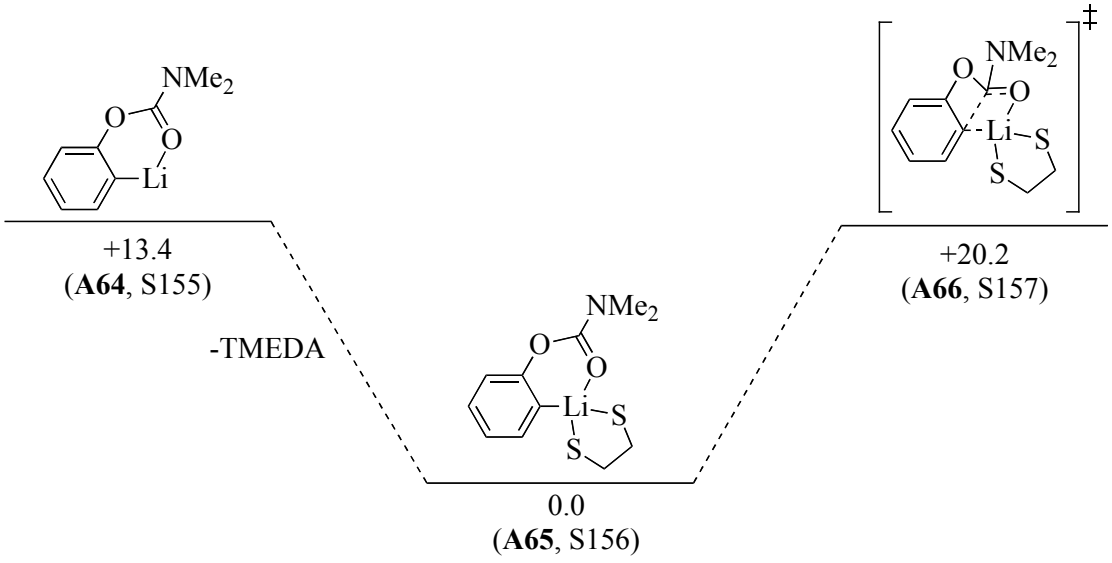


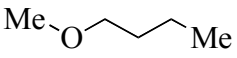
Figure 78. Relative free energies ($\Delta G°$, kcal/mol). S = NMe_2

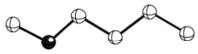
Table 5. Optimized geometry, free energy ($G°$, Hartrees), and cartesian coordinates (X,Y,Z).

$G° = -154.970104$

Atom	X	Y	Z
O	0.000000	-0.590089	0.000004
C	1.170987	0.195371	0.000000
H	2.021836	-0.491272	-0.000151
H	1.232054	0.839804	-0.892910
H	1.232210	0.839598	0.893048
C	-1.170987	0.195371	0.000000
H	-1.231991	0.839904	-0.892842
H	-2.021836	-0.491272	-0.000291
H	-1.232273	0.839498	0.893116

Table 5 (Continued).

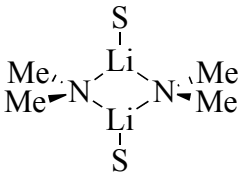


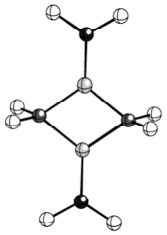


$G°$ = -272.837541

Atom	X	Y	Z
C	-0.718160	0.391824	0.000007
C	0.596507	-0.377710	-0.000006
H	-0.781230	1.046943	0.887608
H	-0.781197	1.047033	-0.887529
C	1.826039	0.539091	-0.000020
H	0.616898	-1.034219	0.879944
H	0.616872	-1.034215	-0.879960
H	1.790202	1.199235	-0.878403
H	1.790190	1.199285	0.878325
C	3.147212	-0.235672	0.000010
H	4.007874	0.442764	0.000069
H	3.229139	-0.878979	0.884609
H	3.229215	-0.878919	-0.884626
O	-1.788791	-0.535788	-0.000060
C	-3.052409	0.089182	0.000047
H	-3.806358	-0.702842	-0.000044
H	-3.198185	0.719847	0.892862
H	-3.198222	0.720083	-0.892596

Table 5 (Continued).

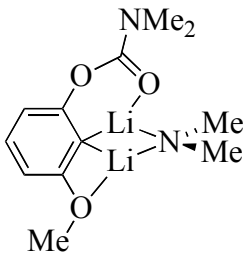


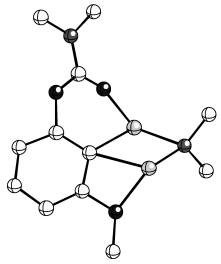


$G°$ = -594.095732
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.136511	-2.431283	1.173404	O	-3.111067	0.000030	-0.087085
H	-1.020755	-3.109124	1.137695	O	3.111459	-0.000164	0.087764
H	0.732546	-3.107438	1.343485	N	0.000005	-1.588870	0.002534
H	-0.243398	-1.821323	2.084300	C	-3.884200	-1.192867	-0.019656
C	0.136331	-2.431260	-1.168356	H	-4.450405	-1.235823	0.921141
H	-0.732822	-3.107320	-1.338380	H	-4.583949	-1.250871	-0.864779
H	0.243193	-1.821290	-2.079255	H	-3.181010	-2.026301	-0.063773
H	1.020486	-3.109225	-1.132764	C	-3.884891	1.192437	-0.019084
C	-0.136240	2.431889	1.173197	H	-4.584677	1.250446	-0.864176
H	-0.243018	1.822120	2.084233	H	-4.451120	1.234618	0.921734
H	0.732794	3.108127	1.343054	H	-3.182197	2.026311	-0.062810
H	-1.020526	3.109669	1.137406	C	3.884396	1.192366	0.012017
C	0.136543	2.431376	-1.168571	H	4.592508	1.250489	0.850131
H	0.243360	1.821213	-2.079350	H	4.441276	1.234591	-0.934371
H	-0.732597	3.107418	-1.338708	H	3.182070	2.026159	0.062599
H	1.020721	3.109319	-1.133145	C	3.884107	-1.192891	0.012183
Li	-1.176805	0.000271	-0.097749	H	4.441018	-1.235357	-0.934176
Li	1.177040	0.000115	0.102833	H	4.592169	-1.251090	0.850334
N	0.000237	1.589228	0.002502	H	3.181577	-2.026507	0.062827

Table 5 (Continued).

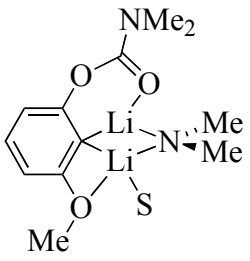


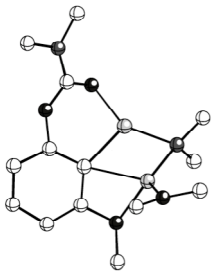


A1
G° = -818.192237
See pp S75 and S83

Atom	X	Y	Z	Atom	X	Y	Z
C	2.270501	-2.533822	-0.182127	H	1.305036	-4.413541	-0.613829
C	1.159825	-3.363728	-0.374591	H	3.270839	-2.945209	-0.265146
C	-0.123650	-2.846909	-0.249645	H	-1.001026	-3.472898	-0.381585
C	-0.263244	-1.488758	0.063712	H	2.626820	2.803936	-1.521787
C	0.772645	-0.583725	0.253390	H	1.498924	4.175230	-1.552338
C	2.032776	-1.192836	0.117127	H	2.851269	4.174900	-0.413689
Li	1.965263	1.194949	0.841356	H	-3.606565	-1.863559	1.025763
O	-1.663274	0.801906	-0.926709	H	-4.651942	-0.610571	1.735841
Li	0.054816	1.378698	-0.528572	H	-5.124333	-1.403235	0.215174
N	1.267670	2.809818	0.092768	H	-5.149281	0.777752	-1.093390
C	0.576787	3.781726	0.924286	H	-4.816987	1.620526	0.439122
C	2.087019	3.515682	-0.878213	H	-3.709624	1.819006	-0.945664
C	-2.231915	-0.066535	-0.246313	H	-0.057204	3.275843	1.669918
O	-1.636691	-1.141825	0.284424	H	1.264843	4.446939	1.488454
N	-3.560169	-0.016356	0.034904	H	-0.085907	4.462972	0.347644
C	-4.353079	1.117380	-0.418777	O	3.100987	-0.291252	0.345884
C	-4.270710	-1.034065	0.797514	C	4.441026	-0.734356	0.186691
H	5.076604	0.133321	0.374408	H	4.684801	-1.527484	0.904272
H	4.614921	-1.100061	-0.832333				

Table 5 (Continued).

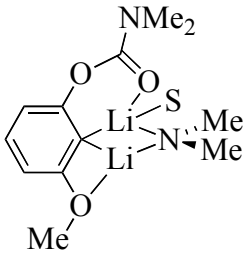


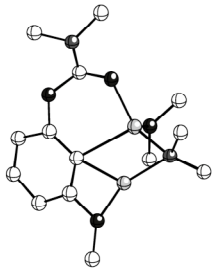


A2
G° = -973.168918
See pp S75 and S78
Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.029163	3.217527	-0.494364	H	4.851929	-0.780213	2.168090
C	0.237888	3.775051	-0.282558	H	5.563331	0.325874	0.971084
C	1.328182	2.951946	-0.026765	H	5.440690	-1.687711	-0.720260
C	1.110852	1.568497	0.012214	H	4.669052	-2.672538	0.545760
C	-0.100074	0.923270	-0.186387	H	3.814988	-2.367489	-0.991137
C	-1.145448	1.826484	-0.446262	H	-0.457650	-3.453153	0.107831
Li	-1.792823	-0.652031	-0.005018	H	-1.997563	-4.023054	-0.573698
O	2.128882	-0.833335	-1.153409	H	-0.531238	-4.072998	-1.555758
Li	0.260446	-0.936160	-1.252080	O	-2.380768	1.181443	-0.643980
N	-1.320883	-2.094293	-1.253395	C	-3.536128	1.954677	-0.922311
C	-1.070137	-3.450012	-0.807883	H	-4.356411	1.245216	-1.048784
C	-2.125136	-2.136461	-2.461038	H	-3.770423	2.639835	-0.096731
C	2.708239	-0.267777	-0.214375	H	-3.412134	2.534347	-1.845601
O	2.300054	0.857596	0.385414	O	-2.583747	-0.967609	1.772165
N	3.866215	-0.745537	0.318751	C	-2.328792	-0.123477	2.888486
C	4.481654	-1.937223	-0.246445	H	-1.867874	0.786627	2.501100
C	4.617328	-0.068817	1.366805	H	-3.263576	0.124122	3.410668
H	0.365552	4.853664	-0.318529	H	-1.640067	-0.609133	3.593948
H	-1.875635	3.867422	-0.691130	C	-3.134908	-2.229618	2.131117
H	2.320319	3.360288	0.141794	H	-2.465165	-2.766263	2.817365
H	-2.329256	-1.117862	-2.825095	H	-4.115364	-2.101909	2.610967
H	-1.642597	-2.687392	-3.298550	H	-3.242908	-2.802353	1.208894
H	-3.112548	-2.631560	-2.318865	H	4.032855	0.750457	1.777517

Table 5 (Continued).

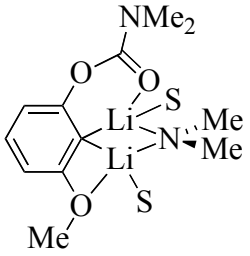


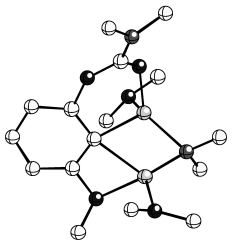


A3
$G°$ = -973.161962
See pg S75
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.131016	-2.786077	0.184986	H	3.762067	-2.221612	-0.951753
C	-1.090786	-3.486031	0.810703	H	5.083910	-1.167492	-1.504581
C	0.211999	-3.003590	0.752578	H	5.062997	-1.758824	0.172874
C	0.443624	-1.806350	0.062177	H	5.123816	0.901226	0.734788
C	-0.521137	-1.033202	-0.564076	H	4.989127	1.217308	-1.011995
C	-1.802148	-1.597927	-0.469333	H	3.727929	1.811187	0.099357
Li	-1.398631	0.487454	-1.791492	H	0.903269	2.167787	-2.441837
O	1.733416	0.725699	0.453063	H	-0.234529	3.370679	-3.088792
Li	-0.087528	1.159914	0.136568	H	0.668903	3.720357	-1.610023
N	-0.904673	2.272571	-1.361959	O	-2.776388	-0.821259	-1.143447
C	0.138079	2.904015	-2.150774	C	-4.109037	-1.300157	-1.230749
C	-1.890518	3.271260	-1.002722	H	-4.664501	-0.564483	-1.816087
C	2.347932	-0.273804	0.063790	H	-4.148518	-2.274699	-1.733855
O	1.837697	-1.510150	-0.040433	H	-4.565577	-1.390611	-0.236841
N	3.664385	-0.236243	-0.286073	O	-0.820139	1.509430	1.988818
C	4.418328	0.994749	-0.102887	C	-2.157598	1.187322	2.342752
C	4.431863	-1.416411	-0.659582	H	-2.848302	1.992271	2.054215
H	-1.304564	-4.414367	1.333587	H	-2.415173	0.271361	1.807922
H	-3.142316	-3.178688	0.218599	H	-2.238871	1.012890	3.425156
H	1.035324	-3.540202	1.214848	C	-0.339551	2.678935	2.638057
H	-2.705924	2.820467	-0.416069	H	-0.930347	3.560481	2.352528
H	-1.475274	4.103944	-0.389083	H	-0.373844	2.557189	3.730060
H	-2.363227	3.767196	-1.878684	H	0.697238	2.814076	2.323137

Table 5 (Continued).

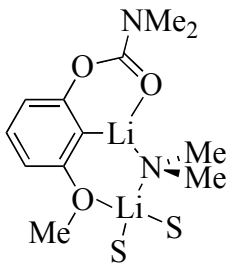


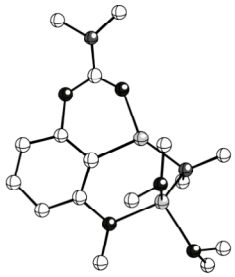


A4
$G°$ = -1128.132284
See pg S75
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	1.476647	3.102685	-0.565074	H	-0.446619	-3.128025	-0.059299
C	0.267918	3.784336	-0.762476	H	0.973204	-4.122531	0.341798
C	-0.930261	3.081551	-0.830257	H	-0.192236	-3.706114	1.601601
C	-0.881536	1.687400	-0.695324	O	2.576984	0.934918	-0.225017
C	0.257628	0.929003	-0.485408	C	3.848912	1.555134	-0.291138
C	1.421507	1.712340	-0.430009	H	4.585933	0.758772	-0.168228
Li	1.521938	-0.884765	-0.514391	H	4.004367	2.050837	-1.258793
O	-2.081312	-0.428842	0.812277	H	3.978708	2.293377	0.511562
Li	-0.208018	-0.501769	1.218661	O	2.111831	-1.594740	-2.278170
N	1.046159	-2.061958	0.973652	C	1.669201	-1.004703	-3.494136
C	0.327057	-3.289470	0.707487	H	1.475741	0.048635	-3.285138
C	2.046389	-2.316307	1.986708	H	2.439431	-1.096651	-4.272978
C	-2.603481	0.026816	-0.209777	H	0.743270	-1.481745	-3.845710
O	-2.160582	1.081758	-0.911550	C	2.360223	-2.991920	-2.390610
N	-3.745664	-0.495337	-0.745372	H	1.456714	-3.525362	-2.716878
C	-4.443750	-1.557660	-0.037973	H	3.171880	-3.183426	-3.106685
C	-4.437526	0.085379	-1.886753	H	2.646156	-3.343414	-1.398301
H	0.270845	4.866160	-0.867848	O	-0.089671	0.423619	3.034617
H	2.407715	3.659371	-0.523354	C	0.982814	1.295496	3.361216
H	-1.876903	3.588977	-0.992464	H	1.877999	0.728355	3.654145
H	2.615225	-1.400427	2.210340	H	1.196582	1.884604	2.467796
H	1.624952	-2.677742	2.954576	H	0.697386	1.967366	4.183732
H	2.793101	-3.092514	1.697594	C	-0.492756	-0.389506	4.128072
H	-3.767826	0.744430	-2.434203	H	0.327822	-1.039996	4.460763
H	-4.774136	-0.718559	-2.551881	H	-0.829014	0.232862	4.969982
H	-5.320455	0.657713	-1.567228	H	-1.325267	-1.003985	3.778875
H	-5.369429	-1.182624	0.421544	H	-3.794934	-1.956980	0.739179
H	-4.707355	-2.357842	-0.739803				

Table 5 (Continued).

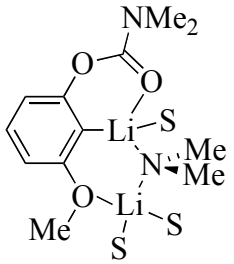


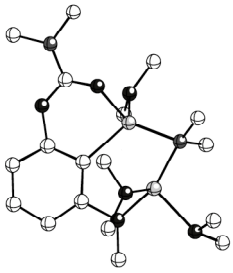


A5
$G°$ = -1128.125069
See pg S75
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.050006	3.370377	-0.646994	H	3.777656	-3.111196	-0.494132
C	1.400765	3.738332	-0.600133	H	-1.449960	-3.356418	0.422003
C	2.376594	2.775747	-0.378629	H	-2.586119	-3.555670	-0.927269
C	1.954931	1.449803	-0.210419	H	-0.882707	-3.969195	-1.143792
C	0.648759	0.990004	-0.239763	O	-1.622286	1.595757	-0.503024
C	-0.273175	2.021355	-0.469839	C	-2.634130	2.571428	-0.707759
Li	-1.954351	-0.346951	0.040473	H	-3.585779	2.041000	-0.649975
O	2.325526	-1.376388	-0.812568	H	-2.606213	3.346252	0.069890
Li	0.481312	-1.021664	-0.766043	H	-2.534884	3.050232	-1.690196
N	-1.272256	-1.855173	-1.049101	O	-4.059093	-0.392604	0.126733
C	-1.554313	-3.221077	-0.665897	C	-4.624322	-1.172375	1.176695
C	-1.414503	-1.742355	-2.491028	H	-4.110920	-0.890860	2.096167
C	3.174292	-0.697978	-0.218047	H	-5.701323	-0.972370	1.269326
O	3.077110	0.598617	0.089680	H	-4.470852	-2.244128	0.989721
N	4.355511	-1.235844	0.209643	C	-4.605772	-0.742454	-1.143217
C	4.674854	-2.614236	-0.130372	H	-4.395877	-1.792207	-1.380787
C	5.434353	-0.450044	0.791208	H	-5.691240	-0.567808	-1.154994
H	1.681060	4.779332	-0.737948	H	-4.126120	-0.107570	-1.890143
H	-0.698776	4.135055	-0.824084	O	-1.629549	-0.322952	2.095008
H	3.430885	3.033967	-0.335880	C	-0.526328	-1.101678	2.553394
H	-1.199011	-0.714662	-2.824083	H	0.420483	-0.599082	2.320024
H	-0.734095	-2.415578	-3.059954	H	-0.602538	-1.271845	3.637151
H	-2.435266	-1.989013	-2.863195	H	-0.569973	-2.058370	2.029791
H	5.053960	0.505283	1.144163	C	-1.656809	0.963075	2.707871
H	5.866111	-0.999078	1.636267	H	-1.741401	0.864898	3.799789
H	6.232531	-0.268943	0.056893	H	-0.753230	1.531754	2.457258
H	5.449784	-2.657315	-0.908761	H	-2.534310	1.486114	2.322581
H	5.049568	-3.136593	0.758025				

Table 5 (Continued).

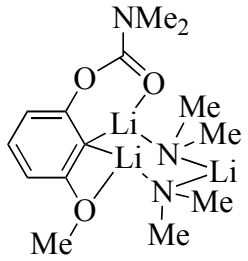


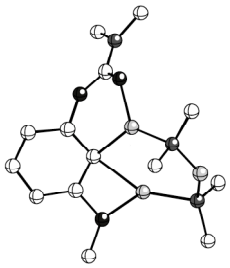


A6
$G°$ = -1283.086394
See pg S75
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.669624	3.221493	1.235059	O	1.891273	1.104910	1.321496
C	-0.520778	3.896578	0.936033	H	-3.648173	-1.857321	-2.089695
C	-1.629005	3.183818	0.494908	H	0.753867	-2.262415	-2.283009
C	-1.506881	1.791782	0.381944	H	1.970620	-3.402669	-1.665842
C	-0.380213	1.036113	0.667766	H	0.255971	-3.695070	-1.361157
C	0.696120	1.830209	1.079840	C	2.955707	1.781090	1.972260
Li	2.028576	-0.342097	-0.194134	H	3.721900	1.033052	2.182600
O	-1.981553	-0.630912	-1.136353	H	3.391983	2.567578	1.341665
Li	-0.576377	-1.034787	0.190671	H	2.618220	2.227483	2.915896
N	1.090827	-2.079373	-0.211151	O	4.162002	-0.673422	-0.296286
C	1.016539	-2.880965	-1.412490	C	4.499786	-1.219367	-1.570879
C	1.438185	-2.945242	0.893815	H	3.975696	-0.624644	-2.318957
C	-2.897070	0.102046	-0.748210	H	5.585240	-1.162866	-1.737918
O	-2.764593	1.201258	0.006907	H	4.171019	-2.264164	-1.642722
N	-4.207108	-0.131065	-1.071083	C	4.776057	-1.405191	0.758203
C	-4.559625	-1.340993	-1.794277	H	4.486793	-2.463120	0.722188
C	-5.316707	0.693186	-0.618423	H	5.871380	-1.323478	0.700367
H	-0.572908	4.976533	1.048059	H	4.432353	-0.975708	1.701105
H	1.528227	3.790601	1.577397	O	2.024208	0.854568	-1.880337
H	-2.564155	3.682126	0.254099	C	0.822502	0.967227	-2.643933
H	1.515960	-2.373247	1.832093	H	0.183602	1.763553	-2.244946
H	0.700505	-3.761780	1.077524	H	1.063680	1.174211	-3.696850
H	2.410307	-3.478410	0.760477	H	0.293867	0.018331	-2.558533
H	-4.943984	1.625476	-0.201952	C	2.752599	2.075108	-1.842868
H	-5.978322	0.915490	-1.465330	H	3.020883	2.397645	-2.859673
H	-5.907241	0.171297	0.148175	H	2.166254	2.864686	-1.354688
H	-5.168059	-2.006875	-1.165799	H	3.663597	1.886603	-1.270726
H	-5.141980	-1.090076	-2.690268	O	-1.824605	-1.889724	1.637409
C	-2.295798	-3.221259	1.511634	H	-1.575998	-3.938916	1.929355
H	-3.263277	-3.344170	2.021677	H	-2.420550	-3.416622	0.444477
C	-1.610540	-1.500896	2.987536	H	-1.242239	-0.474147	2.957811
H	-2.549596	-1.547560	3.558897	H	-0.864947	-2.149523	3.470011

Table 5 (Continued).

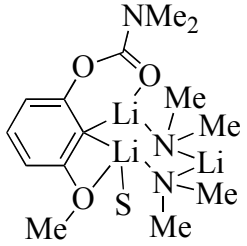


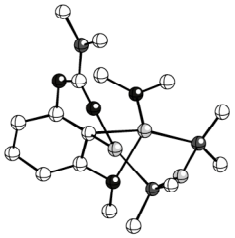


A7
G° = -960.273556
See pg 76

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.907700	3.409275	0.386237	N	-1.204538	-1.966426	1.787872
C	0.408370	3.879664	0.459958	N	-2.495636	-1.696198	-1.620509
C	1.473929	3.025277	0.196954	Li	-2.117228	-2.358124	0.154814
C	1.187363	1.695471	-0.131644	C	-2.037665	-1.286114	2.773588
C	-0.080169	1.131721	-0.207258	H	-1.457740	-0.871832	3.627233
C	-1.097447	2.065130	0.060443	H	-2.570482	-0.441850	2.311118
O	1.968627	-0.767626	0.951664	H	-2.804618	-1.944706	3.234186
C	2.631339	-0.237063	0.048806	C	-0.511223	-3.071090	2.438741
O	2.352110	0.956787	-0.498623	H	-1.199571	-3.818326	2.888012
N	3.741876	-0.807785	-0.483156	H	0.123208	-3.608772	1.718681
C	4.229489	-2.072117	0.050278	H	0.152841	-2.744924	3.267980
C	4.562966	-0.180447	-1.510606	C	-3.909764	-1.568576	-1.948394
H	0.595005	4.918679	0.716952	H	-4.444187	-1.019573	-1.157942
H	-1.734205	4.084927	0.579271	H	-4.092578	-1.024180	-2.899751
H	2.501734	3.373291	0.232327	H	-4.424930	-2.545642	-2.065356
H	4.057283	0.693354	-1.913670	C	-1.830292	-2.434306	-2.687328
H	5.534046	0.122905	-1.096602	H	-0.757009	-2.546241	-2.471187
H	4.743184	-0.896646	-2.321054	H	-2.239308	-3.456059	-2.837057
H	4.313147	-2.811675	-0.755416	H	-1.907977	-1.938168	-3.678128
H	5.221006	-1.937908	0.502174	Li	-1.650953	-0.018505	-1.140237
H	3.535952	-2.434959	0.806273	Li	0.101548	-0.672573	1.065200
O	-2.382247	1.503390	-0.074423	H	-3.592668	2.745959	1.078272
C	-3.527247	2.334698	0.064057	H	-4.391719	1.696049	-0.125023
H	-3.512039	3.157235	-0.662020				

Table 5 (Continued).

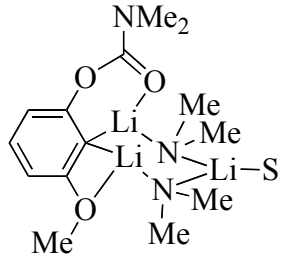


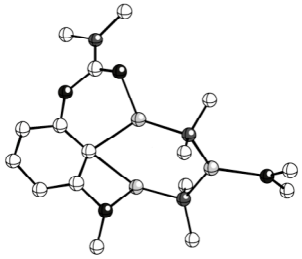


A8
$G°$ = -1115.243685
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.731778	-1.704939	2.800471	N	0.410792	3.134734	0.839332
C	-0.528379	-2.267752	3.035881	N	2.440676	1.167326	-1.644711
C	-1.584781	-2.012892	2.166752	Li	1.738539	2.353931	-0.287740
C	-1.339727	-1.180363	1.068205	C	0.803325	3.309256	2.230640
C	-0.132348	-0.569623	0.757014	H	-0.054546	3.510549	2.909409
C	0.880356	-0.880225	1.680945	H	1.302011	2.403277	2.607162
O	-2.511015	1.205201	0.206309	H	1.505479	4.156439	2.388113
C	-2.920039	0.116163	-0.218453	C	-0.241403	4.350178	0.375819
O	-2.461825	-1.080254	0.186341	H	0.407756	5.249573	0.442335
N	-3.909664	0.010948	-1.142871	H	-0.544365	4.250938	-0.677211
C	-4.588687	1.212685	-1.607615	H	-1.158394	4.603553	0.951072
C	-4.462238	-1.259295	-1.593053	C	3.893105	1.181522	-1.675267
H	-0.678250	-2.907940	3.901042	H	4.306478	0.955200	-0.680269
H	1.549411	-1.916396	3.481433	H	4.336378	0.438621	-2.377097
H	-2.568007	-2.445684	2.325335	H	4.323511	2.158337	-1.989269
H	-3.808924	-2.077330	-1.299630	C	1.939452	1.470311	-2.976092
H	-5.460506	-1.424586	-1.164564	H	0.839154	1.470833	-2.985089
H	-4.555059	-1.247196	-2.685270	H	2.266546	2.460829	-3.361104
H	-4.594554	1.235789	-2.703791	H	2.264233	0.738612	-3.749358
H	-5.628520	1.228805	-1.254302	O	1.777529	-2.158458	-1.548440
H	-4.067235	2.089142	-1.228051	C	1.055494	-3.341414	-1.225912
O	2.114401	-0.305607	1.337198	H	0.448424	-3.668787	-2.081976
C	3.257073	-0.602038	2.129190	H	1.743741	-4.151499	-0.945775
H	3.459932	-1.680563	2.152985	H	0.404167	-3.100014	-0.385826
H	4.095332	-0.085171	1.658587	C	2.643057	-2.325477	-2.665823
H	3.132242	-0.234286	3.154996	H	3.125078	-1.363621	-2.840366
Li	-0.715918	1.536067	0.655811	H	3.402893	-3.092390	-2.457997
Li	1.561214	-0.353417	-0.720461	H	2.072517	-2.619480	-3.558079

Table 5 (Continued).

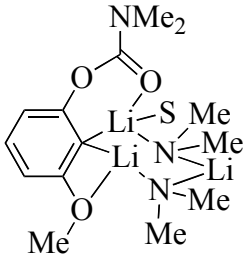


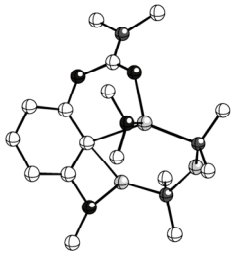


A9
$G°$ = -1115.244712
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.270820	3.409187	-0.448941	Li	0.549807	1.193804	0.919048
C	-3.591172	2.945966	-0.483293	N	1.480679	-0.591933	-1.582832
C	-3.870558	1.608445	-0.225469	N	2.151721	0.505616	1.736495
C	-2.799110	0.753918	0.060082	Li	2.624866	-0.411851	0.027900
C	-1.458777	1.114686	0.097426	C	1.739026	0.432230	-2.584968
C	-1.266103	2.482402	-0.166093	H	1.036276	0.398431	-3.448107
O	-1.795628	-1.682116	-0.951273	H	1.651670	1.435666	-2.144133
C	-2.682098	-1.666823	-0.085726	H	2.752739	0.365549	-3.042198
O	-3.235605	-0.556634	0.424548	C	1.582277	-1.899491	-2.216764
N	-3.213593	-2.801094	0.440897	H	2.577211	-2.100371	-2.673294
C	-2.770956	-4.098978	-0.047635	H	1.401349	-2.700718	-1.484997
C	-4.290878	-2.813894	1.421347	H	0.852787	-2.049980	-3.043733
H	-4.399018	3.637410	-0.706694	C	3.085883	1.542446	2.141139
H	-2.061102	4.456320	-0.639789	H	3.314308	2.211750	1.297279
H	-4.888201	1.229977	-0.233197	H	2.707725	2.183374	2.968650
H	-4.483088	-1.806182	1.780643	H	4.061039	1.148992	2.505797
H	-5.209881	-3.220761	0.978001	C	1.885835	-0.358208	2.874405
H	-4.007911	-3.449592	2.269113	H	1.172243	-1.150745	2.602929
H	-2.416203	-4.713593	0.788937	H	2.793453	-0.868299	3.271573
H	-3.600458	-4.626119	-0.537336	H	1.454948	0.177630	3.748747
H	-1.962930	-3.957582	-0.762653	O	4.488867	-1.076119	-0.086668
O	0.089765	2.855027	-0.082601	C	5.270810	-1.337010	1.072803
C	0.446274	4.225365	-0.198325	H	5.621873	-2.378802	1.076926
H	-0.058302	4.833356	0.563180	H	6.139290	-0.665056	1.116597
H	1.526080	4.273008	-0.047283	H	4.629499	-1.157748	1.936222
H	0.200263	4.612683	-1.194350	C	5.215396	-1.241183	-1.298067
Li	-0.390695	-0.441641	-1.002547	H	6.075917	-0.557606	-1.329805
H	5.574273	-2.274869	-1.400409	H	4.531222	-1.010798	-2.115298

Table 5 (Continued).

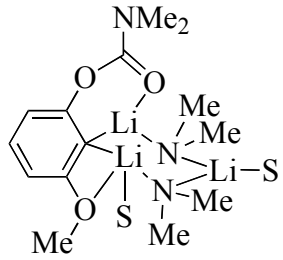


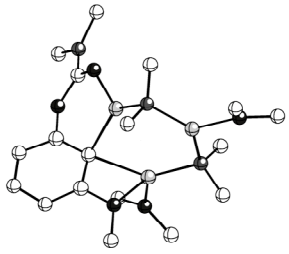


A10
G° = -1115.240119
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	1.319547	-3.043859	-1.246822	N	0.711351	1.882435	2.021701
C	0.054746	-3.616533	-1.431669	N	2.114642	2.649260	-1.294754
C	-1.087826	-2.821902	-1.392084	Li	1.357305	2.781886	0.474770
C	-0.928215	-1.450838	-1.158733	C	1.784893	1.564239	2.952108
C	0.275807	-0.800413	-0.935776	H	1.478192	0.854780	3.751160
C	1.375913	-1.668510	-1.006033	H	2.634944	1.103147	2.424396
O	-2.007095	0.274729	0.766844	H	2.184936	2.452974	3.487587
C	-2.521857	0.173302	-0.353033	C	-0.364899	2.520520	2.767162
O	-2.144467	-0.716026	-1.287646	H	-0.047446	3.448121	3.291672
N	-3.569702	0.938252	-0.758777	H	-1.192179	2.793231	2.096579
C	-4.181293	1.873995	0.173659	H	-0.797335	1.869408	3.559200
C	-4.220188	0.799115	-2.054815	C	3.538503	2.941346	-1.379852
H	-0.030847	-4.683457	-1.619579	H	4.094203	2.399971	-0.599101
H	2.207430	-3.665633	-1.301590	H	3.988394	2.653137	-2.354765
H	-2.075542	-3.241809	-1.558586	H	3.775874	4.019352	-1.254426
H	-3.621479	0.169840	-2.708691	C	1.418014	3.389661	-2.338145
H	-5.219103	0.355256	-1.943126	H	0.337141	3.185034	-2.303973
H	-4.333738	1.788653	-2.513210	H	1.542390	4.490621	-2.255436
H	-4.225263	2.873248	-0.276076	H	1.760957	3.131330	-3.363244
H	-5.204920	1.559933	0.419195	O	0.011028	-1.399750	2.468171
H	-3.588011	1.913004	1.085236	C	1.237780	-2.089640	2.662489
O	2.600187	-0.985632	-0.836219	H	1.302588	-2.483318	3.686955
C	3.818479	-1.673278	-1.086420	H	1.337629	-2.917412	1.946915
H	3.838272	-2.093518	-2.100060	H	2.040853	-1.368562	2.502997
H	4.614486	-0.933970	-0.980436	C	-1.122159	-2.235200	2.674033
H	3.974339	-2.479493	-0.358857	H	-1.140948	-2.608489	3.707976
Li	-0.133748	0.210279	1.228619	H	-2.004143	-1.623414	2.483342
Li	1.651368	0.766692	-1.261608	H	-1.111169	-3.086763	1.979797

Table 5 (Continued).

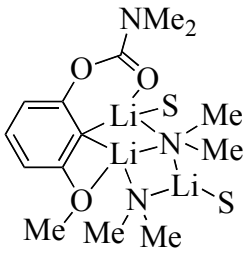


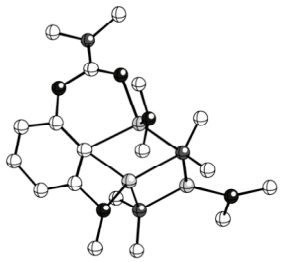


A11
G° = -1270.211974
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	1.936956	-2.259988	-2.440031	H	-1.662997	-0.113248	-2.740092
C	3.215454	-1.699748	-2.553461	H	-2.798019	1.153139	-3.262467
C	3.584783	-0.627697	-1.748544	C	-1.884382	2.983331	-1.526577
C	2.638447	-0.137773	-0.839892	H	-2.864261	3.288938	-1.958237
C	1.347302	-0.613645	-0.665174	H	-1.819529	3.443995	-0.529557
C	1.056298	-1.698305	-1.511538	H	-1.121532	3.486765	-2.161831
O	1.458130	2.354649	-0.273224	C	-3.099478	-1.862873	1.279560
C	2.519243	2.018234	0.266189	H	-3.216780	-2.250190	0.255640
O	3.179254	0.876008	0.016186	H	-2.865586	-2.739932	1.927791
N	3.158207	2.796928	1.181253	H	-4.110516	-1.536491	1.613296
C	2.627798	4.115015	1.497624	C	-1.966345	-0.341480	2.684883
C	4.445579	2.461344	1.772548	H	-1.211207	0.456619	2.747872
H	3.920705	-2.109457	-3.271649	H	-2.906852	0.077076	3.113280
H	1.663092	-3.102003	-3.067148	H	-1.657448	-1.132604	3.405980
H	4.574360	-0.184703	-1.809950	O	0.692756	-2.671198	1.861926
H	4.697828	1.425610	1.559170	C	2.073889	-2.540943	2.177502
H	5.237315	3.112669	1.376824	H	2.206007	-2.303483	3.243229
H	4.396373	2.603294	2.858903	H	2.614275	-3.470697	1.948750
H	2.504385	4.217987	2.582685	H	2.464003	-1.730618	1.561962
H	3.314482	4.899203	1.151158	C	0.060167	-3.700535	2.608947
H	1.663867	4.240886	1.008476	H	-0.989402	-3.717598	2.313149
O	-0.233429	-2.206903	-1.305971	H	0.521910	-4.676036	2.396459
C	-0.652888	-3.348804	-2.036352	H	0.127419	-3.500927	3.687830
H	-0.003451	-4.212480	-1.841130	O	-4.573749	1.157706	0.147830
H	-1.666447	-3.571162	-1.697119	C	-5.407371	1.155956	1.297264
H	-0.668222	-3.145284	-3.114311	H	-5.745508	2.175469	1.533669
Li	0.099583	1.151592	-0.795844	H	-6.286843	0.514277	1.143696
Li	-0.329169	-1.397671	0.625584	H	-4.814279	0.764057	2.124355
N	-1.706827	1.544038	-1.439885	C	-5.232063	1.647162	-1.014313
N	-2.096876	-0.814455	1.318902	H	-4.501043	1.625662	-1.822194
Li	-2.648485	0.586012	0.001694	H	-6.094038	1.012608	-1.267348
C	-1.811706	0.975640	-2.773286	H	-5.578554	2.678837	-0.861082
H	-1.064606	1.383000	-3.492322				

Table 5 (Continued).

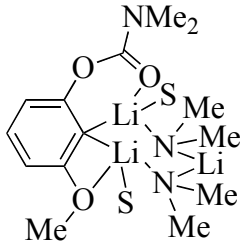


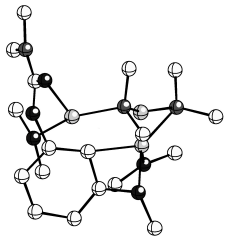


A12
$G°$ = -1270.212974
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.194676	-3.179667	-0.889861	H	1.921139	-1.371644	2.255732
C	-3.416135	-2.643362	-1.317700	H	2.943640	-0.010030	2.760944
C	-3.596581	-1.264706	-1.373997	C	1.450024	1.859071	1.564635
C	-2.522411	-0.449839	-0.994718	H	2.453317	2.257185	1.844687
C	-1.286990	-0.886848	-0.548754	H	1.106411	2.436849	0.695213
C	-1.187014	-2.285305	-0.517713	H	0.790612	2.139156	2.416263
O	-1.821352	1.748290	0.695108	C	3.214880	-1.937020	-1.845814
C	-2.328974	1.911995	-0.422460	H	3.419281	-2.453758	-0.894240
O	-2.794387	0.938477	-1.216120	H	2.622771	-2.641298	-2.472796
N	-2.505999	3.146918	-0.972309	H	4.195617	-1.842307	-2.368969
C	-2.191661	4.334168	-0.193207	C	2.308060	-0.025184	-2.885845
C	-3.150349	3.371884	-2.258949	H	1.796514	0.939169	-2.742525
H	-4.223188	-3.309455	-1.611597	H	3.237110	0.189793	-3.465070
H	-2.061324	-4.256427	-0.857012	H	1.671293	-0.624904	-3.572800
H	-4.530636	-0.827619	-1.715114	O	-1.501772	-0.441453	2.865516
H	-3.189269	2.444568	-2.825196	C	-2.728022	0.126333	3.309612
H	-4.171960	3.755667	-2.126710	H	-3.581238	-0.336054	2.793836
H	-2.575610	4.114266	-2.824959	H	-2.843734	-0.009513	4.394494
H	-1.532945	4.995620	-0.769035	H	-2.694715	1.188809	3.067804
H	-3.107111	4.889735	0.054077	C	-1.439710	-1.845011	3.092699
H	-1.691733	4.037607	0.726821	H	-0.483156	-2.192089	2.700786
O	0.068398	-2.722046	-0.058158	H	-1.502382	-2.064127	4.168221
C	0.432589	-4.079603	-0.261107	H	-2.253985	-2.361204	2.566299
H	0.323522	-4.366646	-1.314334	O	4.817109	1.062269	0.141706
H	1.481176	-4.163170	0.030122	C	5.624546	0.889457	-1.023369
H	-0.171328	-4.753968	0.360724	H	5.966033	1.862956	-1.401503
Li	-0.645033	0.291474	1.172741	H	6.497751	0.262737	-0.795969
Li	0.911728	-0.773280	-0.462660	H	4.992227	0.395713	-1.762055
N	1.447061	0.430997	1.265256	C	5.512076	1.672530	1.220696
N	2.552167	-0.671594	-1.611748	H	6.373950	1.061294	1.523147
Li	3.002695	0.347232	-0.032892	H	5.863611	2.675364	0.940642
C	1.910912	-0.288499	2.445706	H	4.811206	1.752448	2.053499
H	1.279020	-0.121907	3.343085				

Table 5 (Continued).

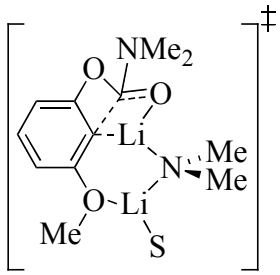


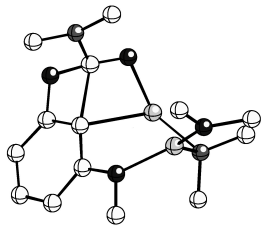


A13
$G°$ = -1270.209295
See pg S76
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.229621	-1.944379	-2.494973	H	-0.696164	-3.241994	1.215646
C	-0.650851	-1.156924	-3.250484	H	-0.593039	-3.238250	2.989269
C	-0.994457	0.121585	-2.819551	C	-1.852384	-0.911860	3.298346
C	-0.437627	0.575494	-1.617245	H	-1.298326	-1.194405	4.220992
C	0.428698	-0.128960	-0.795628	H	-1.919960	0.186201	3.289718
C	0.732730	-1.404574	-1.305631	H	-2.887405	-1.296877	3.451367
O	-2.140062	1.360671	0.390765	C	3.169358	-1.034906	2.875484
C	-1.497604	2.213851	-0.235083	H	3.107662	-2.028923	2.406735
O	-0.736797	1.943506	-1.308700	H	4.253576	-0.779179	2.941547
N	-1.516096	3.534231	0.081231	H	2.838077	-1.155978	3.930528
C	-2.356416	4.005326	1.172000	C	2.479693	1.220736	2.781365
C	-0.780173	4.551650	-0.655962	H	1.891780	1.974856	2.233837
H	-1.057611	-1.545614	-4.180403	H	2.105047	1.219238	3.829239
H	0.507165	-2.931844	-2.850763	H	3.520279	1.617387	2.848412
H	-1.663862	0.753848	-3.395387	O	3.914829	0.573833	-0.837321
H	-0.110591	4.081674	-1.371995	C	3.948418	0.958846	-2.204152
H	-1.471158	5.217246	-1.191257	H	4.095815	2.044003	-2.299711
H	-0.191768	5.157704	0.043616	H	4.757308	0.439251	-2.737118
H	-1.749787	4.558124	1.899510	H	2.985415	0.682235	-2.637211
H	-3.139418	4.675578	0.792516	C	5.101449	0.899219	-0.119500
H	-2.817449	3.151182	1.663976	H	4.930171	0.598025	0.915053
O	1.659635	-2.081369	-0.503564	H	5.964958	0.359651	-0.533226
C	2.105736	-3.370947	-0.895297	H	5.296260	1.979803	-0.162831
H	2.601136	-3.344936	-1.875102	O	-3.528969	-1.284109	-0.480005
H	2.820358	-3.688455	-0.134038	C	-4.768217	-0.850053	0.069852
H	1.272891	-4.084682	-0.930931	H	-5.578359	-0.972903	-0.662597
Li	-1.933317	-0.537631	0.479698	H	-5.014121	-1.413302	0.980864
Li	2.389592	-0.076876	0.195153	H	-4.652330	0.208065	0.311548
N	-1.230481	-1.395378	2.078742	C	-3.541576	-2.656876	-0.856219
N	2.388091	-0.070070	2.129415	H	-2.566270	-2.875058	-1.294855
Li	0.531199	-0.614627	1.701612	H	-3.708658	-3.302856	0.016171
C	-1.172171	-2.842748	2.124872	H	-4.325778	-2.841853	-1.603773
H	-2.173309	-3.328180	2.202990				

Table 5 (Continued).

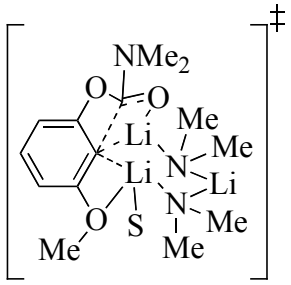


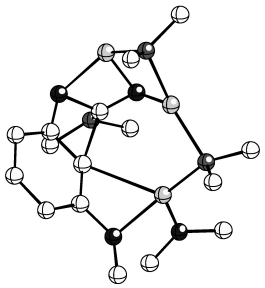


A14
$G°$ = -973.117585
See pg S78
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	1.614050	-2.335510	-1.242218	H	2.654885	3.462665	-1.381485
C	2.904934	-2.449544	-0.710876	H	3.405882	1.958052	-0.821141
C	3.449968	-1.481716	0.139873	H	1.955508	1.891976	-1.858468
C	2.617649	-0.402353	0.422991	H	-0.272773	2.861387	-0.707873
C	1.321319	-0.238541	-0.056556	H	-0.059119	3.370554	0.991913
C	0.828761	-1.214595	-0.912609	H	0.704824	4.298945	-0.323657
O	2.868658	0.714336	1.156989	H	-3.802387	-0.996271	2.410959
C	1.497028	1.333315	0.937841	H	-2.622212	-0.993368	3.721722
O	0.748948	1.384899	1.963387	H	-2.816982	0.455502	2.716215
Li	-0.039670	-0.227032	2.073230	H	-0.927161	-2.921262	1.090528
N	-1.751143	-1.094243	1.756843	H	-1.500631	-2.979045	2.768566
Li	-1.729529	-0.391260	-0.045565	H	-2.668879	-3.019777	1.444817
O	-3.056433	0.672515	-0.976577	H	-1.792041	1.196823	-2.481235
C	-2.781959	1.480119	-2.119856	H	-3.530184	1.303337	-2.904170
C	-4.325608	0.955966	-0.385197	H	-2.783459	2.544379	-1.850884
C	-2.780992	-0.643321	2.680217	H	-4.377427	2.006425	-0.070737
C	-1.712562	-2.551255	1.766141	H	-4.425346	0.308102	0.486564
N	1.644585	2.501862	0.164208	H	-5.134315	0.749371	-1.098534
C	2.454011	2.441551	-1.040111	O	-0.478060	-1.045927	-1.408825
C	0.436745	3.295703	0.024880	C	-0.950129	-1.973915	-2.386769
H	1.244859	-3.118211	-1.895246	H	-1.942188	-1.625482	-2.682142
H	4.457095	-1.563846	0.535204	H	-0.289469	-1.984286	-3.260179
H	3.498473	-3.321127	-0.975434	H	-1.027645	-2.985305	-1.971954

Table 5 (Continued).

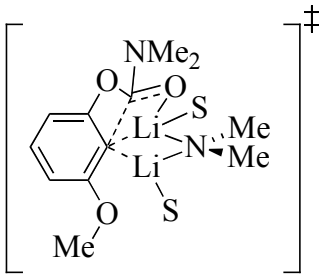


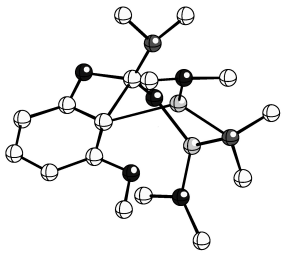


A15
$G°$ = -1115.202413
See pg S78
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.199747	-2.300179	2.451583	N	-3.409306	1.277884	-0.319043
C	-1.316982	-3.039992	2.047620	N	0.149885	2.393275	0.735659
C	-1.835515	-2.933770	0.752527	Li	-1.416241	1.611630	-0.192468
C	-1.161124	-2.055137	-0.085763	C	-4.099993	1.002030	0.929090
C	-0.043201	-1.306853	0.227060	H	-3.644722	0.141597	1.441310
C	0.422827	-1.438791	1.532736	H	-4.072077	1.854524	1.641689
O	-0.877865	0.426859	-1.791371	H	-5.177089	0.765317	0.793380
C	-0.442918	-0.756837	-1.702161	C	-4.047253	2.411680	-0.970919
O	-1.506771	-1.760752	-1.408685	H	-5.119631	2.241116	-1.206265
N	0.478092	-1.244423	-2.606075	H	-4.023628	3.340081	-0.359008
C	1.404548	-0.267777	-3.166760	H	-3.547022	2.646258	-1.924564
C	1.021421	-2.580402	-2.416166	C	-0.109466	2.682932	2.137523
H	-1.792756	-3.706224	2.762018	H	-0.364672	1.761793	2.682644
H	0.162447	-2.402626	3.468823	H	0.757565	3.143718	2.662973
H	-2.705958	-3.498420	0.433723	H	-0.955180	3.386762	2.293529
H	1.757779	-2.608783	-1.597512	C	0.448984	3.640702	0.054210
H	0.217566	-3.280140	-2.188983	H	0.624541	3.467318	-1.019313
H	1.506484	-2.895940	-3.344663	H	-0.369318	4.391345	0.124722
H	1.846133	-0.686085	-4.076273	H	1.349378	4.164164	0.450974
H	0.860484	0.642884	-3.415282	O	3.182616	0.938300	-0.159857
H	2.214198	-0.016747	-2.463270	C	4.115991	-0.134533	-0.086132
O	1.526221	-0.645708	1.862720	H	4.477229	-0.405635	-1.087898
C	1.929701	-0.567019	3.228108	H	4.975165	0.143245	0.540168
H	2.301683	-1.534999	3.583651	H	3.593522	-0.980065	0.362005
H	2.735869	0.167924	3.263174	C	3.754052	2.131380	-0.693012
H	1.102370	-0.233776	3.864300	H	2.974897	2.893220	-0.681643
Li	-2.734034	-0.096516	-1.424814	H	4.601033	2.461186	-0.076248
Li	1.296933	0.847720	0.504206	H	4.101464	1.967141	-1.722423

Table 5 (Continued).

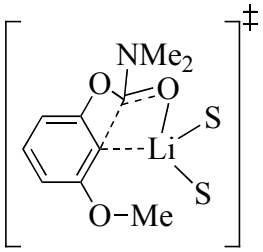


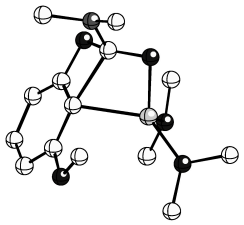


A16
$G°$ = -1128.087599
See pg S78
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.185534	2.960308	-1.759267	H	-1.963512	1.275710	3.390669
C	0.110458	3.979943	-0.846688	H	-2.199742	1.342131	1.628572
C	0.313342	3.719411	0.512822	H	0.149801	-1.790173	3.107295
C	0.201261	2.384282	0.887762	H	-0.614488	-0.715395	4.303651
C	-0.098127	1.327006	0.042055	H	-1.614885	-1.835485	3.343412
C	-0.287495	1.629342	-1.305771	H	-0.722078	-4.221367	0.153328
O	0.378047	1.864399	2.146241	H	1.035567	-4.326451	0.237675
C	0.292638	0.442792	1.807014	H	0.145356	-3.421797	1.480827
O	1.361611	-0.208668	1.847591	H	0.475242	-1.818015	-2.372260
Li	1.736207	-1.261791	0.356878	H	1.238054	-3.389478	-2.017678
N	0.301329	-2.391205	-0.355393	H	-0.517365	-3.274964	-2.141096
Li	-0.944295	-0.889555	0.061070	H	-2.667582	-3.079156	-0.257738
O	-2.893482	-1.062724	-0.371799	H	-4.372768	-2.527507	-0.325661
C	-3.356473	-2.365918	-0.711803	H	-3.356560	-2.507542	-1.801309
C	-3.674663	-0.029348	-0.958318	H	-3.687497	-0.123847	-2.052771
C	0.186958	-3.624583	0.401485	H	-4.706441	-0.063319	-0.581116
C	0.377584	-2.727218	-1.765062	H	-3.212550	0.919860	-0.684363
O	3.550585	-0.911052	-0.223143	H	3.645626	0.561361	1.167479
C	4.254920	0.196634	0.340025	H	5.241561	-0.122088	0.702739
C	4.193751	-1.475077	-1.358404	H	4.310230	-0.724141	-2.152277
N	-0.909067	-0.192584	2.249831	H	5.183132	-1.869709	-1.088855
C	-2.067714	0.670842	2.479186	H	3.559891	-2.288467	-1.717070
C	-0.732276	-1.188366	3.315975	O	-0.603475	0.565185	-2.134176
H	4.381229	0.990242	-0.408841	C	-0.743847	0.808707	-3.523384
H	-0.336299	3.213526	-2.803229	H	-1.583205	1.485393	-3.735194
H	0.550153	4.505809	1.222139	H	0.172399	1.235971	-3.951673
H	0.185310	5.001702	-1.211148	H	-0.936931	-0.162550	-3.983394
H	-2.958221	0.040637	2.569499				

Table 5 (Continued).

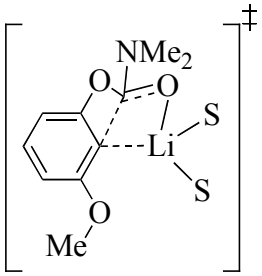


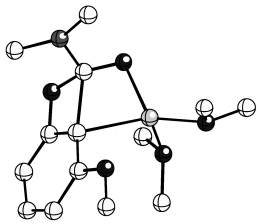


A17
$G°$ = -986.010498
See pg S78
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.430940	0.561780	1.877742	H	3.741782	0.490232	-0.671172
C	0.829180	0.338171	0.560453	H	3.556768	-0.668249	0.670555
C	1.151782	1.459094	-0.205869	H	4.575376	-1.074223	-0.737492
C	1.086720	2.779744	0.220406	H	-3.027102	1.669356	0.246174
C	0.656044	2.960566	1.547490	H	-1.941909	2.878892	-0.493745
C	0.328628	1.884207	2.368547	H	-3.528159	2.508773	-1.249107
O	1.533714	0.980842	-1.427606	H	-2.431507	1.766409	-3.350518
C	1.305297	-0.481061	-1.131522	H	-0.887416	2.290564	-2.596302
O	0.307807	-1.017290	-1.705009	H	-1.063323	0.609910	-3.151363
Li	-1.003204	-0.397217	-0.578591	H	-3.166804	-3.468436	-0.216938
O	-2.076150	1.028110	-1.437741	H	-3.922465	-2.022672	-0.958047
C	-1.590446	1.457717	-2.714748	H	-2.329523	-2.602620	-1.539009
C	-2.674603	2.088541	-0.699161	H	-2.315001	-0.855633	2.125795
O	-2.266239	-1.654012	0.257154	H	-3.906531	-0.877288	1.288143
C	-2.974842	-1.430682	1.473394	H	-3.218578	-2.387595	1.954475
C	-2.970118	-2.484175	-0.662766	O	0.087308	-0.426237	2.775167
N	2.533746	-1.151109	-1.136817	C	0.511926	-1.747899	2.462772
C	3.656552	-0.567515	-0.423591	H	0.239665	-2.361245	3.325726
C	2.463214	-2.601780	-1.060242	H	0.016501	-2.134994	1.565055
H	1.367643	3.616439	-0.411736	H	1.597252	-1.786625	2.310804
H	0.588493	3.968573	1.950727	H	2.306387	-2.963154	-0.028205
H	0.020652	2.040020	3.398740	H	3.404737	-3.024888	-1.427374
H	1.643286	-2.953679	-1.684851				

Table 5 (Continued).

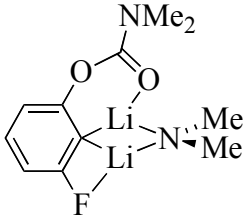


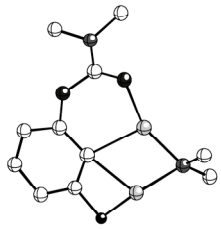


A18
$G°$ = -986.010510
See pg S78
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.862353	-1.000804	1.340371	H	-1.676612	4.326281	0.289417
C	-0.932514	-0.174669	0.220081	H	-0.814157	3.129883	1.290367
C	-1.624580	-0.639694	-0.891378	H	-3.510769	1.398312	-0.731229
C	-2.221403	-1.893423	-1.003104	H	-3.003519	1.609720	0.966246
C	-2.105564	-2.708462	0.130467	H	-3.607004	2.999659	0.023446
C	-1.442859	-2.288241	1.290151	H	2.371029	-2.436386	-0.155741
O	-1.616487	0.387489	-1.788388	H	0.938772	-2.938457	-1.103117
C	-0.840659	1.351067	-0.913915	H	2.583879	-3.095044	-1.803357
O	0.335384	1.630083	-1.301181	H	2.041330	-1.538738	-3.682840
Li	1.206991	0.278515	-0.439342	H	0.367683	-1.598825	-3.035497
O	1.856695	-1.149713	-1.646503	H	1.185166	-0.026523	-3.204496
C	1.333185	-1.082305	-2.977794	H	3.933544	2.043357	-0.292369
C	1.936943	-2.485621	-1.157125	H	4.831000	0.829193	0.672824
O	2.758516	0.643467	0.713724	H	4.020590	0.343849	-0.848514
C	2.537390	1.433952	1.882345	H	1.599740	1.087978	2.318934
C	3.957361	0.992447	0.027058	H	3.360547	1.293270	2.596468
N	-1.687889	2.401418	-0.516495	H	2.461023	2.498074	1.621160
C	-3.020200	2.076616	-0.033341	O	-0.195760	-0.517050	2.449558
C	-1.026740	3.445520	0.251685	C	-0.154091	-1.325943	3.612995
H	-2.763199	-2.211438	-1.888331	H	0.381726	-0.745019	4.367177
H	-2.552678	-3.700048	0.119708	H	-1.162236	-1.553510	3.983325
H	-1.394835	-2.961619	2.138978	H	0.382463	-2.268518	3.437649
H	-0.089517	3.712228	-0.235370				

Table 5 (Continued).

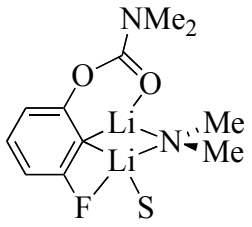


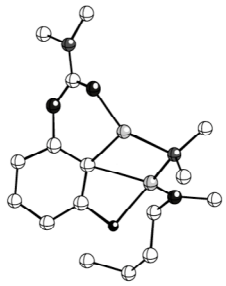


A19
G° = -802.947297
See pg S81

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.980240	3.037104	-0.108775	C	4.144269	0.244636	0.738974
C	-0.738046	3.641279	-0.318432	H	-0.677950	4.703311	-0.537063
C	0.425203	2.875906	-0.238279	H	-2.911365	3.592547	-0.150392
C	0.319313	1.511535	0.050122	H	1.402459	3.324994	-0.387070
C	-0.875190	0.819638	0.259407	H	-3.471727	-2.005417	-1.513292
C	-1.952904	1.678053	0.157254	H	-2.700834	-3.604923	-1.547319
F	-3.231253	1.075476	0.382153	H	-4.018923	-3.286991	-0.412395
Li	-2.478072	-0.614815	0.846838	H	3.614480	1.092182	1.166123
O	1.178152	-1.052735	-0.890017	H	4.646452	-0.306511	1.542375
Li	-0.623223	-1.264466	-0.501205	H	4.909710	0.611254	0.041698
N	-2.158200	-2.341376	0.106100	H	4.535182	-1.728153	-1.174389
C	-1.726586	-3.453079	0.939649	H	4.199138	-2.458946	0.413991
C	-3.118874	-2.827923	-0.872371	H	2.957422	-2.498237	-0.866257
C	1.931278	-0.305702	-0.247266	H	-0.994405	-3.115947	1.690807
O	1.600685	0.908141	0.218701	H	-2.557677	-3.933576	1.497529
N	3.210433	-0.642783	0.056612	H	-1.244176	-4.271797	0.363648
C	3.755284	-1.906341	-0.422405				

Table 5 (Continued).

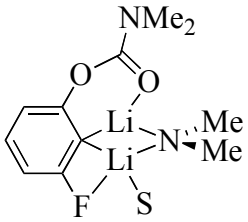


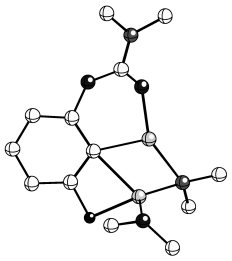


A20
$G°$ = -1075.788321
S = *n*-BuOMe

Atom	X	Y	Z	Atom	X	Y	Z
C	0.955631	-2.158682	2.084912	H	-1.922320	-3.564231	0.919340
C	-0.022199	-3.133119	1.866414	H	0.471784	2.749845	2.896238
C	-1.149392	-2.824173	1.104406	H	1.097156	4.184876	2.056286
C	-1.266709	-1.535563	0.574429	H	-0.587807	4.142956	2.589853
C	-0.346459	-0.501575	0.739823	H	-1.334565	4.583214	0.256645
C	0.720764	-0.915714	1.513805	H	0.346479	4.625747	-0.279280
F	1.723378	0.059997	1.739289	H	-0.792244	3.488077	-1.033687
Li	-1.413973	1.392561	0.942867	H	-3.609928	-2.253321	-1.939840
O	-3.080922	0.655247	0.509048	H	-5.365749	-2.105126	-1.678352
C	-3.215642	-0.320892	-0.242686	H	-4.592159	-1.250844	-3.032913
O	-2.417264	-1.399808	-0.260953	H	-5.311316	1.002526	-2.257888
N	-4.223934	-0.410422	-1.149813	H	-6.201046	0.278522	-0.896459
C	-5.220403	0.648956	-1.223786	H	-4.916104	1.474005	-0.582985
C	-4.457111	-1.574440	-1.993952	H	2.240766	3.401346	-1.137535
Li	0.960174	1.373957	0.372091	H	2.907511	2.628187	-2.606079
O	2.274499	1.375024	-1.071540	H	3.143923	0.290172	-2.607130
C	2.915676	0.175758	-1.536355	H	2.155633	-0.602837	-1.432854
C	4.172328	-0.176455	-0.740385	H	3.887983	-0.294034	0.312431
C	4.044678	-2.734740	-1.089775	H	4.881602	0.659819	-0.789326
C	2.872865	2.592807	-1.508645	H	3.156267	-2.731298	-1.731424
H	3.887996	2.712811	-1.110907	H	4.637619	-3.615764	-1.360129
N	-0.165991	2.890853	0.889886	H	3.701445	-2.865192	-0.056396
C	-0.496826	3.927682	-0.067839	C	4.873791	-1.452301	-1.239760
C	0.214163	3.513277	2.146319	H	5.811363	-1.565349	-0.680734
H	0.094387	-4.127150	2.288499	H	5.164419	-1.322812	-2.292397
H	1.845945	-2.355341	2.674052				

Table 5 (Continued).

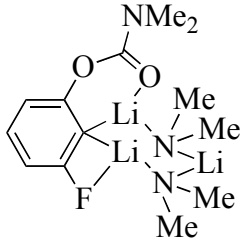


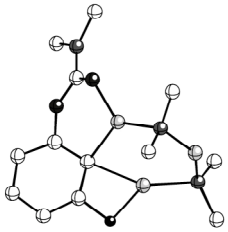


A21
G° = -957.923830
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.740073	3.274978	-0.926923	H	-1.954606	-2.785007	-3.066967
C	0.569989	3.724294	-0.741461	H	-3.439881	-2.345964	-2.215341
C	1.560499	2.825503	-0.344230	H	3.930833	0.566074	1.884338
C	1.208162	1.488144	-0.138584	H	4.623425	-0.974282	2.442581
C	-0.067578	0.949544	-0.300110	H	5.423709	-0.061703	1.142542
C	-0.962470	1.923886	-0.701427	H	5.110606	-2.303096	-0.283306
Li	-1.958417	-0.336977	-0.058412	H	4.244151	-3.008462	1.102841
O	1.961632	-1.139813	-0.939548	H	3.422163	-2.842418	-0.472000
Li	0.101117	-1.070642	-1.126281	H	-1.097489	-3.225883	0.493774
N	-1.638178	-1.959122	-1.104086	H	-2.674776	-3.627331	-0.219673
C	-1.650577	-3.257484	-0.458213	H	-1.191409	-4.063893	-1.071036
C	-2.376752	-2.045612	-2.351831	O	-3.015533	-0.281402	1.583604
C	2.579645	-0.527130	-0.057007	C	-3.073182	0.856434	2.436400
O	2.301214	0.716740	0.362298	H	-2.159494	1.429021	2.266889
N	3.645383	-1.063226	0.594563	H	-3.947416	1.479033	2.201302
C	4.132738	-2.380898	0.210749	H	-3.122921	0.545809	3.489065
C	4.448825	-0.336031	1.568653	C	-4.150312	-1.134315	1.702244
H	0.816665	4.769340	-0.905453	H	-4.240047	-1.514947	2.728806
H	-1.541256	3.939645	-1.234396	H	-5.071037	-0.597542	1.433853
H	2.585417	3.150517	-0.191833	H	-3.993707	-1.966851	1.014444
H	-2.386244	-1.072818	-2.866714	F	-2.296356	1.484220	-0.888152

Table 5 (Continued).

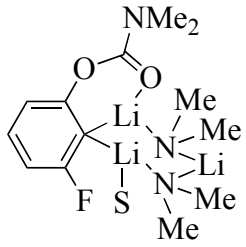


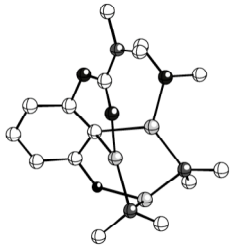


A22
G° = -945.029227
See pg S77

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.334318	3.643524	0.483214	Li	-1.809827	0.550562	-1.082418
C	1.045959	3.841191	0.565733	N	-1.761470	-1.567680	1.732119
C	1.918138	2.789387	0.278931	N	-3.048843	-0.835604	-1.591112
C	1.384069	1.549844	-0.082062	Li	-2.818224	-1.663855	0.139216
C	0.021533	1.253809	-0.170157	C	-2.369648	-0.750946	2.778806
C	-0.743733	2.367250	0.127399	H	-1.679520	-0.535863	3.623343
O	1.612371	-1.070455	0.879897	H	-2.691353	0.220571	2.374714
C	2.390590	-0.646266	0.014480	H	-3.261779	-1.221890	3.242844
O	2.378384	0.609732	-0.467723	C	-1.350322	-2.842598	2.309236
N	3.368363	-1.405166	-0.537636	H	-2.191996	-3.415761	2.752661
C	3.570879	-2.770777	-0.071355	H	-0.890786	-3.485030	1.543397
C	4.320013	-0.911608	-1.525652	H	-0.604442	-2.734546	3.125741
H	1.440536	4.813705	0.844780	C	-4.393245	-0.341818	-1.869860
H	-1.047943	4.436044	0.683105	H	-4.749470	0.300078	-1.050573
H	2.994330	2.925965	0.321839	H	-4.452946	0.260702	-2.800681
H	4.011221	0.064542	-1.891137	H	-5.140897	-1.153185	-1.994762
H	5.323885	-0.832653	-1.087633	C	-2.614131	-1.675117	-2.701911
H	4.365733	-1.611994	-2.367744	H	-1.599057	-2.061782	-2.523409
H	3.503068	-3.468527	-0.914695	H	-3.270693	-2.554551	-2.871062
H	4.563927	-2.872142	0.384936	H	-2.586419	-1.136943	-3.672725
H	2.809112	-3.016559	0.665809	F	-2.143011	2.174000	0.002247
Li	-0.193448	-0.612211	1.026274				

Table 5 (Continued).

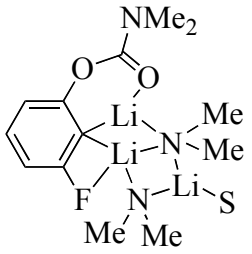


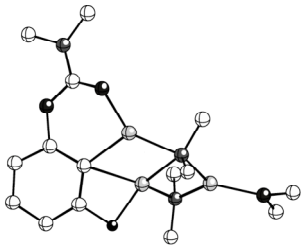


A23
G° = -1100.001665
See pg S77
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.744505	-1.853916	2.931853	C	-2.379549	-3.325173	-0.902755
C	0.585351	-2.187785	3.199172	H	-1.852910	-4.177596	-1.385667
C	1.603644	-1.701160	2.376667	H	-2.141750	-3.370463	0.170852
C	1.249829	-0.868239	1.313866	H	-3.462698	-3.556668	-1.002074
C	-0.042788	-0.456085	0.987245	C	-2.339441	-2.022868	-2.877100
C	-0.975579	-1.021860	1.842956	H	-3.418460	-2.193726	-3.081434
O	1.615249	-1.279583	-1.386839	H	-2.080255	-1.054394	-3.329292
C	2.438466	-0.604479	-0.754136	H	-1.802615	-2.806153	-3.455849
O	2.365569	-0.367274	0.571609	C	-3.671908	2.106445	0.168812
N	3.523829	-0.032851	-1.331719	H	-3.629356	1.742360	1.206438
C	3.766766	-0.224788	-2.755951	H	-3.591286	3.217084	0.214705
C	4.555993	0.683434	-0.593719	H	-4.702773	1.911119	-0.200288
H	0.825354	-2.835450	4.037299	C	-2.747003	1.965204	-2.002353
H	-1.563605	-2.226294	3.538774	H	-1.987032	1.495626	-2.644466
H	2.643683	-1.957753	2.554331	H	-3.733207	1.759748	-2.470966
H	4.271598	0.782701	0.450713	H	-2.608483	3.067664	-2.094943
H	5.510077	0.143676	-0.655990	O	0.110201	3.022029	0.591626
H	4.697440	1.681209	-1.026742	C	1.238925	3.149333	1.448276
H	3.911201	0.747671	-3.241266	H	1.995814	3.804538	0.994678
H	4.669360	-0.829680	-2.912468	H	0.943639	3.564294	2.422075
H	2.913256	-0.731046	-3.202233	H	1.652141	2.149063	1.584082
Li	-0.215527	-1.505134	-0.987519	C	-0.525735	4.267748	0.308457
Li	-0.877048	1.389138	0.181525	H	-1.386401	4.045480	-0.322856
N	-2.014835	-2.030376	-1.458760	H	-0.862036	4.749568	1.236558
N	-2.641230	1.475929	-0.639289	H	0.165108	4.939837	-0.218728
Li	-2.683288	-0.486520	-0.457285	F	-2.325056	-0.731114	1.586007

Table 5 (Continued).

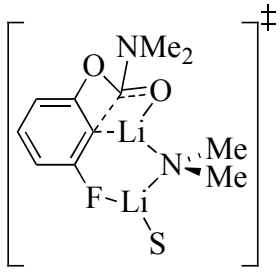


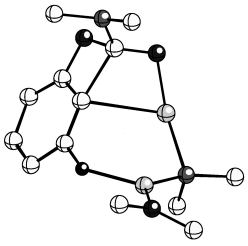


A24
$G°$ = -1100.002591
See pg S77
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.583192	3.585892	-0.797299	C	1.598100	-0.574296	-2.474944
C	-2.970281	3.477920	-0.665507	H	0.845637	-1.040312	-3.151644
C	-3.542059	2.253756	-0.318196	H	1.555983	0.509787	-2.645587
C	-2.698916	1.159305	-0.103440	H	2.579800	-0.926233	-2.859872
C	-1.309703	1.173459	-0.210874	C	1.462513	-2.323309	-0.868901
C	-0.853118	2.428393	-0.570982	H	0.700634	-2.895921	-1.443704
O	-2.226282	-1.575138	-0.816158	H	2.437118	-2.761409	-1.178644
C	-3.118440	-1.248117	-0.016569	H	1.317341	-2.579821	0.190829
O	-3.420823	0.007875	0.337202	C	3.041856	2.114572	1.721912
N	-3.918012	-2.161436	0.593585	H	3.217007	2.630076	0.766064
C	-3.775577	-3.574470	0.272823	H	2.406366	2.787035	2.338215
C	-5.013142	-1.812253	1.489626	H	4.022637	2.078054	2.250763
H	-3.602444	4.345273	-0.832420	C	2.217354	0.173908	2.784980
H	-1.098200	4.519804	-1.062578	H	1.759799	-0.819972	2.653255
H	-4.617041	2.146140	-0.208986	H	3.145284	0.019563	3.383092
H	-4.960298	-0.759779	1.755815	H	1.538087	0.752219	3.448609
H	-5.981793	-2.016446	1.013629	F	0.546175	2.542246	-0.713876
H	-4.943727	-2.417012	2.401457	O	4.849093	-0.929468	-0.149137
H	-3.637327	-4.153585	1.193829	C	5.723963	-0.522687	0.904243
H	-4.674540	-3.944645	-0.237761	H	5.105264	-0.000354	1.635067
H	-2.912375	-3.711400	-0.375209	H	6.200860	-1.397900	1.365927
Li	-0.609794	-0.667531	-0.953382	H	6.499435	0.153344	0.519576
Li	0.918355	0.798728	0.257125	C	5.517663	-1.605275	-1.206617
N	1.383072	-0.875627	-1.061806	H	6.272570	-0.953382	-1.667380
N	2.450579	0.808967	1.501169	H	6.006209	-2.517693	-0.838012
Li	3.001913	-0.372606	0.067016	H	4.763196	-1.871688	-1.949156

Table 5 (Continued).

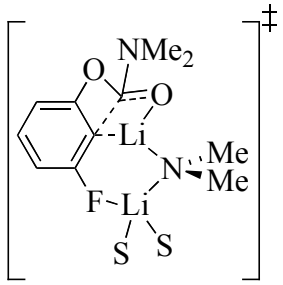


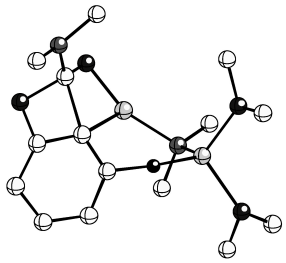


A25
$G°$ = -957.874164
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.938724	-2.254905	-1.681127	H	4.028884	-2.451581	-0.186822
C	2.199659	-2.750480	-1.331889	H	2.526463	-3.695002	-1.758538
C	3.049842	-2.064762	-0.449516	H	3.349947	3.144241	-1.204054
C	2.563782	-0.863274	0.055944	H	3.815366	1.460134	-0.907039
C	1.315048	-0.315630	-0.249216	H	2.319642	1.822139	-1.812490
C	0.546263	-1.037754	-1.119472	H	0.396950	3.012083	-0.344441
O	3.130237	0.039268	0.894458	H	0.836587	3.262972	1.369488
C	1.907544	0.969210	0.904058	H	1.672359	4.177620	0.090129
O	1.261788	1.010924	1.997337	H	-3.837473	-0.634763	2.506791
Li	-0.048800	-0.210864	1.888367	H	-2.530850	-0.574563	3.689325
N	-1.868290	-0.886628	1.664524	H	-2.772263	0.789685	2.580803
Li	-2.077919	-0.334810	-0.168520	H	-1.214265	-2.809368	1.070388
O	-3.474161	0.598416	-1.101892	H	-1.614980	-2.704116	2.796508
C	-3.338205	1.192634	-2.392936	H	-2.911540	-2.773335	1.599579
C	-4.749849	0.837646	-0.505540	H	-2.334533	0.957307	-2.749451
C	-2.781871	-0.308606	2.641401	H	-4.083118	0.780636	-3.085927
C	-1.904836	-2.341952	1.787983	H	-3.463083	2.281379	-2.329122
N	2.264041	2.187344	0.292301	H	-4.921021	1.915283	-0.385876
C	2.968898	2.142934	-0.978364	H	-4.742237	0.357290	0.474127
C	1.232406	3.210848	0.355955	H	-5.548608	0.408151	-1.123956
H	0.286208	-2.788187	-2.364762	F	-0.741764	-0.565590	-1.480543

Table 5 (Continued).

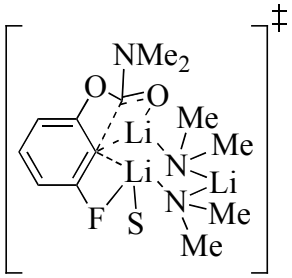


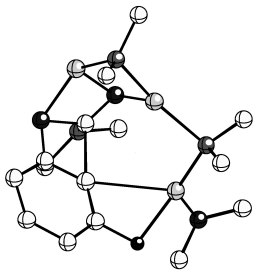


A26
$G°$ = -1112.843260
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.548279	-2.597506	-1.114210	H	-3.159934	0.653645	2.966829
C	1.628119	-3.371361	-0.675649	H	-1.685967	0.773576	3.930914
C	2.713180	-2.809059	0.014556	H	-1.974229	1.927585	2.615609
C	2.651765	-1.435477	0.227243	H	-1.009115	-2.053444	1.681269
C	1.607704	-0.607441	-0.191178	H	-1.119697	-1.565792	3.385687
C	0.577576	-1.224182	-0.850632	H	-2.588768	-1.704998	2.419670
O	3.528717	-0.599119	0.836045	F	-0.537808	-0.476690	-1.271465
C	2.668940	0.654666	0.628925	O	-3.539397	-0.712186	-0.656026
O	2.145016	1.148540	1.674273	C	-3.510846	-1.800775	-1.574052
Li	0.539357	0.321701	1.772217	H	-3.449918	-2.759092	-1.040554
N	-1.376410	0.014857	1.939633	H	-4.409099	-1.797270	-2.206778
Li	-1.901527	0.231165	0.053334	C	-1.331141	3.144946	-0.208147
C	-2.069764	0.867878	2.892866	H	-1.911189	4.072523	-0.109429
C	-1.528113	-1.371240	2.370496	H	-0.502855	3.305654	-0.910418
N	3.352607	1.514409	-0.252417	O	-2.168392	2.078758	-0.649807
C	3.910643	0.960535	-1.475019	C	-2.735721	2.322885	-1.931821
C	2.742220	2.821644	-0.424966	H	-1.951698	2.425226	-2.694975
H	-0.286981	-3.043649	-1.644403	H	-3.369278	1.465834	-2.165129
H	3.547496	-3.413475	0.354898	H	-3.344791	3.237180	-1.917065
H	1.620862	-4.439939	-0.874182	C	-4.651115	-0.773048	0.235800
H	4.581939	1.701418	-1.921808	H	-5.595177	-0.705223	-0.321998
H	4.489683	0.066300	-1.245422	H	-4.634692	-1.705479	0.814410
H	3.133905	0.703447	-2.216765	H	-4.563739	0.074083	0.918208
H	1.861926	2.789158	-1.095997	H	-2.622601	-1.671500	-2.193394
H	2.433818	3.205940	0.546669	H	-0.931036	2.858342	0.765226
H	3.476631	3.503965	-0.866211				

Table 5 (Continued).

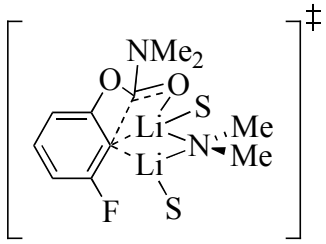


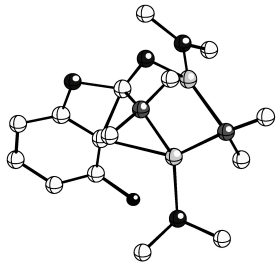


A27
G° = -1099.955863
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.322475	-2.003541	2.768553	C	-4.013270	1.209791	0.694382
C	-1.435372	-2.767563	2.406523	H	-3.618341	0.396697	1.321312
C	-1.891921	-2.807300	1.079223	H	-3.984242	2.134553	1.309669
C	-1.168651	-2.052955	0.167365	H	-5.091191	0.997239	0.529877
C	-0.043173	-1.289133	0.440669	C	-3.812847	2.399768	-1.340867
C	0.330101	-1.292712	1.761530	H	-4.878672	2.242975	-1.612100
O	-0.698109	0.219036	-1.757987	H	-3.780692	3.386952	-0.830182
C	-0.304769	-0.955862	-1.511714	H	-3.258458	2.512031	-2.286811
O	-1.430256	-1.903463	-1.194192	C	-0.132544	2.969200	1.909471
N	0.660455	-1.559871	-2.293161	H	-0.446678	2.147717	2.569983
C	1.684519	-0.664063	-2.821805	H	0.680887	3.515738	2.435305
C	1.132863	-2.888783	-1.934198	H	-0.983833	3.681151	1.860013
H	-1.961692	-3.332951	3.170015	C	0.664258	3.575854	-0.232651
H	0.024382	-1.954628	3.795617	H	0.960583	3.228008	-1.234832
H	-2.761064	-3.391358	0.793744	H	-0.142676	4.326982	-0.382333
H	1.797900	-2.864117	-1.055964	H	1.521024	4.158013	0.176992
H	0.285633	-3.538562	-1.716334	O	3.325451	0.807246	0.256212
H	1.681855	-3.305154	-2.783797	C	4.195946	-0.261339	0.620365
H	2.215681	-1.177393	-3.628585	H	4.786815	-0.588705	-0.245696
H	1.210482	0.234250	-3.215895	H	4.875511	0.051089	1.424491
H	2.412295	-0.372133	-2.047113	H	3.569186	-1.080479	0.972822
Li	-2.587664	-0.185313	-1.465615	C	4.029975	1.958118	-0.210076
Li	1.413009	0.920880	0.732955	H	3.284713	2.718026	-0.445216
N	-3.253367	1.321004	-0.539511	H	4.708237	2.335414	0.566703
N	0.265941	2.456064	0.604673	H	4.610826	1.713218	-1.109506
Li	-1.256875	1.602796	-0.344057	F	1.423599	-0.496608	2.142343

Table 5 (Continued).

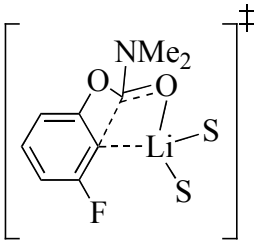


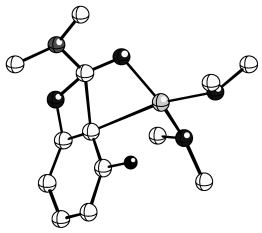


A28
G° = -1112.843762
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.767815	2.566473	-2.277980	H	-0.813043	4.700167	-2.042660
C	-0.696688	3.746985	-1.533450	H	-3.025677	-0.191060	2.429079
C	-0.478141	3.730221	-0.146641	H	-2.290106	1.304668	3.069215
C	-0.335026	2.474714	0.430425	H	-2.519451	1.097928	1.317949
C	-0.401993	1.261478	-0.248780	H	0.362668	-1.322370	3.160463
C	-0.615013	1.346968	-1.607373	H	-0.600736	-0.258870	4.214310
O	-0.092756	2.174918	1.745865	H	-1.366208	-1.659947	3.421269
C	0.103515	0.722938	1.587142	H	0.047966	-4.222358	0.400655
O	1.276547	0.304656	1.710047	H	1.786114	-3.957954	0.528168
Li	1.893148	-0.842812	0.377603	H	0.686025	-3.161338	1.674012
N	0.695402	-2.266257	-0.239615	H	0.804476	-1.827589	-2.297299
Li	-0.834884	-1.041618	0.059758	H	1.871948	-3.166425	-1.803345
O	-2.666251	-1.581007	-0.512123	H	0.137545	-3.438446	-1.958760
C	-2.793015	-2.951887	-0.885864	H	-2.051956	-3.511761	-0.314147
C	-3.558447	-0.736972	-1.234441	H	-3.801981	-3.320068	-0.654083
C	0.807243	-3.435011	0.615788	H	-2.594261	-3.080672	-1.957951
C	0.883800	-2.685659	-1.617780	H	-3.382324	-0.819311	-2.314532
O	3.651191	-0.281505	-0.194709	H	-4.601232	-1.001813	-1.012051
C	4.165386	0.973940	0.250892	H	-3.363960	0.287880	-0.915917
C	4.438910	-0.889750	-1.211094	H	3.460702	1.351203	0.992836
N	-0.964666	-0.073364	2.112775	H	5.158752	0.843059	0.701002
C	-2.269485	0.578538	2.245056	H	4.510544	-0.234796	-2.090294
C	-0.617668	-0.870745	3.299056	H	5.449975	-1.107600	-0.840483
H	4.236887	1.677771	-0.589348	H	3.941587	-1.820540	-1.490205
H	-0.938415	2.580673	-3.350040	F	-0.724585	0.190592	-2.346484
H	-0.417743	4.645001	0.433931				

Table 5 (Continued).

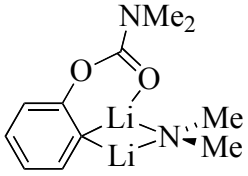


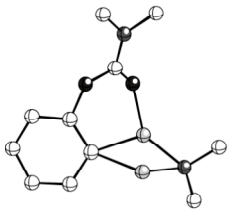


A29
$G°$ = -970.764758
See pg S79
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.759649	-0.778526	1.669241	H	-1.096027	-2.501439	2.927355
C	-0.968478	-0.164561	0.454076	H	-0.130075	3.502368	-0.844901
C	-1.751428	-0.854729	-0.471563	H	-1.659029	4.256851	-0.332638
C	-2.315804	-2.108658	-0.263215	H	-0.723513	3.280563	0.826695
C	-2.058778	-2.690522	0.990071	H	-3.604898	1.234290	-0.547333
C	-1.284864	-2.047037	1.959652	H	-2.949800	1.784065	1.019413
O	-1.829680	-0.027349	-1.547834	H	-3.616695	2.960050	-0.144149
C	-0.959084	1.069518	-0.932245	H	2.843010	-2.129914	0.491939
O	0.184129	1.227886	-1.463230	H	1.454685	-3.157324	0.023295
Li	1.183143	0.168407	-0.370739	H	2.981368	-3.225943	-0.914300
O	1.853723	-1.493576	-1.165838	H	1.832953	-2.467108	-3.006184
C	1.149694	-1.932098	-2.333036	H	0.316669	-2.588374	-2.052328
C	2.304102	-2.570287	-0.349997	H	0.755905	-1.036671	-2.814797
O	2.748389	0.851285	0.605900	H	3.659212	2.235012	-0.662299
C	2.575335	1.733404	1.716014	H	4.774595	1.229138	0.316721
C	3.828978	1.234737	-0.241979	H	3.876034	0.501083	-1.049117
N	-1.758713	2.205970	-0.703511	H	1.726862	1.356598	2.286439
C	-3.047270	2.029240	-0.052366	H	3.476900	1.735317	2.343240
C	-1.023047	3.370741	-0.234943	H	2.370377	2.755590	1.370551
H	-2.930416	-2.604035	-1.008116	F	0.009882	-0.179094	2.633393
H	-2.476234	-3.668589	1.216531				

Table 5 (Continued).

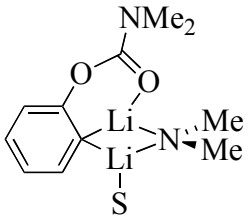


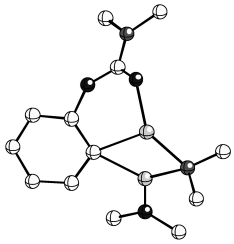


A30
G° = -703.680871
See pg S84

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.354312	3.020300	-0.153635	H	-1.072430	4.682686	-0.676292
C	-1.123486	3.642079	-0.366564	H	-3.278118	3.576747	-0.297260
C	0.050564	2.910605	-0.183756	H	1.026582	3.360611	-0.344891
C	-0.053207	1.580494	0.219388	H	-3.857039	-1.746685	-0.510626
C	-1.237093	0.882696	0.467528	H	-3.270219	-3.230162	-1.288623
C	-2.390413	1.677894	0.242378	H	-3.916715	-3.297221	0.354817
Li	-1.858718	-0.891703	1.384683	H	3.272314	1.119906	1.305407
O	0.892985	-0.701207	-1.079103	H	4.076294	-0.410194	1.730305
Li	-0.924383	-1.003573	-0.763557	H	4.683583	0.563664	0.371528
N	-1.972003	-2.384359	0.204160	H	4.320996	-1.341341	-1.287292
C	-1.270839	-3.637257	0.435777	H	3.795424	-2.365833	0.070267
C	-3.296626	-2.676843	-0.325716	H	2.701460	-2.086755	-1.311536
C	1.612706	-0.099285	-0.264516	H	-0.262680	-3.450167	0.836137
O	1.225065	0.965185	0.452085	H	-1.786389	-4.302800	1.159482
N	2.894203	-0.467364	-0.010908	H	-1.144047	-4.243465	-0.486342
C	3.458691	-1.633943	-0.674731	H	-3.379322	1.232239	0.382567
C	3.777318	0.245732	0.902573				

Table 5 (Continued).

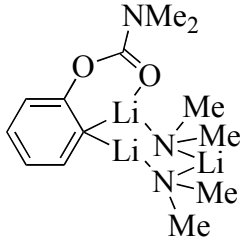


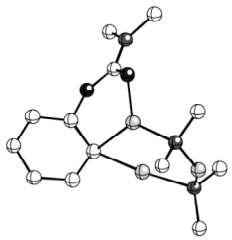


A31
G° = -858.662455
See pg S80
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.482676	3.555467	-1.124155	H	-1.253595	4.823733	-0.877700
C	-0.837079	3.826497	-0.760346	H	1.108768	4.346621	-1.532213
C	-1.626125	2.796849	-0.246506	H	-2.659367	2.969123	0.043828
C	-1.056011	1.532008	-0.105676	H	2.830762	-0.618098	-2.624795
C	0.253031	1.172576	-0.430647	H	3.740348	-1.978586	-1.930618
C	0.990397	2.259854	-0.965697	H	2.516312	-2.278722	-3.168799
Li	0.043625	-0.761698	-1.513756	H	1.337095	-3.836030	-1.634997
O	-1.783242	-0.975829	-1.139770	H	2.550229	-3.541874	-0.384943
C	-2.273815	-0.562664	-0.077182	H	0.832810	-3.245188	-0.037484
O	-1.949822	0.592629	0.519009	H	-3.515299	0.225508	2.057170
N	-3.220221	-1.258308	0.607507	H	-4.935032	-0.797233	1.725439
C	-3.643189	-2.566515	0.130020	H	-3.578046	-1.442382	2.676650
C	-3.843252	-0.787061	1.836362	H	-3.441073	-3.331854	0.890555
Li	1.750777	-0.295332	0.061281	H	-4.720511	-2.563289	-0.079620
O	3.016764	-0.030490	1.484240	H	-3.099010	-2.808750	-0.780628
C	2.991192	1.038991	2.424214	H	4.001158	-1.710699	0.912214
C	4.089376	-0.946368	1.686177	H	4.018656	-1.412473	2.678478
H	5.056981	-0.434402	1.595052	H	2.861099	0.653994	3.444940
N	1.709942	-1.754505	-1.243376	H	2.145318	1.674460	2.156544
C	1.605263	-3.135791	-0.814416	H	2.025323	2.094004	-1.279247
C	2.730006	-1.656942	-2.272537	H	3.921411	1.621037	2.373192

Table 5 (Continued).

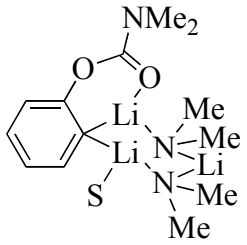


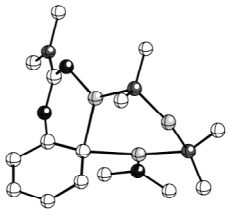


A32
G° = -845.768828
See pg S77

Atom	X	Y	Z	Atom	X	Y	Z
C	0.479457	3.893332	-0.194105	Li	-1.208247	0.249050	-1.603558
C	1.859369	3.710877	-0.093490	N	-2.231850	-0.266524	1.909685
C	2.391022	2.425810	-0.212952	N	-2.792145	-0.839554	-1.701648
C	1.513489	1.367250	-0.439796	Li	-3.000866	-0.776473	0.230933
C	0.125498	1.460054	-0.568943	C	-2.871398	0.886588	2.534586
C	-0.350406	2.787788	-0.420236	H	-2.302517	1.286391	3.401457
O	1.133048	-0.809402	1.198549	H	-2.973615	1.712635	1.814930
C	1.933425	-0.889038	0.254493	H	-3.887691	0.668940	2.926300
O	2.169275	0.104620	-0.620280	C	-2.118041	-1.332227	2.898890
N	2.667830	-2.000896	0.001511	H	-3.097904	-1.660559	3.306147
C	2.523502	-3.173944	0.852619	H	-1.636779	-2.218904	2.460552
C	3.638212	-2.104096	-1.080861	H	-1.511732	-1.044595	3.784429
H	2.519590	4.556611	0.079922	C	-3.894249	-0.229746	-2.439538
H	0.053637	4.889653	-0.098238	H	-4.083896	0.793622	-2.081878
H	3.460375	2.247462	-0.138984	H	-3.705045	-0.159927	-3.531149
H	3.686560	-1.168126	-1.631489	H	-4.849060	-0.787517	-2.340426
H	4.630394	-2.334631	-0.672345	C	-2.576456	-2.190182	-2.210828
H	3.352840	-2.911608	-1.766974	H	-1.750905	-2.681919	-1.673605
H	2.203753	-4.037351	0.255688	H	-3.465651	-2.846271	-2.103971
H	3.483197	-3.416577	1.326182	H	-2.319182	-2.215808	-3.290510
H	1.782753	-2.971033	1.623541	H	-1.424242	2.976249	-0.485755
Li	-0.461170	0.205932	1.194005				

Table 5 (Continued).

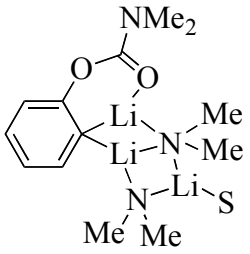


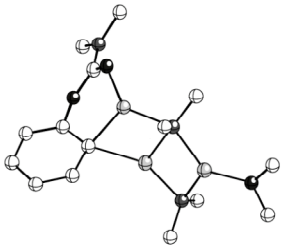


A33
$G°$ = -1000.741527
See pg S77
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	0.226655	-0.014404	3.700017	C	1.728343	3.877467	0.814100
C	-1.151556	-0.176365	3.850369	H	0.894348	4.574190	1.049179
C	-1.952998	-0.293133	2.713589	H	1.917539	3.290297	1.725311
C	-1.334175	-0.252016	1.464839	H	2.616479	4.525723	0.655271
C	0.032398	-0.106332	1.218494	C	1.193755	3.818160	-1.493414
C	0.782912	0.026566	2.414529	H	2.051167	4.469293	-1.767169
O	-1.795198	1.552649	-0.571100	H	0.980598	3.185057	-2.368218
C	-2.404832	0.474278	-0.563035	H	0.326710	4.503410	-1.375676
O	-2.244548	-0.478508	0.372394	C	4.257476	-0.770380	-0.098855
N	-3.324121	0.141438	-1.505092	H	4.076676	-0.636390	0.978225
C	-3.579161	1.047292	-2.616779	H	4.507168	-1.844508	-0.248462
C	-4.079127	-1.103636	-1.498662	H	5.193933	-0.221762	-0.340162
H	-1.603010	-0.207449	4.838592	C	3.390342	-0.524984	-2.288405
H	0.862202	0.081789	4.577825	H	2.539902	-0.198067	-2.905848
H	-3.029831	-0.418546	2.791846	H	4.282803	0.033895	-2.644996
H	-3.906578	-1.642069	-0.569955	H	3.589865	-1.585402	-2.560261
H	-5.149799	-0.883804	-1.591963	O	0.910421	-2.893966	-0.589053
H	-3.784810	-1.738958	-2.344706	C	-0.293883	-3.534217	-0.179208
H	-3.334869	0.559070	-3.569013	H	-0.690831	-4.159263	-0.991601
H	-4.638544	1.332174	-2.634782	H	-0.118598	-4.162787	0.704832
H	-2.967521	1.939743	-2.500183	H	-1.006650	-2.747246	0.066763
Li	-0.045070	1.791592	0.098214	C	1.933456	-3.817762	-0.948640
Li	1.375554	-1.016952	-0.202982	H	2.809551	-3.230967	-1.224866
N	1.444155	3.000698	-0.314534	H	2.178265	-4.474526	-0.102069
N	3.107515	-0.327163	-0.873981	H	1.615273	-4.433735	-1.801100
Li	2.625336	1.518385	-0.551781	H	1.865218	0.162349	2.346505

Table 5 (Continued).

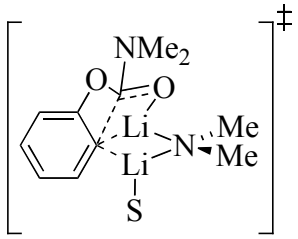


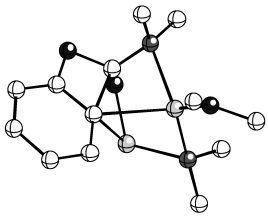


A34
$G°$ = -1000.742460
See pg S77
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.866681	3.668685	-1.049816	C	1.636630	-0.471570	-2.477428
C	-3.213118	3.433552	-0.768760	H	0.893614	-0.885522	-3.200849
C	-3.599348	2.184519	-0.282593	H	1.647702	0.617829	-2.622582
C	-2.614889	1.216142	-0.087136	H	2.614812	-0.856621	-2.838125
C	-1.248873	1.365455	-0.331617	C	1.384281	-2.255271	-0.928012
C	-0.929951	2.649700	-0.840199	H	2.360664	-2.709597	-1.206378
O	-2.183874	-1.435753	-0.979331	H	1.185280	-2.534826	0.116334
C	-2.916349	-1.197380	-0.002868	H	0.632453	-2.788634	-1.550078
O	-3.147179	0.017246	0.505471	C	2.765718	2.426511	1.406975
N	-3.578030	-2.179366	0.664237	H	2.790006	2.821213	0.379082
C	-3.437514	-3.564997	0.242292	H	2.106609	3.101646	1.993699
C	-4.478600	-1.935337	1.783075	H	3.786624	2.577027	1.827664
H	-3.958357	4.209145	-0.925800	C	2.300853	0.568839	2.789202
H	-1.550029	4.637717	-1.429999	H	1.967248	-0.480346	2.834998
H	-4.638543	1.964669	-0.052584	H	3.292509	0.607686	3.296163
H	-4.489726	-0.877144	2.030690	H	1.617187	1.151092	3.444377
H	-5.496359	-2.258491	1.527231	H	0.111185	2.880427	-1.083216
H	-4.147082	-2.505926	2.659676	O	4.795208	-0.701393	-0.124310
H	-3.071193	-4.177588	1.075838	C	5.675693	-0.114172	0.834759
H	-4.407593	-3.965104	-0.080417	H	6.182516	-0.894418	1.418599
H	-2.732846	-3.619259	-0.585025	H	6.427501	0.510457	0.333643
Li	-0.629044	-0.448943	-1.242891	H	5.055548	0.500507	1.488340
Li	0.699594	0.697376	0.368924	C	5.460897	-1.537926	-1.061989
N	1.352134	-0.802412	-1.083220	H	6.207202	-0.966934	-1.631351
N	2.330138	1.042258	1.417552	H	5.959270	-2.373899	-0.552207
Li	2.928051	-0.195789	0.045894	H	4.702568	-1.927694	-1.743455

Table 5 (Continued).

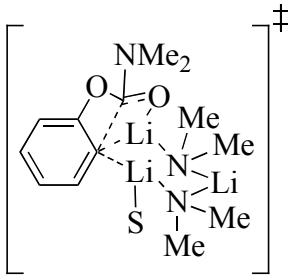


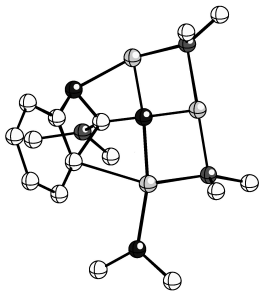


A35
$G°$ = -858.612196
See pg S80
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.452356	-2.366032	-0.796544	H	-4.578447	0.115686	0.258368
C	-3.635681	-1.737914	-0.402048	H	-4.561223	-2.307977	-0.378368
C	-3.660646	-0.380886	-0.041144	H	0.357146	1.237737	2.982596
C	-2.444810	0.283184	-0.101674	H	-1.177570	2.071001	2.613947
C	-1.233082	-0.297408	-0.476623	H	-0.963692	0.361249	2.180735
C	-1.238698	-1.648801	-0.836635	H	1.289952	3.176736	0.038765
O	-2.184370	1.596391	0.180829	H	0.278604	3.786737	1.369914
C	-0.758727	1.601677	-0.185853	H	1.721497	2.803149	1.729023
O	-0.431676	2.212026	-1.232147	H	3.889638	0.735994	-1.311438
Li	0.162529	0.712268	-2.131273	H	3.270968	1.095845	-2.924750
N	1.903847	-0.016329	-1.689512	H	2.620251	1.964372	-1.520765
Li	1.078654	-0.069828	0.123891	H	1.621712	-2.067454	-2.122332
O	1.811327	-1.287607	1.482294	H	2.659600	-1.232907	-3.292015
C	3.217153	-1.526983	1.430975	H	3.297630	-1.657391	-1.702139
C	1.113745	-2.243492	2.275153	H	3.643958	-0.785681	0.753563
C	2.954432	0.976517	-1.867094	H	3.661584	-1.422932	2.430068
C	2.384947	-1.281713	-2.217256	H	3.424369	-2.532405	1.042202
N	0.120767	1.690903	0.955824	H	1.279916	-3.259106	1.891293
C	-0.455948	1.325491	2.254739	H	1.443723	-2.194468	3.321646
C	0.894699	2.942772	1.025278	H	0.051447	-2.003361	2.211445
H	-2.467764	-3.415998	-1.078550	H	-0.331556	-2.163112	-1.150711

Table 5 (Continued).

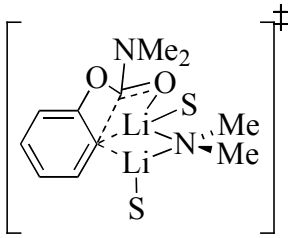


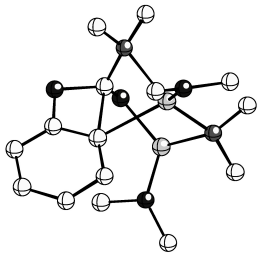


A36
G° = -1000.703234
See pg S80
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.592875	-1.929156	-2.843391	C	4.291567	-0.618814	-0.958901
C	-0.802639	-3.055434	-2.605984	H	3.572556	-0.901539	-1.741845
C	-0.122561	-3.206959	-1.388125	H	4.890763	0.224746	-1.361792
C	-0.286646	-2.176005	-0.478076	H	5.001964	-1.464811	-0.850565
C	-1.051036	-1.030221	-0.641176	C	4.584383	0.077070	1.288364
C	-1.724157	-0.925062	-1.866461	H	5.310340	-0.733556	1.508947
O	0.653482	0.045243	1.361135	H	5.200843	0.956116	1.001298
C	-0.199570	-0.895359	1.330362	H	4.092166	0.331119	2.240860
O	0.304205	-2.156801	0.805246	C	1.139774	2.732097	-2.048963
N	-1.110127	-1.071284	2.335663	H	0.974089	1.846259	-2.678522
C	-1.484140	0.101558	3.118796	H	0.441400	3.519764	-2.412138
C	-2.119127	-2.116447	2.226523	H	2.155850	3.113697	-2.288815
H	-0.713055	-3.826457	-3.366583	C	1.210498	3.590492	0.155907
H	-2.111690	-1.829410	-3.794119	H	1.088873	3.371598	1.229033
H	0.485801	-4.082313	-1.177583	H	2.233277	4.010073	0.023856
H	-2.938572	-1.818553	1.556077	H	0.527217	4.440700	-0.068323
H	-1.667431	-3.030124	1.842487	O	-2.315618	2.024377	-0.158290
H	-2.524769	-2.314970	3.222495	C	-3.604970	1.481610	0.089702
H	-1.845960	-0.230557	4.096236	H	-4.102161	2.012308	0.914640
H	-0.610300	0.737497	3.255193	H	-4.236117	1.551119	-0.807416
H	-2.279393	0.685328	2.631817	H	-3.466439	0.431770	0.351263
Li	2.115489	-1.291483	0.870939	C	-2.367298	3.375295	-0.615805
Li	-0.482937	1.163665	-0.135455	H	-1.340353	3.669923	-0.825080
N	3.600018	-0.287765	0.278341	H	-2.972210	3.446189	-1.530397
N	0.962076	2.402247	-0.645254	H	-2.800856	4.028894	0.153935
Li	2.185537	1.088595	0.112263	H	-2.347657	-0.060068	-2.090810

Table 5 (Continued).

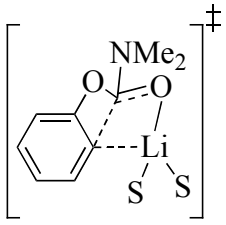


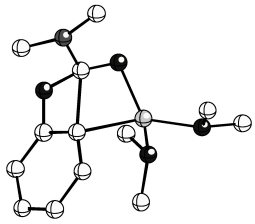


A37
$G°$ = -1013.590873
See pg S80
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.015283	-2.175790	-2.450551	H	-1.915898	-4.121758	-2.262724
C	-1.475743	-3.280951	-1.731779	H	3.096888	-1.435932	1.846314
C	-1.389484	-3.324892	-0.330725	H	1.822712	-2.427434	2.606942
C	-0.819292	-2.216268	0.277798	H	1.852603	-2.211129	0.842895
C	-0.324499	-1.096659	-0.388799	H	0.890557	1.164403	3.131119
C	-0.439585	-1.075229	-1.781752	H	1.323991	-0.312214	4.026058
O	-0.653372	-2.001966	1.623401	H	2.570145	0.568059	3.104198
C	-0.163428	-0.623991	1.571916	H	1.914408	3.752156	0.364329
O	-0.944441	0.279968	1.946371	H	0.246838	4.259877	0.636964
Li	-1.182440	1.426124	0.472901	H	0.968555	3.012791	1.674678
N	0.434561	2.302778	-0.240421	H	-0.026325	2.069404	-2.287538
Li	1.275263	0.519917	-0.042414	H	-0.342438	3.706669	-1.675031
O	2.943876	0.195619	-1.058037	H	1.314768	3.196604	-1.994078
C	3.780683	1.323452	-1.299680	H	3.330463	2.169464	-0.778486
C	3.367350	-0.974104	-1.748512	H	4.795831	1.142010	-0.919705
C	0.905055	3.362802	0.634618	H	3.830608	1.543847	-2.374435
C	0.343281	2.832966	-1.587418	H	3.424128	-0.784897	-2.829286
O	-3.067221	1.628613	0.060654	H	4.351726	-1.305397	-1.389370
C	-3.973988	0.651819	0.573736	H	2.622338	-1.747749	-1.557615
C	-3.602274	2.385768	-1.017420	H	-3.442856	0.122265	1.365395
N	1.229898	-0.499370	1.895993	H	-4.871586	1.139565	0.977373
C	2.039535	-1.716512	1.798176	H	-3.883653	1.729711	-1.852824
C	1.515685	0.273889	3.114215	H	-4.485037	2.953108	-0.691751
H	-4.264377	-0.053734	-0.216082	H	-2.822992	3.077461	-1.343375
H	-1.101288	-2.164775	-3.534868	H	-0.091378	-0.226879	-2.370733
H	-1.757234	-4.173149	0.239113				

Table 5 (Continued).

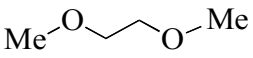


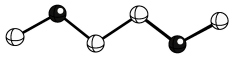


A38
G° = -871.514409
See pg S80
S = Me_2O

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.662526	-0.776277	1.949085	H	-2.093812	-3.841253	1.454809
C	-0.877060	-0.225896	0.685685	H	-0.931263	-2.531737	3.196211
C	-1.553072	-0.999886	-0.257794	H	-0.487225	3.513455	-0.807125
C	-2.006065	-2.296510	-0.046541	H	-2.115544	4.087885	-0.368966
C	-1.756385	-2.831868	1.229766	H	-1.097178	3.294176	0.858116
C	-1.098685	-2.091933	2.215440	H	-3.644949	0.826539	-0.478631
O	-1.690494	-0.219055	-1.370199	H	-3.099592	1.509281	1.076006
C	-0.999303	1.000739	-0.826551	H	-3.891173	2.549652	-0.139837
O	0.127397	1.284403	-1.334875	H	2.416636	-2.277899	0.654205
Li	1.141326	0.255836	-0.214157	H	1.050124	-3.009566	-0.233405
O	1.943606	-1.331246	-1.085900	H	2.732239	-3.240404	-0.819348
C	1.472982	-1.549673	-2.420673	H	2.207740	-2.138721	-2.986170
C	2.036609	-2.541137	-0.335235	H	0.509125	-2.071867	-2.406242
O	2.595748	1.013296	0.878524	H	1.335064	-0.567538	-2.872722
C	2.301231	2.086938	1.767974	H	3.940668	2.072506	-0.313176
C	3.875536	1.139618	0.263509	H	4.669623	1.125961	1.022295
N	-1.938817	2.025953	-0.637608	H	3.988961	0.285405	-0.405926
C	-3.207760	1.704728	-0.004275	H	1.301764	1.907633	2.167994
C	-1.374378	3.296793	-0.213178	H	3.028216	2.113704	2.590979
H	-2.541112	-2.859715	-0.806195	H	2.314998	3.048332	1.237482
H	-0.162366	-0.218005	2.741708				

Table 5 (Continued).

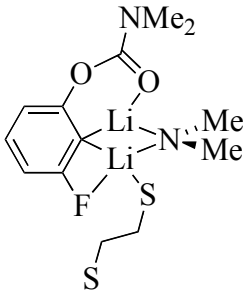


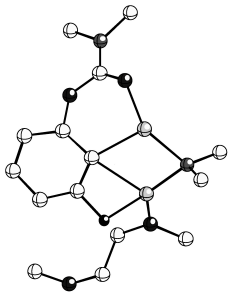


$G°$ = -308.745832

Atom	X	Y	Z
C	-2.980716	-0.113688	0.000155
O	-1.719840	0.519179	-0.000163
C	-0.646509	-0.400872	-0.000111
C	0.646509	0.400871	0.000009
O	1.719840	-0.519178	-0.000041
C	2.980716	0.113688	0.000070
H	-3.121127	-0.744728	-0.892514
H	-3.120974	-0.744118	0.893279
H	-3.738156	0.674708	-0.000058
H	-0.679961	-1.051702	-0.889275
H	-0.680084	-1.051755	0.889009
H	0.679991	1.051643	0.889215
H	0.680053	1.051814	-0.889069
H	3.121011	0.744346	0.893027
H	3.738156	-0.674708	0.000037
H	3.121091	0.744500	-0.892766

Table 5 (Continued).

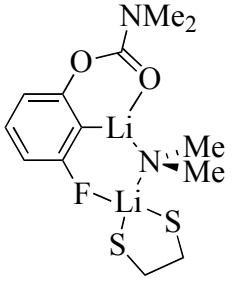


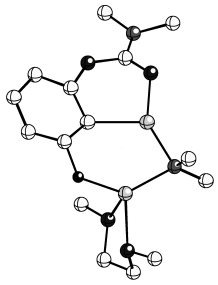


A39
$G°$ = -1111.696585
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	1.043457	-2.140472	2.066541	H	0.210530	-4.122926	2.252874
C	0.077826	-3.125939	1.842698	H	1.940415	-2.331625	2.647290
C	-1.058207	-2.823768	1.091184	H	-1.821510	-3.572543	0.901508
C	-1.197585	-1.530642	0.577553	H	0.447751	2.800134	2.941150
C	-0.291132	-0.485287	0.750497	H	1.062781	4.238591	2.099701
C	0.786917	-0.894235	1.512099	H	-0.630551	4.171317	2.603100
F	1.781459	0.090960	1.738074	H	-1.339604	4.580267	0.252095
Li	-1.385969	1.397138	0.968644	H	0.350120	4.643650	-0.254973
O	-3.042229	0.636369	0.536654	H	-0.758138	3.481730	-1.017760
C	-3.167146	-0.336104	-0.221411	H	-3.533302	-2.255359	-1.941904
O	-2.353175	-1.403643	-0.250885	H	-5.287418	-2.152212	-1.649571
N	-4.177671	-0.434352	-1.124562	H	-4.557553	-1.266491	-3.008238
C	-5.192683	0.608448	-1.184032	H	-5.293907	0.970553	-2.214153
C	-4.397338	-1.596640	-1.975088	H	-6.165213	0.217505	-0.856553
Li	0.990053	1.415716	0.410907	H	-4.900217	1.432246	-0.536166
O	2.266713	1.392140	-1.063733	H	2.308509	3.418275	-1.152489
C	2.770840	0.165406	-1.606023	H	2.731087	2.606859	-2.688422
C	4.082686	-0.271111	-0.941526	H	2.911270	0.267945	-2.690264
O	4.529805	-1.501566	-1.485669	H	1.988024	-0.576783	-1.428345
C	4.021761	-2.644433	-0.817382	H	3.936643	-0.339431	0.146136
C	2.849093	2.580929	-1.597144	H	4.874058	0.462192	-1.133468
H	3.913757	2.658064	-1.345841	H	2.923352	-2.688935	-0.824083
N	-0.156085	2.912454	0.922420	H	4.412707	-3.517057	-1.347166
C	-0.486162	3.935238	-0.051352	H	4.361834	-2.679086	0.229032
C	0.190433	3.552408	2.179928				

Table 5 (Continued).

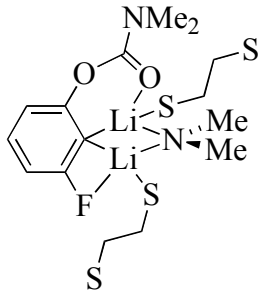


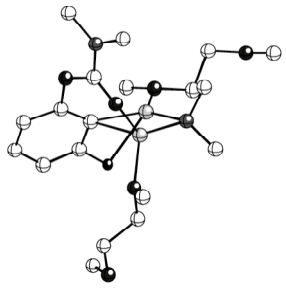


A40
G° = -1111.704715
See pp S81 and 82
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.167286	3.306337	-1.056926	N	1.344325	-1.804978	-1.013125
C	-1.517160	3.659022	-0.963733	C	1.585754	-1.992785	-2.432481
C	-2.458172	2.701343	-0.586089	C	1.662156	-3.035281	-0.316362
C	-2.011912	1.405214	-0.305182	H	-1.832442	4.674282	-1.187489
C	-0.692182	0.967179	-0.364328	H	0.595164	4.019974	-1.353903
C	0.146306	1.987930	-0.757695	H	-3.512895	2.949471	-0.508982
F	1.527522	1.666696	-0.870840	H	1.352348	-1.073650	-2.992343
Li	-0.460460	-1.081130	-0.750360	H	2.640819	-2.254908	-2.676342
O	-2.309360	-1.449447	-0.644749	H	0.977472	-2.808103	-2.884045
C	-3.138215	-0.760790	-0.035906	H	1.068756	-3.911174	-0.661833
O	-3.082281	0.567204	0.142075	H	2.726624	-3.351661	-0.428257
N	-4.249117	-1.303574	0.539640	H	1.475139	-2.930348	0.763381
C	-4.514187	-2.725998	0.382898	H	-4.961685	0.499656	1.336413
C	-5.296656	-0.522768	1.182141	H	-6.207878	-0.513863	0.567758
Li	1.963366	-0.121487	-0.192238	H	-5.543105	-0.970473	2.152576
O	4.060558	0.037552	-0.093571	H	-4.720943	-3.175301	1.361855
C	4.774379	-0.654867	-1.115927	H	-5.387448	-2.889034	-0.263630
C	4.399479	-0.399376	1.216694	H	-3.645203	-3.206627	-0.061984
C	3.531686	0.369849	2.191021	H	1.457999	1.899893	2.669695
O	2.174641	0.121817	1.848524	H	0.257807	0.652129	2.241846
C	1.245163	0.821932	2.672373	H	1.286987	0.445578	3.703876
H	3.744257	1.447565	2.123195	H	4.422303	-0.259974	-2.069842
H	3.739323	0.037231	3.219548	H	5.854253	-0.475486	-1.019248
H	5.461956	-0.204889	1.428470	H	4.569747	-1.731683	-1.073329
H	4.214405	-1.479806	1.311139				

Table 5 (Continued).

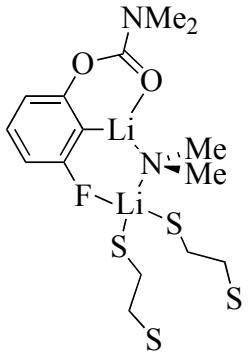


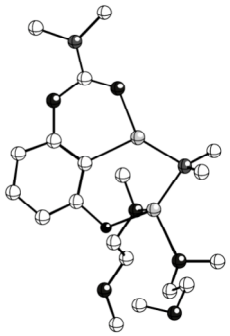


A41
$G°$ = -1420.433448
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	1.995063	-1.340418	2.615380	H	3.304751	1.803302	2.792698
C	2.845447	-0.304099	3.011303	H	-0.952681	-2.024084	-2.246986
C	2.657829	0.981480	2.499971	H	-2.552452	-1.372816	-2.656800
C	1.604942	1.194763	1.606464	H	-1.141292	-0.885426	-3.599265
C	0.709530	0.226561	1.159556	H	-1.640046	1.504165	-3.083399
C	0.993020	-1.010014	1.709522	H	-3.047221	0.995928	-2.143209
Li	0.683715	0.418890	-1.161099	H	-1.785693	1.988936	-1.379809
O	1.422075	2.189837	-1.015555	H	0.942022	4.634132	1.902637
C	1.306713	2.941881	-0.040641	H	1.858586	5.850577	0.978952
O	1.447654	2.565512	1.243080	H	0.082871	5.813184	0.884405
N	1.039070	4.270553	-0.159530	H	0.013908	5.450780	-1.557993
C	0.938949	4.866877	-1.483366	H	1.788373	5.537545	-1.672840
C	0.980760	5.189557	0.968946	H	0.929064	4.077628	-2.232431
Li	-1.200777	-0.280225	0.298440	H	-1.854964	-0.610218	3.137106
N	-1.222501	-0.027864	-1.628371	H	-2.738037	-2.127985	2.802601
C	-1.472809	-1.106480	-2.559299	H	-4.096916	-2.205035	0.869808
C	-1.944365	1.147825	-2.073017	H	-3.588453	-1.125570	-0.452627
O	-2.804509	-0.641088	1.344339	H	-4.980830	0.723763	0.524032
C	-2.768155	-1.034000	2.715521	H	-5.494389	-0.349463	1.842757
C	-3.910781	-1.158847	0.590853	H	-5.416163	-0.747117	-1.876264
C	-5.182026	-0.324983	0.792818	H	-7.189202	-0.875664	-1.752697
O	-6.265030	-0.850509	0.046662	H	-6.377482	0.670698	-1.378171
C	-6.298966	-0.425205	-1.306056	H	2.788260	0.833225	-3.044423
O	2.152798	-0.716323	-1.904608	H	3.956672	-0.507534	-2.947288
C	2.108460	-2.138494	-1.752706	H	2.491430	-0.677147	-3.961047
C	3.393071	-2.705116	-1.135268	H	1.913267	-2.616891	-2.722270
O	3.273859	-4.108042	-0.957508	H	1.260755	-2.338662	-1.093582
C	2.721960	-4.483481	0.294008	H	3.604238	-2.192137	-0.185695
C	2.892910	-0.253468	-3.029985	H	4.248038	-2.548420	-1.802575
F	0.155580	-2.065590	1.305337	H	1.745378	-4.018347	0.485546
H	-3.634428	-0.648433	3.266015	H	2.599619	-5.569769	0.269558
H	3.649724	-0.497938	3.715503	H	3.398351	-4.219437	1.122017
H	2.105829	-2.351411	2.995682				

Table 5 (Continued).

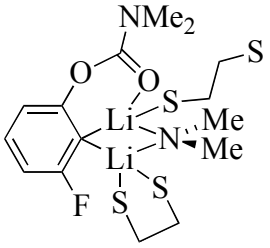


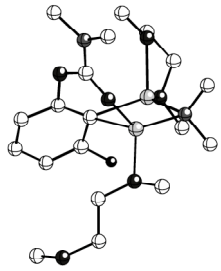


A42
G° = -1420.429740
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	0.388916	-0.538848	3.078493	H	3.761184	-0.246974	3.472367
C	1.624012	-0.477277	3.731654	H	-0.084745	-2.762382	-1.482908
C	2.789790	-0.296849	2.988778	H	-1.089713	-2.537608	-2.931772
C	2.682804	-0.177819	1.597735	H	0.654808	-2.761327	-3.097568
C	1.499661	-0.224021	0.866875	H	0.863037	-0.632277	-4.319054
C	0.419053	-0.413582	1.696733	H	-0.882561	-0.390794	-4.196527
F	-0.861346	-0.494605	1.070903	H	0.225899	0.853101	-3.585582
Li	1.665228	-0.599512	-1.177611	H	5.956537	1.023378	1.376062
O	3.549404	-0.585366	-1.163397	H	7.208711	-0.077963	0.751603
C	4.284246	-0.123005	-0.281475	H	7.068387	1.571009	0.100754
O	3.962619	0.063457	1.006060	H	6.614422	0.945556	-2.225252
N	5.567189	0.265104	-0.540135	H	6.883764	-0.768606	-1.828180
C	6.130737	0.031111	-1.861573	H	5.334979	-0.256552	-2.545721
C	6.498127	0.717159	0.484553	H	0.594040	2.227256	-1.799249
Li	-1.018580	-0.052773	-0.882466	H	0.727296	2.593935	-0.058487
N	0.084579	-0.832286	-2.323650	H	-1.336588	2.827654	1.130341
C	-0.114449	-2.264445	-2.465526	H	-2.578477	1.665389	0.622921
C	0.072870	-0.235341	-3.643990	H	-3.441711	3.312280	-1.064918
O	-2.997470	-0.529308	-0.940984	H	-2.208267	4.483812	-0.560163
C	-3.684190	-1.391720	-0.028466	H	-4.637204	2.432433	1.438809
C	-3.484876	-2.883512	-0.329242	H	-5.396166	3.996899	1.817338
O	-4.115419	-3.676763	0.663566	H	-5.445548	3.365572	0.147992
C	-3.301961	-3.940141	1.793755	H	-3.032558	0.314090	-2.788765
C	-3.565625	-0.470956	-2.250078	H	-3.440503	-1.415476	-2.790745
O	-1.132982	1.972826	-0.760928	H	-4.633458	-0.218568	-2.191112
C	0.091832	2.687490	-0.946906	H	-4.757509	-1.153586	-0.030087
C	-1.956675	2.497463	0.286619	H	-3.276442	-1.152057	0.955487
C	-2.832285	3.653675	-0.212917	H	-2.411540	-3.110654	-0.406357
O	-3.646603	4.181284	0.820168	H	-3.954009	-3.153555	-1.281071
C	-4.832389	3.446475	1.059614	H	-3.008703	-3.025419	2.329673
H	-0.094631	3.745502	-1.167829	H	-3.893722	-4.565191	2.467698
H	1.675263	-0.570054	4.812816	H	-2.387406	-4.483530	1.511373
H	-0.541040	-0.680885	3.621018				

Table 5 (Continued).

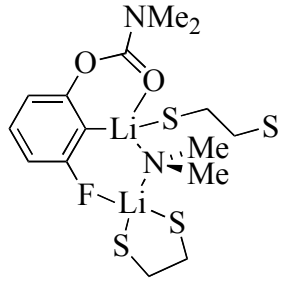


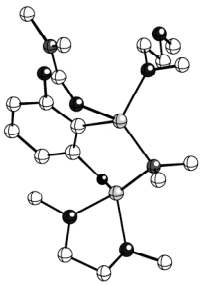


A43
G° = -1420.440459
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.397971	-1.308186	-2.731742	H	4.501653	-2.406671	0.606535
C	-1.732450	-0.079349	-3.307922	H	-2.394016	-0.040983	-4.169198
C	-1.210938	1.099345	-2.771250	H	-1.784699	-2.246654	-3.118496
C	-0.351246	0.997731	-1.674026	H	-1.456020	2.069666	-3.193519
C	0.049956	-0.177322	-1.044463	H	0.113494	-2.711877	2.120496
C	-0.539761	-1.286785	-1.634797	H	1.660862	-2.746850	3.002592
F	-0.255811	-2.522632	-1.074628	H	0.248679	-1.986687	3.736803
Li	-0.335628	0.087089	1.177541	H	1.508674	0.140968	3.980723
O	-0.432578	2.029620	0.924856	H	2.928696	-0.621765	3.255256
C	0.109903	2.662361	0.014479	H	2.256763	0.858155	2.537176
O	0.184475	2.263831	-1.267277	H	1.328927	4.128480	-1.774890
N	0.715783	3.870356	0.213501	H	0.452878	5.518595	-1.090516
C	0.623317	4.495903	1.525504	H	2.126756	5.189835	-0.589449
C	1.178367	4.720812	-0.875441	H	1.585722	4.954356	1.778859
Li	1.707462	-1.000988	0.222591	H	-0.148116	5.279147	1.538102
N	1.116002	-0.861373	2.117060	H	0.374281	3.739423	2.267331
C	0.776028	-2.110754	2.761086	H	3.216633	1.324752	-1.741393
C	1.976533	-0.101811	2.997638	H	3.044885	1.856068	-0.045282
O	3.567993	-0.092614	-0.252761	H	4.675225	1.601603	-0.732113
C	3.635092	1.244928	-0.729149	H	1.354530	-4.080160	-0.112927
C	4.341075	-1.000527	-1.024820	H	2.946528	-4.741135	-0.593031
C	4.146504	-2.381433	-0.435034	H	2.708900	-4.074764	1.056804
O	2.758010	-2.671828	-0.486775	H	-2.670779	0.937326	3.287105
C	2.432271	-3.971332	-0.000562	H	-3.175511	-0.758699	3.563638
O	-2.202588	-0.385526	1.745141	H	-1.445968	-0.326300	3.622464
C	-2.398299	-0.116146	3.132331	H	-2.904323	0.020329	-0.104758
C	-3.312504	-0.056314	0.905657	H	-3.724801	0.922771	1.187181
C	-4.413140	-1.123709	0.958696	H	-4.832697	-1.193576	1.968279
O	-5.494934	-0.789217	0.104632	H	-3.987120	-2.105764	0.701829
C	-5.319620	-1.204253	-1.239136	H	-5.224111	-2.299387	-1.309672
H	4.006890	-0.985455	-2.073682	H	-6.215698	-0.891846	-1.782491
H	5.406666	-0.725239	-0.992636	H	-4.439886	-0.749563	-1.715472
H	4.718670	-3.118688	-1.019131				

Table 5 (Continued).

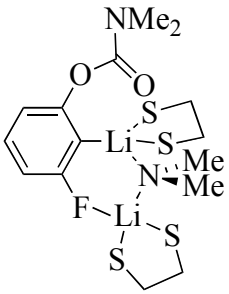


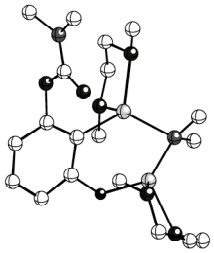


A44
$G°$ = -1420.439104
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.397971	-1.308186	-2.731742	H	4.501653	-2.406671	0.606535
C	-1.732450	-0.079349	-3.307922	H	-2.394016	-0.040983	-4.169198
C	-1.210938	1.099345	-2.771250	H	-1.784699	-2.246654	-3.118496
C	-0.351246	0.997731	-1.674026	H	-1.456020	2.069666	-3.193519
C	0.049956	-0.177322	-1.044463	H	0.113494	-2.711877	2.120496
C	-0.539761	-1.286785	-1.634797	H	1.660862	-2.746850	3.002592
F	-0.255811	-2.522632	-1.074628	H	0.248679	-1.986687	3.736803
Li	-0.335628	0.087089	1.177541	H	1.508674	0.140968	3.980723
O	-0.432578	2.029620	0.924856	H	2.928696	-0.621765	3.255256
C	0.109903	2.662361	0.014479	H	2.256763	0.858155	2.537176
O	0.184475	2.263831	-1.267277	H	1.328927	4.128480	-1.774890
N	0.715783	3.870356	0.213501	H	0.452878	5.518595	-1.090516
C	0.623317	4.495903	1.525504	H	2.126756	5.189835	-0.589449
C	1.178367	4.720812	-0.875441	H	1.585722	4.954356	1.778859
Li	1.707462	-1.000988	0.222591	H	-0.148116	5.279147	1.538102
N	1.116002	-0.861373	2.117060	H	0.374281	3.739423	2.267331
C	0.776028	-2.110754	2.761086	H	3.216633	1.324752	-1.741393
C	1.976533	-0.101811	2.997638	H	3.044885	1.856068	-0.045282
O	3.567993	-0.092614	-0.252761	H	4.675225	1.601603	-0.732113
C	3.635092	1.244928	-0.729149	H	1.354530	-4.080160	-0.112927
C	4.341075	-1.000527	-1.024820	H	2.946528	-4.741135	-0.593031
C	4.146504	-2.381433	-0.435034	H	2.708900	-4.074764	1.056804
O	2.758010	-2.671828	-0.486775	H	-2.670779	0.937326	3.287105
C	2.432271	-3.971332	-0.000562	H	-3.175511	-0.758699	3.563638
O	-2.202588	-0.385526	1.745141	H	-1.445968	-0.326300	3.622464
C	-2.398299	-0.116146	3.132331	H	-2.904323	0.020329	-0.104758
C	-3.312504	-0.056314	0.905657	H	-3.724801	0.922771	1.187181
C	-4.413140	-1.123709	0.958696	H	-4.832697	-1.193576	1.968279
O	-5.494934	-0.789217	0.104632	H	-3.987120	-2.105764	0.701829
C	-5.319620	-1.204253	-1.239136	H	-5.224111	-2.299387	-1.309672
H	4.006890	-0.985455	-2.073682	H	-6.215698	-0.891846	-1.782491
H	5.406666	-0.725239	-0.992636	H	-4.439886	-0.749563	-1.715472
H	4.718670	-3.118688	-1.019131				

Table 5 (Continued).

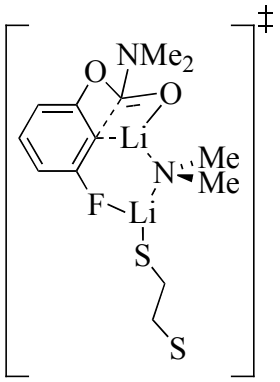


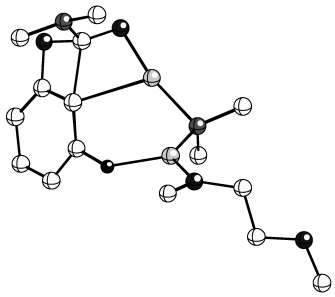


A45
G° = -1420.437512
See pg S81
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.761677	-1.735954	2.870188	H	0.375839	4.677783	0.335043
C	0.416832	-2.451097	3.097135	H	0.450157	-3.226549	3.857547
C	1.551088	-2.156851	2.337171	H	-1.669034	-1.924585	3.436882
C	1.472164	-1.147935	1.374673	H	2.482398	-2.694567	2.493327
C	0.346737	-0.377496	1.082896	H	-2.703198	2.888754	-0.103472
C	-0.708526	-0.759048	1.883188	H	-1.776310	3.581803	-1.454733
F	-1.953220	-0.079451	1.668385	H	-3.296325	2.741633	-1.771257
Li	-2.274383	-0.142586	-0.281947	H	-2.202412	1.161659	-3.298084
O	-2.203379	-2.075989	-1.002974	H	-0.668250	2.003396	-3.055483
C	-1.126932	-3.007726	-0.837183	H	-0.782803	0.255982	-2.730300
C	-3.481245	-2.683305	-0.899459	H	4.806569	-0.068673	0.709739
O	-4.333769	-0.563196	-0.265333	H	5.930401	-1.371239	0.252990
C	-5.233847	0.521739	-0.466757	H	5.835411	0.104419	-0.732673
C	-4.524708	-1.625618	-1.192167	H	5.199974	-1.142960	-2.796646
Li	-0.015108	1.429947	-0.074516	H	5.291213	-2.705226	-1.949324
N	-1.666821	1.442761	-1.230998	H	3.763882	-2.203781	-2.714914
C	-2.378805	2.697429	-1.138466	H	3.094888	1.345899	-1.321168
C	-1.319419	1.210377	-2.619062	H	1.833903	1.500093	-2.577207
O	0.198649	2.920135	1.421036	H	3.006956	2.826592	-2.333520
C	-0.849249	3.315334	2.294203	H	-1.401716	2.408319	2.543923
C	0.989894	3.993232	0.940354	H	-0.442284	3.765768	3.211020
C	2.098986	3.392542	0.098755	H	-1.522343	4.033949	1.806208
O	1.489379	2.619134	-0.924434	H	-5.106586	0.956348	-1.466523
C	2.419944	2.042493	-1.833828	H	-6.273446	0.189232	-0.337054
O	2.706824	-0.864488	0.709089	H	-4.995930	1.275492	0.285117
C	2.936693	-1.473524	-0.479891	H	-1.181324	-3.482618	0.150964
O	2.132053	-2.170315	-1.078147	H	-1.180306	-3.778047	-1.618783
N	4.198352	-1.183375	-0.955749	H	-0.191464	-2.456189	-0.920060
C	5.246057	-0.599453	-0.131936	H	-5.533584	-2.053134	-1.086771
C	4.637968	-1.847734	-2.171806	H	-4.407733	-1.249956	-2.220157
H	2.745369	2.753795	0.719351	H	-3.578611	-3.505510	-1.625162
H	2.711410	4.197124	-0.337545	H	-3.624735	-3.095951	0.111365
H	1.426983	4.561546	1.776573				

Table 5 (Continued).

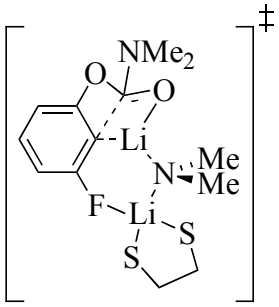


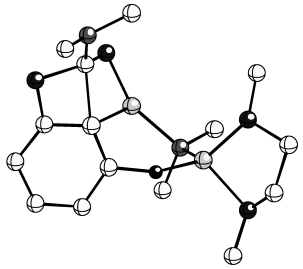


A46
G° = -1111.647492
See pg S82
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.600313	2.430939	-1.450158	H	-3.321850	-1.474070	-2.078176
C	-2.834707	3.006811	-1.130302	H	-1.607588	-2.958982	-0.629898
C	-3.802114	2.321564	-0.377828	H	-2.174416	-3.330450	1.023798
C	-3.459937	1.036354	0.030419	H	-2.997843	-4.045593	-0.384261
C	-2.245276	0.405967	-0.252092	H	2.709881	-0.116636	2.816241
C	-1.356784	1.133351	-0.994229	H	1.320357	-0.156787	3.902149
O	-4.159350	0.115201	0.737603	H	1.488406	-1.400025	2.648063
C	-3.022978	-0.920187	0.729080	H	0.463865	2.513611	1.507290
O	-2.459665	-1.121550	1.849687	H	0.715500	2.159138	3.228134
Li	-1.040681	-0.024355	1.931872	H	2.100433	2.210466	2.133985
N	0.849842	0.469508	1.895974	H	1.442400	-0.921419	-2.643879
Li	1.136087	0.106508	0.029186	H	3.186683	-0.692959	-2.939824
O	2.549436	-0.757755	-0.944990	H	2.577386	-2.276764	-2.368586
C	2.444124	-1.189784	-2.305504	H	4.180278	-2.018754	-0.659959
C	3.808821	-1.045500	-0.316915	H	3.614940	-1.105901	0.756467
C	1.617921	-0.325762	2.846335	F	-0.093082	0.578883	-1.323565
C	1.039854	1.884788	2.202558	C	4.840132	0.045807	-0.595675
N	-3.438456	-2.038931	-0.020260	H	4.991999	0.177643	-1.681085
C	-4.050094	-1.812548	-1.319511	H	4.479470	1.007204	-0.192556
C	-2.499185	-3.149728	-0.000116	O	6.033930	-0.359190	0.033740
H	-0.856750	2.964278	-2.033433	C	7.072714	0.594089	-0.081241
H	-4.759782	2.771262	-0.137428	H	6.794521	1.553189	0.382310
H	-3.046637	4.014879	-1.476488	H	7.338310	0.778326	-1.134259
H	-4.496979	-2.750201	-1.665766	H	7.941295	0.184287	0.439456
H	-4.839939	-1.066794	-1.230629				

Table 5 (Continued).

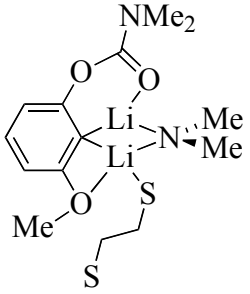


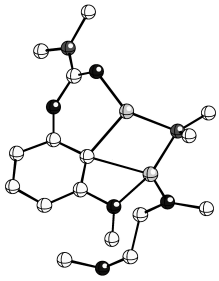


A47
G° = -1111.6585722
See pg S82
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	0.983124	-2.671379	-1.037359	H	2.553756	3.900638	-1.087901
C	2.233627	-3.193846	-0.690139	H	-3.056584	0.178020	3.042059
C	3.231532	-2.402459	-0.099575	H	-1.647148	0.284888	4.102736
C	2.902110	-1.067566	0.113272	H	-1.887572	1.503476	2.837979
C	1.675716	-0.485279	-0.212628	H	-0.699267	-2.378673	1.765454
C	0.748448	-1.316971	-0.782319	H	-0.944527	-1.984589	3.478360
O	3.637654	-0.052791	0.635851	H	-2.342594	-2.146206	2.412128
C	2.527720	0.992139	0.507555	F	-0.526139	-0.823984	-1.116312
O	2.006951	1.389010	1.594597	O	-3.507465	-0.806379	-0.590937
Li	0.644170	0.226897	1.865115	C	-3.894654	0.130388	-1.592502
N	-1.191285	-0.348802	2.097934	H	-3.257091	0.012869	-2.481517
Li	-1.782639	-0.122706	0.248592	H	-4.941996	-0.030410	-1.886517
C	-1.971694	0.427334	3.050669	C	-3.733768	1.516906	-1.001477
C	-1.298258	-1.759773	2.450167	H	-3.954383	2.276224	-1.765978
N	2.928105	1.953926	-0.438621	H	-4.425425	1.657584	-0.157535
C	3.474456	1.498879	-1.706612	O	-2.388606	1.637783	-0.550941
C	2.034633	3.094018	-0.559311	C	-2.095479	2.906486	0.033686
H	0.217054	-3.291149	-1.492596	H	-2.744511	3.097226	0.898223
H	4.200205	-2.812362	0.166868	H	-1.054350	2.873754	0.357348
H	2.433593	-4.244682	-0.882658	H	-2.224973	3.707443	-0.705986
H	3.933285	2.351698	-2.217830	C	-3.642767	-2.166601	-0.998014
H	4.244913	0.749124	-1.528338	H	-4.691784	-2.397396	-1.224918
H	2.702973	1.069303	-2.369430	H	-3.022409	-2.374939	-1.879844
H	1.116006	2.850384	-1.127640	H	-3.308123	-2.778986	-0.159244
H	1.757133	3.439553	0.436227				

Table 5 (Continued).

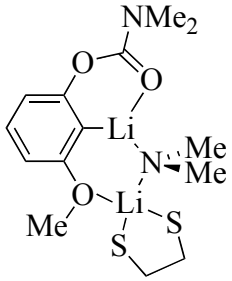


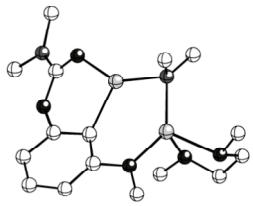


A48
G° = -1126.938909
See pg S83
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	1.085514	-1.838118	2.372796	H	0.521308	3.185447	2.580925
C	0.098353	-2.826128	2.266571	H	1.114146	4.534795	1.586672
C	-1.025788	-2.606452	1.479291	H	-0.575943	4.499229	2.102068
C	-1.128506	-1.380007	0.809221	H	-1.296538	4.639466	-0.275901
C	-0.209444	-0.342306	0.853295	H	0.391328	4.666043	-0.795396
C	0.891469	-0.644308	1.674205	H	-0.706933	3.414054	-1.419128
Li	-1.295143	1.549314	0.836780	H	-3.587792	-2.446412	-1.453719
O	-2.974881	0.775194	0.532782	H	-5.344993	-2.198161	-1.301683
C	-3.113226	-0.283091	-0.097985	H	-4.477148	-1.566901	-2.719696
O	-2.284539	-1.334739	-0.038729	H	-5.280839	0.770251	-2.185737
N	-4.159883	-0.496144	-0.940797	H	-6.135308	0.208389	-0.728728
C	-5.164529	0.542007	-1.118996	H	-4.853154	1.438912	-0.587325
C	-4.401183	-1.750198	-1.640455	H	2.412950	3.210007	-1.718037
Li	1.036954	1.508878	0.213305	H	2.212071	2.289622	-3.234506
O	2.055076	1.231906	-1.448553	H	2.012258	-0.030456	-3.103145
C	2.139963	-0.082555	-2.013667	H	1.298488	-0.635054	-1.588538
C	3.466575	-0.768831	-1.666508	H	3.598300	-0.770796	-0.573171
O	3.525203	-2.081835	-2.193265	H	4.308043	-0.222788	-2.107662
C	2.880597	-3.057486	-1.389372	H	1.798358	-2.890547	-1.299194
C	2.644472	2.271592	-2.225450	H	3.048705	-4.022140	-1.875277
H	3.732801	2.154216	-2.300893	H	3.308850	-3.086515	-0.375764
N	-0.089091	3.069825	0.566801	O	1.839975	0.394583	1.713939
C	-0.435841	3.975020	-0.510826	C	2.955120	0.290347	2.584482
C	0.251776	3.847905	1.743917	H	3.609829	-0.545209	2.303296
H	0.214300	-3.764570	2.802161	H	3.506106	1.228317	2.490443
H	1.961459	-2.017934	2.987589	H	2.632881	0.159960	3.624914
H	-1.804752	-3.356783	1.380634				

Table 5 (Continued).

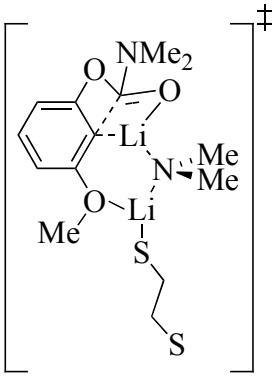


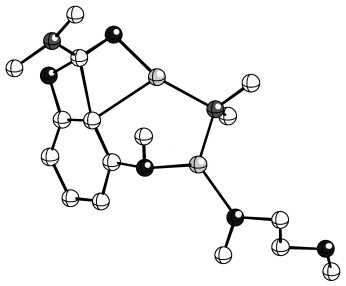


A49
G° = -1126.945642
See pg S83
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.207049	3.409903	-0.647079	H	-1.877864	4.773487	-0.588460
C	-1.560216	3.738358	-0.494321	H	0.509108	4.196790	-0.859510
C	-2.491745	2.744262	-0.223849	H	-3.546563	2.971899	-0.099417
C	-2.025178	1.427428	-0.113248	H	1.372365	-0.825981	-3.083845
C	-0.712004	1.005609	-0.246559	H	2.537951	-2.149892	-2.866469
C	0.161952	2.067731	-0.522988	H	0.848754	-2.519843	-3.218821
Li	-0.571659	-0.969025	-0.951170	H	0.705797	-3.890764	-1.161794
O	-2.418672	-1.320465	-0.916940	H	2.388816	-3.529485	-0.773278
C	-3.197463	-0.733922	-0.153009	H	1.107906	-3.139091	0.397883
O	-3.090008	0.534592	0.257653	H	-4.914475	0.284881	1.527432
N	-4.296186	-1.350580	0.372501	H	-6.211979	-0.477303	0.575088
C	-4.614878	-2.709884	-0.037799	H	-5.578343	-1.288980	2.024933
C	-5.304329	-0.663731	1.166858	H	-4.854507	-3.314854	0.844779
Li	1.777413	-0.250322	-0.135895	H	-5.482565	-2.723402	-0.712384
O	3.936737	-0.327390	0.142615	H	-3.757483	-3.139563	-0.552119
C	4.632111	-0.944712	-0.939493	H	1.294264	1.303847	3.032368
C	4.081587	-1.044466	1.363633	H	0.009164	0.316038	2.285322
C	3.219802	-0.363963	2.406448	H	0.871438	-0.283108	3.749878
O	1.882304	-0.366711	1.931530	H	4.450174	-0.333732	-1.825193
C	0.964318	0.279311	2.810269	H	5.711522	-0.978775	-0.733890
H	3.559789	0.670620	2.569239	H	4.252591	-1.957249	-1.118570
H	3.295009	-0.906884	3.361351	O	1.509926	1.672436	-0.663401
H	5.133144	-1.044559	1.690002	C	2.489032	2.656791	-0.957587
H	3.757141	-2.085968	1.224640	H	2.286118	3.144606	-1.919372
N	1.190929	-1.794123	-1.220013	H	2.538539	3.421352	-0.171093
C	1.496341	-1.825153	-2.637626	H	3.444196	2.131012	-1.005777
C	1.352257	-3.125869	-0.675452				

Table 5 (Continued).

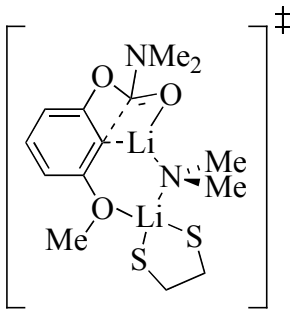


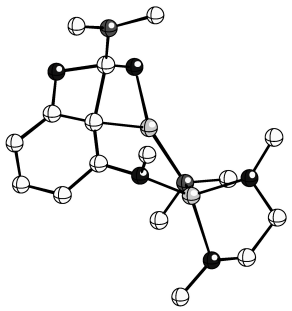


A50
G° = -1126.893815
See pg S140
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.387250	-2.374388	0.052222	H	-4.298171	2.696618	0.521563
C	-0.924750	-2.982971	-1.085527	H	-5.691449	1.937044	1.330609
C	-2.020433	-2.436241	-1.769978	H	2.145861	3.269378	0.088572
C	-2.535124	-1.257534	-1.239380	H	0.733859	3.891417	-0.769443
C	-2.047728	-0.604760	-0.106457	H	0.543567	3.202566	0.854448
C	-0.961432	-1.179140	0.531221	H	1.349908	0.623040	-2.364405
O	-3.560360	-0.486446	-1.681888	H	1.208720	2.365283	-2.675973
C	-3.381009	0.613147	-0.640530	H	2.623841	1.740901	-1.827096
O	-2.890870	1.704446	-1.064854	H	2.016844	-1.598206	2.592798
Li	-1.101504	1.456421	-0.963937	H	3.640665	-2.052992	2.002056
N	0.814076	1.741164	-0.650075	H	3.467240	-0.778081	3.245434
Li	1.148096	0.279925	0.572786	H	4.695797	0.593196	1.791093
O	2.841969	-0.234046	1.336107	H	3.747448	1.392698	0.516403
C	3.013321	-1.224853	2.351600	C	4.795179	-0.374297	-0.144865
C	4.048508	0.423844	0.921497	H	5.021867	-1.394186	0.211570
C	1.068573	3.068644	-0.103606	H	4.166276	-0.468174	-1.045262
C	1.522489	1.614882	-1.919843	O	5.981499	0.336707	-0.418691
N	-4.525478	0.656255	0.167371	C	6.751595	-0.246556	-1.451634
C	-5.044731	-0.581828	0.718869	H	6.194593	-0.283288	-2.400516
C	-4.640887	1.807119	1.048433	H	7.068664	-1.269257	-1.192377
H	0.441681	-2.829996	0.587808	H	7.637808	0.379102	-1.581675
H	-2.434385	-2.906559	-2.655920	O	-0.299979	-0.590504	1.629134
H	-0.482692	-3.909611	-1.442993	C	-1.097115	0.262361	2.463285
H	-6.059600	-0.405588	1.090677	H	-1.430969	1.152870	1.921873
H	-5.089587	-1.343086	-0.059770	H	-1.970971	-0.283302	2.831937
H	-4.430982	-0.963800	1.553925	H	-0.456036	0.552393	3.298795
H	-4.053060	1.692817	1.977944				

Table 5 (Continued).

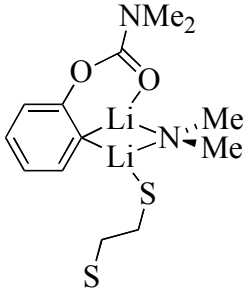


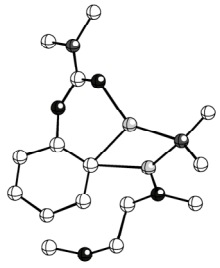


A51
G° = -1126.902988
See pg. S83
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.829353	2.622393	-0.908856	H	1.570953	-0.886668	3.981263
C	-1.962500	3.293871	-0.440267	H	1.729344	-1.962946	2.583453
C	-3.020544	2.611577	0.180155	H	0.780127	2.081166	1.993572
C	-2.866542	1.234266	0.296935	H	0.982665	1.461018	3.644001
C	-1.761200	0.512182	-0.151555	H	2.401573	1.682530	2.615144
C	-0.741790	1.227078	-0.755479	C	4.343087	0.069293	-1.058728
O	-3.704605	0.311287	0.843174	O	3.568470	0.911146	-0.215813
C	-2.787081	-0.874627	0.625587	H	4.041603	0.205027	-2.108985
O	-2.245122	-1.363965	1.661488	H	5.412732	0.310870	-0.970276
Li	-0.708328	-0.403852	1.768582	C	4.103594	-1.360957	-0.618505
N	1.162156	0.003777	2.067264	H	4.646200	-2.050997	-1.281519
Li	1.759034	0.030704	0.196457	H	4.457798	-1.510118	0.411719
C	1.886237	-0.926128	2.917210	O	2.700624	-1.603987	-0.687124
C	1.338322	1.349782	2.597649	C	2.343237	-2.940885	-0.336418
N	-3.382350	-1.750376	-0.300833	H	2.660412	-3.174944	0.687128
C	-3.966433	-1.196993	-1.509950	H	1.255953	-3.007375	-0.403102
C	-2.661675	-2.995010	-0.504088	H	2.798527	-3.655430	-1.035268
H	-0.019400	3.164939	-1.389342	C	3.703356	2.298789	-0.509218
H	-3.900144	3.132659	0.544730	H	4.748117	2.616878	-0.394660
H	-2.023687	4.372885	-0.558813	H	3.363914	2.518757	-1.530619
H	-4.577641	-1.967568	-1.991750	H	3.080212	2.833247	0.208998
H	-4.609071	-0.354342	-1.256059	O	0.439751	0.589360	-1.206276
H	-3.203554	-0.856390	-2.232701	C	0.281523	-0.074646	-2.466217
H	-1.756105	-2.860681	-1.129276	H	0.055596	0.654435	-3.253662
H	-2.362834	-3.399819	0.462135	H	1.226514	-0.578126	-2.679386
H	-3.316893	-3.711374	-1.010914	H	-0.527311	-0.811391	-2.412303
H	2.987273	-0.751239	2.933236				

Table 5 (Continued).

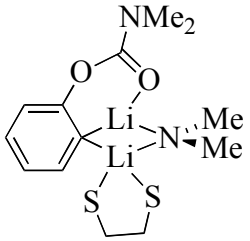


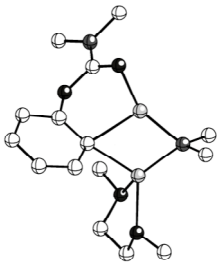


A52
$G°$ = -1012.433018
See pg S84
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	1.280377	-1.898088	2.604000	H	2.060412	-2.031930	3.351130
C	0.517531	-2.990362	2.187009	H	-1.108391	-3.620974	0.897831
C	-0.488660	-2.796019	1.239827	H	0.443073	3.002048	2.786520
C	-0.683878	-1.510411	0.734595	H	0.659157	4.461530	1.795115
C	0.038923	-0.367119	1.078803	H	-0.855586	4.207156	2.668765
C	1.027271	-0.631973	2.060986	H	-2.122635	4.394096	0.536128
Li	-1.484854	1.226744	1.348404	H	-0.612321	4.648690	-0.344472
O	-2.912886	0.198955	0.687217	H	-1.693220	3.316759	-0.809223
C	-2.742853	-0.644487	-0.206744	H	-2.613126	-2.449862	-2.063214
O	-1.689344	-1.469866	-0.293084	H	-4.379066	-2.467660	-2.293289
N	-3.633840	-0.826817	-1.216838	H	-3.370742	-1.350304	-3.240526
C	-4.813251	0.022228	-1.303212	H	-4.825997	0.555088	-2.262617
C	-3.485235	-1.831737	-2.260382	H	-5.724532	-0.585453	-1.232627
Li	0.585178	1.555117	0.243910	H	-4.796961	0.743518	-0.488628
O	2.049299	1.605921	-1.006332	H	2.098684	3.634019	-0.985297
C	2.577737	0.403415	-1.584992	H	2.578112	2.904299	-2.546018
C	3.865018	-0.062222	-0.893625	H	2.753779	0.555558	-2.658114
O	4.314100	-1.285349	-1.448502	H	1.793825	-0.347358	-1.461309
C	3.737083	-2.436272	-0.848863	H	3.685848	-0.153509	0.188136
C	2.653852	2.819243	-1.454098	H	4.671393	0.664025	-1.046376
H	3.707642	2.878061	-1.157500	H	2.644034	-2.469936	-0.956386
N	-0.602768	2.931083	0.953863	H	4.168954	-3.301648	-1.358162
C	-1.277743	3.851788	0.058895	H	3.977412	-2.491216	0.222998
C	-0.073970	3.675077	2.084149	H	1.639793	0.195430	2.431005
H	0.693177	-3.981517	2.597523				

Table 5 (Continued).

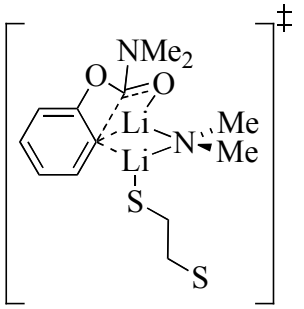


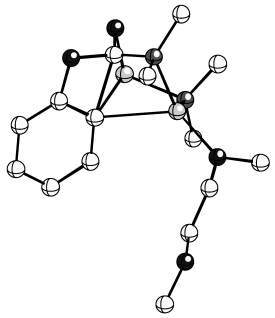


A53
$G°$ = -1012.440900
See pg S84
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	0.521290	3.415230	-1.393676	C	2.056642	-2.229893	-2.436419
C	-0.755301	3.837827	-1.018522	C	0.966452	-3.352291	-0.674071
C	-1.647483	2.906395	-0.488255	H	-1.058640	4.874706	-1.140353
C	-1.218384	1.586293	-0.345284	H	1.227802	4.127575	-1.816142
C	0.036938	1.075431	-0.678341	H	-2.652539	3.193920	-0.189586
C	0.882802	2.072438	-1.229663	H	2.227824	-1.266518	-2.944361
Li	-0.342259	-0.879484	-1.572533	H	3.060244	-2.637740	-2.172881
O	-2.210854	-0.873082	-1.303970	H	1.657958	-2.927043	-3.206654
C	-2.683069	-0.352553	-0.282876	H	0.507656	-4.104394	-1.353622
O	-2.217693	0.762159	0.297613	H	1.903934	-3.825752	-0.303558
N	-3.748094	-0.882890	0.379445	H	0.295649	-3.261050	0.195013
C	-4.356202	-2.114754	-0.101696	H	-3.868006	0.664472	1.786201
C	-4.386204	-0.255392	1.527344	H	-5.435392	-0.025828	1.298030
Li	1.514568	-0.541037	-0.062000	H	-4.366627	-0.935257	2.389121
O	3.424988	0.166269	0.275438	H	-4.383290	-2.860351	0.703008
C	4.556359	-0.226095	-0.494573	H	-5.385693	-1.928767	-0.435412
C	3.689832	0.236194	1.670872	H	-3.772970	-2.500926	-0.935301
C	2.379375	0.519119	2.375508	H	-0.300046	0.493575	2.370436
O	1.484096	-0.535989	2.040074	H	-0.368333	-1.289856	2.380199
C	0.217508	-0.420478	2.683862	H	0.341408	-0.428426	3.775963
H	1.963605	1.482965	2.047360	H	4.228543	-0.289205	-1.532416
H	2.543408	0.554645	3.463193	H	5.361693	0.515896	-0.403630
H	4.414653	1.035465	1.887686	H	4.927348	-1.208409	-0.172269
H	4.107279	-0.720549	2.019662	H	1.889731	1.790784	-1.546049
N	1.177847	-2.060260	-1.296379				

Table 5 (Continued).

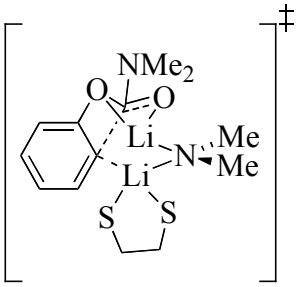


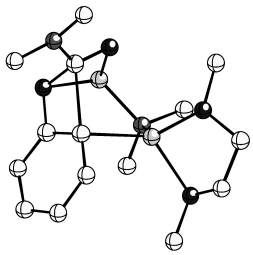


A54
G° = -1012.383881
See pg S84
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	0.609726	2.665393	1.855775	H	-3.274332	-1.711418	-1.476906
C	0.094826	3.779341	1.189044	H	-3.330738	-0.712185	-2.948300
C	-0.914063	3.652910	0.220412	H	-2.092445	-1.984770	-2.784725
C	-1.357380	2.362060	-0.026094	H	-1.487209	-4.046891	1.024253
C	-0.871213	1.215284	0.601622	H	-2.679531	-3.477982	2.193820
C	0.129645	1.371279	1.565805	H	-2.784532	-2.948044	0.503335
O	-2.327506	1.953990	-0.900557	H	0.241151	-1.428252	2.984274
C	-2.312921	0.521227	-0.562678	H	-0.954040	-2.561236	3.641167
O	-3.298646	0.063339	0.063978	H	0.291006	-3.144936	2.536613
Li	-2.335655	-0.362907	1.577950	H	0.714038	-3.479356	0.206459
N	-1.256636	-1.978151	1.594851	H	1.850923	-3.654450	-1.170164
Li	-0.452967	-1.090554	-0.006217	H	2.446803	-3.135985	0.437363
O	1.314744	-1.719967	-0.614827	H	2.961284	-1.691004	-1.884559
C	1.610113	-3.077669	-0.267815	H	1.964776	-0.224189	-1.835521
C	2.402948	-1.015874	-1.223596	H	0.544954	0.520684	2.103979
C	-2.077679	-3.149825	1.320083	C	3.341950	-0.404114	-0.185697
C	-0.393433	-2.287019	2.722621	H	2.797393	0.342728	0.413788
N	-1.722434	-0.298657	-1.594663	H	3.719062	-1.177613	0.505143
C	-0.877671	0.396441	-2.572805	O	4.403227	0.189121	-0.903310
C	-2.666381	-1.228671	-2.239597	C	5.322323	0.864648	-0.067969
H	1.383319	2.798023	2.608293	H	4.837782	1.679917	0.491346
H	-1.323968	4.515450	-0.295917	H	6.094979	1.285774	-0.715939
H	0.477576	4.768816	1.426893	H	5.793926	0.178661	0.653703
H	-0.343497	-0.353758	-3.164989	H	-0.146450	1.022858	-2.056831
H	-1.462171	1.032874	-3.250039				

Table 5 (Continued).

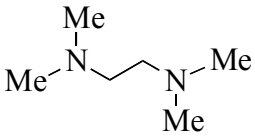


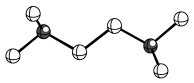


A55
$G°$ = -1012.400729
See pg S84
S = OMe

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.679931	2.842215	-1.529461	H	-3.943692	-2.989855	-1.210733
C	-1.277865	3.416517	-0.404878	H	3.256876	-0.717644	2.299450
C	-1.808560	2.611745	0.615730	H	2.371595	-0.874719	3.820998
C	-1.676546	1.242872	0.433825	H	1.973483	-1.940990	2.459304
C	-1.065345	0.600902	-0.637682	H	0.862755	2.097918	2.285228
C	-0.580802	1.441390	-1.649034	H	1.682406	1.488290	3.739719
O	-2.211723	0.269309	1.287582	H	2.595478	1.690708	2.242460
C	-1.986480	-0.951745	0.488740	O	2.747470	0.662282	-0.734215
O	-1.199980	-1.777941	1.016766	C	3.113671	-0.155673	-1.836815
Li	-0.567691	-0.553186	2.316816	H	2.447077	0.042419	-2.690202
N	1.236546	0.023935	2.228521	H	4.148988	0.051753	-2.146842
Li	1.081224	-0.165758	0.220369	C	2.995392	-1.599144	-1.389124
C	2.241615	-0.904930	2.718135	H	3.179529	-2.270368	-2.241627
C	1.605595	1.367841	2.637930	H	3.734715	-1.818661	-0.604211
N	-3.117899	-1.369682	-0.188540	O	1.681719	-1.783731	-0.881063
C	-4.000937	-0.388900	-0.802936	C	1.409573	-3.123384	-0.467975
C	-2.954307	-2.598427	-0.955702	H	2.139464	-3.452322	0.284396
H	-0.299930	3.486290	-2.320657	H	0.409865	-3.109844	-0.034196
H	-2.309562	3.042503	1.478501	H	1.447540	-3.802529	-1.330809
H	-1.352013	4.498251	-0.323796	C	2.959533	2.052667	-0.960584
H	-4.946933	-0.882234	-1.046579	H	4.024940	2.251575	-1.141057
H	-4.203017	0.420836	-0.102515	H	2.367754	2.407485	-1.813699
H	-3.567642	0.034336	-1.722005	H	2.638147	2.570059	-0.056389
H	-2.392684	-2.422015	-1.888113	H	-0.121712	1.026579	-2.548311
H	-2.422082	-3.333799	-0.353324				

Table 5 (Continued).

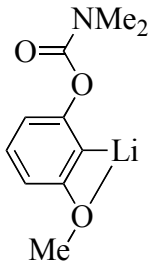


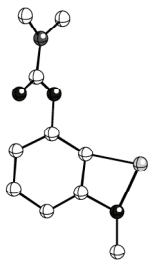


$G° = -347.557034$

Atom	X	Y	Z
C	-2.936402	-0.711691	-0.659111
H	-2.669726	-1.216714	-1.593644
H	-3.136598	-1.488965	0.105899
H	-3.866922	-0.157380	-0.825188
C	-2.258336	0.964362	0.912787
H	-1.504543	1.720776	1.148262
H	-3.205232	1.483824	0.729427
H	-2.389286	0.320696	1.806625
C	-0.598439	-0.480567	-0.124398
C	0.598431	0.480551	-0.124384
H	-0.470842	-1.150691	-0.981694
H	-0.597912	-1.116121	0.783684
H	0.470835	1.150691	-0.981667
H	0.597895	1.116091	0.783710
N	-1.878067	0.214677	-0.278431
N	1.878065	-0.214681	-0.278430
C	2.936381	0.711701	-0.659126
H	3.136576	1.488979	0.105880
H	3.866906	0.157402	-0.825216
H	2.669683	1.216719	-1.593656
C	2.258366	-0.964357	0.912784
H	3.205272	-1.483795	0.729412
H	2.389311	-0.320688	1.806620
H	1.504596	-1.720790	1.148268

Table 5 (Continued).

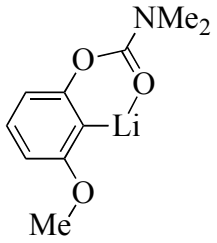


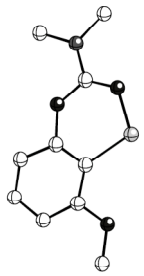


A56
G° = -676.071559
See pg S85

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.780773	1.145154	-0.220583	H	-5.334379	-1.714849	0.688299
C	-2.436753	-0.189992	-0.029009	H	-4.867906	-0.086735	1.260605
C	-1.148796	-0.728440	-0.082312	C	2.131704	0.217203	0.304683
C	-0.168507	0.211799	-0.355814	O	1.950971	1.022578	1.201122
C	-0.417641	1.573880	-0.565357	N	3.352042	-0.327014	-0.014699
C	-1.729817	2.031811	-0.492600	C	4.504495	0.026662	0.793092
H	-3.801582	1.510668	-0.168132	H	4.888346	-0.849876	1.335230
H	0.398623	2.259068	-0.767803	H	5.312575	0.415405	0.158532
H	-1.945336	3.085559	-0.648102	H	4.206667	0.790311	1.510160
Li	-1.980355	-2.458450	0.373116	C	3.563131	-1.326959	-1.046148
O	1.153967	-0.262261	-0.517087	H	4.362021	-1.002737	-1.727212
O	-3.421796	-1.199977	0.260253	H	3.866609	-2.287865	-0.604113
C	-4.773668	-0.810112	0.441376	H	2.648573	-1.472885	-1.615800
H	-5.182842	-0.370373	-0.476381				

Table 5 (Continued).

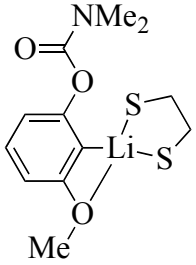


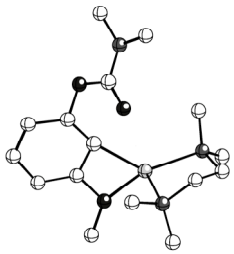


A57
$G°$ = -676.095932
See pg S85

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.960875	1.073834	0.003639	H	-5.071028	-2.176591	-0.018239
C	-2.429060	-0.221031	-0.002951	H	-4.984217	-0.638754	0.883460
C	-1.049992	-0.498257	-0.001629	C	1.998039	-0.453177	-0.003135
C	-0.257523	0.631082	0.006701	O	1.664375	-1.656240	0.017418
C	-0.706529	1.959770	0.014285	N	3.313132	-0.093928	-0.046485
C	-2.079396	2.163919	0.012545	C	3.774827	1.287228	-0.022795
H	-4.029731	1.260054	0.002502	H	4.545359	1.425020	-0.790627
H	-0.006118	2.789761	0.021648	H	2.947110	1.962625	-0.222264
H	-2.476997	3.175705	0.017894	H	4.213799	1.535569	0.953381
Li	-0.058307	-2.198981	0.011293	C	4.347816	-1.114470	0.021560
O	1.190734	0.599448	0.009984	H	5.047360	-0.994110	-0.814826
O	-3.233919	-1.350452	-0.010443	H	4.913771	-1.028924	0.959251
C	-4.636040	-1.173928	-0.011974	H	3.887567	-2.098746	-0.031043
H	-4.981004	-0.629030	-0.902767				

Table 5 (Continued).

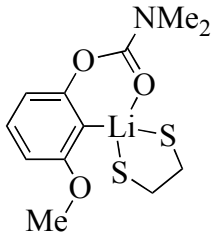


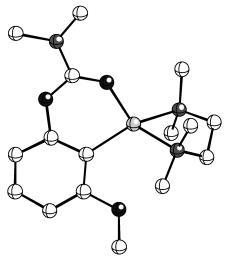


A58
G° = -1023.659337
See pg S85
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.777355	3.641734	-0.190746	H	4.235159	0.482229	-1.449742
C	-0.933692	2.288926	-0.503021	N	-2.022845	-0.984324	1.380675
C	0.075554	1.322430	-0.501930	N	-1.337385	-2.163268	-1.247479
C	1.302318	1.833441	-0.123703	C	-2.101980	-2.401933	-2.476973
C	1.564223	3.168190	0.208288	H	-3.157072	-2.159155	-2.313863
C	0.507360	4.073495	0.165991	H	-1.719293	-1.753929	-3.271339
H	-1.596447	4.354393	-0.215881	H	-2.033695	-3.449184	-2.820859
H	2.566925	3.482631	0.484995	C	0.093248	-2.424078	-1.484318
H	0.675509	5.119144	0.411347	H	0.449559	-1.768627	-2.283258
Li	-1.309519	-0.176873	-0.452430	H	0.672714	-2.192981	-0.588681
O	2.479537	1.021872	-0.138969	H	0.269070	-3.475657	-1.774169
O	-2.197900	1.732810	-0.843278	C	-1.853746	-2.970161	-0.123087
C	-3.336600	2.571930	-0.814675	H	-2.941060	-3.039229	-0.232601
H	-3.253392	3.385444	-1.547697	H	-1.470475	-4.004889	-0.164231
H	-4.195133	1.946856	-1.073895	C	-1.506320	-2.358174	1.239436
H	-3.493671	3.010215	0.181114	H	-1.891651	-3.020327	2.037011
C	2.508777	-0.207675	0.409847	H	-0.420243	-2.305214	1.359770
O	1.678368	-0.679740	1.180095	C	-3.477505	-0.949968	1.555944
N	3.632082	-0.895513	0.006507	H	-3.799818	-1.474702	2.473429
C	3.980686	-2.131517	0.683902	H	-3.805573	0.091562	1.620991
H	4.189568	-2.922256	-0.048476	H	-3.985732	-1.408088	0.702323
H	4.877004	-2.001186	1.308632	C	-1.359428	-0.287033	2.496932
H	3.147587	-2.432398	1.317124	H	-0.284423	-0.251806	2.310460
C	4.657427	-0.321677	-0.850947	H	-1.734609	0.739359	2.548595
H	5.500513	0.076252	-0.265882	H	-1.558625	-0.782131	3.464090
H	5.045049	-1.101085	-1.518369				

Table 5 (Continued).

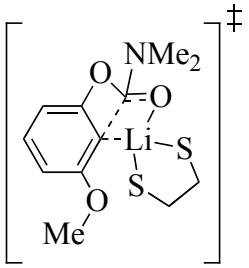


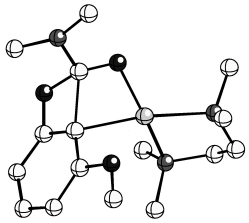


A59
G° = -1023.673569
See pg S85
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	0.589027	3.737077	0.057724	H	-3.022953	-2.883742	-0.240797
C	0.928390	2.379201	0.068788	N	1.753145	-1.513367	-1.461069
C	0.000854	1.322168	0.061211	N	1.432006	-1.796633	1.477513
C	-1.306556	1.764447	0.026001	C	2.877697	-1.810627	-0.558058
C	-1.741506	3.098460	0.007958	H	3.660660	-2.404546	-1.066476
C	-0.767832	4.086936	0.026616	H	3.330795	-0.853940	-0.281362
H	1.335362	4.525038	0.070101	C	2.433619	-2.552316	0.707347
H	-2.799968	3.342344	-0.018355	H	3.324727	-2.784625	1.318928
H	-1.054499	5.135657	0.016375	H	1.989076	-3.514693	0.432690
Li	0.324471	-0.705705	-0.063856	C	1.264096	-2.706478	-2.157330
O	-2.453453	0.881278	0.030503	H	0.930540	-3.462855	-1.441735
O	2.270182	1.969411	0.084264	H	0.404203	-2.433529	-2.775762
C	3.272398	2.965631	0.122270	H	2.036413	-3.157013	-2.807697
H	3.194388	3.593677	1.021416	C	2.120040	-0.471056	-2.429832
H	4.230800	2.439038	0.139653	H	1.253578	-0.244334	-3.058221
H	3.240658	3.617805	-0.762519	H	2.396816	0.438105	-1.891267
C	-2.466640	-0.441347	-0.102571	H	2.953458	-0.786103	-3.084213
O	-1.491973	-1.189741	-0.269817	C	0.634320	-2.680815	2.331622
N	-3.742190	-0.941554	-0.024105	H	-0.133460	-2.091882	2.842150
C	-4.928567	-0.102206	0.054246	H	0.132283	-3.435722	1.718546
H	-5.649842	-0.562044	0.740133	H	1.242584	-3.195884	3.097329
H	-4.664206	0.884906	0.425261	C	2.048183	-0.730787	2.281982
H	-5.410474	0.003329	-0.928970	H	2.541697	-0.001508	1.636983
C	-3.972666	-2.353754	-0.276774	H	1.264014	-0.194650	2.822855
H	-4.647878	-2.761774	0.485264	H	2.773481	-1.136789	3.011207
H	-4.433565	-2.511049	-1.263128				

Table 5 (Continued).

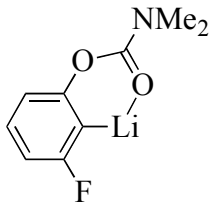


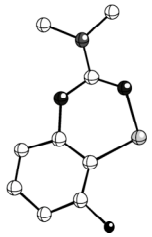


A60
G° = -1023.638034
See pg S85
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.795704	-2.434651	0.982727	H	-0.629775	3.712958	0.099293
C	-1.259963	-1.140502	1.169457	N	2.613838	0.919947	0.772460
C	-1.313701	-0.223167	0.123109	N	1.941098	-1.035908	-1.331206
C	-1.927662	-0.610655	-1.061122	C	3.550991	-0.138172	0.349012
C	-2.469520	-1.869800	-1.309724	H	4.601805	0.180814	0.470985
C	-2.384610	-2.773384	-0.242204	H	3.404510	-0.994442	1.015814
H	-1.761937	-3.178604	1.771560	C	3.320925	-0.572745	-1.103246
H	-2.949294	-2.130064	-2.247898	H	4.061671	-1.348052	-1.369896
H	-2.794639	-3.773959	-0.360527	H	3.500410	0.274053	-1.773439
Li	0.811194	0.413528	-0.257040	C	2.983326	2.232721	0.219729
O	-1.911692	0.493654	-1.859942	H	2.991809	2.200176	-0.871973
O	-0.637253	-0.738123	2.335876	H	2.233580	2.970361	0.515078
C	-0.697468	-1.605477	3.455688	H	3.975529	2.562139	0.575683
H	-0.157187	-2.545868	3.277769	C	2.528890	0.996947	2.236644
H	-0.220823	-1.070305	4.280191	H	1.806324	1.769099	2.515383
H	-1.734711	-1.839386	3.729041	H	2.173875	0.043276	2.636436
C	-1.227532	1.396359	-0.853068	H	3.500715	1.242601	2.699878
O	-0.044943	1.759908	-1.136280	C	1.576472	-0.966337	-2.754703
N	-2.143724	2.370749	-0.410987	H	0.537612	-1.284546	-2.871706
C	-3.488082	1.950716	-0.048914	H	1.650049	0.067071	-3.103371
H	-4.117016	2.841380	0.055367	H	2.219288	-1.610382	-3.379996
H	-3.904096	1.325186	-0.838385	C	1.722645	-2.396915	-0.821943
H	-3.514547	1.390889	0.901777	H	1.962362	-2.451224	0.243762
C	-1.575432	3.350912	0.501533	H	0.668782	-2.661129	-0.940197
H	-2.269718	4.192327	0.598714	H	2.342407	-3.139269	-1.355843
H	-1.399402	2.932205	1.510650				

Table 5 (Continued).

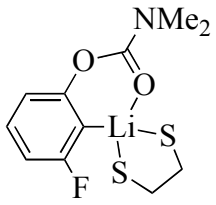


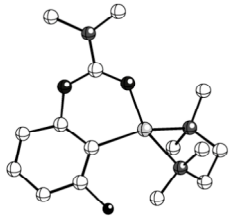


A61
G° = -660.850820
See pg S86

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.442433	0.624823	-0.000564	O	1.433475	-1.619597	0.018663
C	-2.758451	-0.586645	-0.008080	N	2.916932	0.100499	-0.044348
C	-1.378755	-0.752051	-0.004600	C	3.237922	1.521603	-0.023294
C	-0.702682	0.459397	0.007366	H	3.989098	1.734037	-0.793058
C	-1.292606	1.728782	0.016361	H	2.346797	2.111039	-0.221917
C	-2.683657	1.799092	0.012191	H	3.652049	1.812872	0.951629
H	-4.528103	0.646860	-0.004126	C	4.050214	-0.810615	0.020422
H	-0.680955	2.626121	0.026676	H	4.731391	-0.618370	-0.817370
H	-3.177430	2.767031	0.018620	H	4.605757	-0.668041	0.957095
Li	-0.220170	-2.346236	0.009198	H	3.692357	-1.836514	-0.032247
O	0.735744	0.577174	0.013122	F	-3.533469	-1.718609	-0.018926
C	1.646866	-0.389881	-0.000869				

Table 5 (Continued).

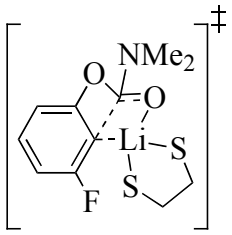


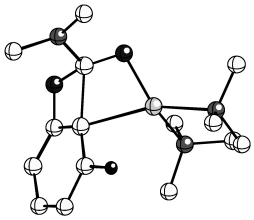


A62
G° = -1008.432441
See pg S86
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	0.519181	3.855405	-0.118039	C	-3.420636	-0.425914	0.554664
C	-0.183882	2.655787	-0.119625	H	-4.372594	-0.653325	1.069793
C	0.337478	1.372632	-0.101891	H	-3.466002	0.623170	0.247933
C	1.723082	1.389596	-0.062655	C	-3.299525	-1.317335	-0.685276
C	2.536938	2.529525	-0.055103	H	-4.212434	-1.205406	-1.298227
C	1.915319	3.776418	-0.086335	H	-3.258146	-2.368693	-0.381306
H	0.000400	4.809635	-0.138527	C	-2.288964	-1.828817	2.203009
H	3.619364	2.439978	-0.025345	H	-2.276884	-2.679461	1.515936
H	2.514223	4.683282	-0.083689	H	-1.393381	-1.893856	2.827863
Li	-0.639769	-0.425417	0.057792	H	-3.178103	-1.918459	2.853520
O	2.529706	0.195882	-0.045310	C	-2.207582	0.570894	2.397632
C	2.110949	-1.060415	0.107742	H	-1.320243	0.469820	3.029598
O	0.944688	-1.447886	0.271726	H	-2.118965	1.498882	1.829996
N	3.156764	-1.944518	0.056439	H	-3.098215	0.618818	3.049806
C	4.551150	-1.534848	-0.031128	C	-1.713295	-2.163945	-2.314397
H	5.086830	-2.226905	-0.691219	H	-0.779981	-1.934541	-2.837239
H	4.621647	-0.529128	-0.437889	H	-1.547509	-3.050426	-1.694088
H	5.037377	-1.556175	0.955140	H	-2.484288	-2.402285	-3.069174
C	2.919451	-3.351001	0.336263	C	-2.245132	0.184970	-2.289965
H	3.405339	-3.970003	-0.427839	H	-2.399126	1.061334	-1.658534
H	3.329003	-3.631883	1.317367	H	-1.324009	0.356548	-2.852823
H	1.848174	-3.541590	0.330107	H	-3.085760	0.087001	-3.000935
N	-2.268828	-0.563351	1.463461	F	-1.573624	2.780696	-0.131730
N	-2.086098	-1.026135	-1.468290				

Table 5 (Continued).

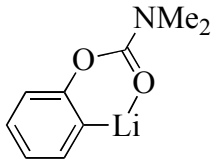


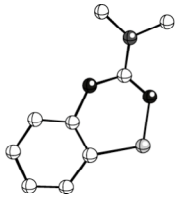


A63
$G°$ = -1008.392406
See pg S86
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	0.519181	3.855405	-0.118039	C	-3.420636	-0.425914	0.554664
C	-0.183882	2.655787	-0.119625	H	-4.372594	-0.653325	1.069793
C	0.337478	1.372632	-0.101891	H	-3.466002	0.623170	0.247933
C	1.723082	1.389596	-0.062655	C	-3.299525	-1.317335	-0.685276
C	2.536938	2.529525	-0.055103	H	-4.212434	-1.205406	-1.298227
C	1.915319	3.776418	-0.086335	H	-3.258146	-2.368693	-0.381306
H	0.000400	4.809635	-0.138527	C	-2.288964	-1.828817	2.203009
H	3.619364	2.439978	-0.025345	H	-2.276884	-2.679461	1.515936
H	2.514223	4.683282	-0.083689	H	-1.393381	-1.893856	2.827863
Li	-0.639769	-0.425417	0.057792	H	-3.178103	-1.918459	2.853520
O	2.529706	0.195882	-0.045310	C	-2.207582	0.570894	2.397632
C	2.110949	-1.060415	0.107742	H	-1.320243	0.469820	3.029598
O	0.944688	-1.447886	0.271726	H	-2.118965	1.498882	1.829996
N	3.156764	-1.944518	0.056439	H	-3.098215	0.618818	3.049806
C	4.551150	-1.534848	-0.031128	C	-1.713295	-2.163945	-2.314397
H	5.086830	-2.226905	-0.691219	H	-0.779981	-1.934541	-2.837239
H	4.621647	-0.529128	-0.437889	H	-1.547509	-3.050426	-1.694088
H	5.037377	-1.556175	0.955140	H	-2.484288	-2.402285	-3.069174
C	2.919451	-3.351001	0.336263	C	-2.245132	0.184970	-2.289965
H	3.405339	-3.970003	-0.427839	H	-2.399126	1.061334	-1.658534
H	3.329003	-3.631883	1.317367	H	-1.324009	0.356548	-2.852823
H	1.848174	-3.541590	0.330107	H	-3.085760	0.087001	-3.000935
N	-2.268828	-0.563351	1.463461	F	-1.573624	2.780696	-0.131730
N	-2.086098	-1.026135	-1.468290				

Table 5 (Continued).

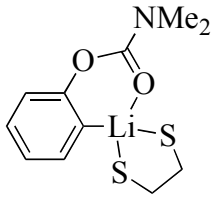


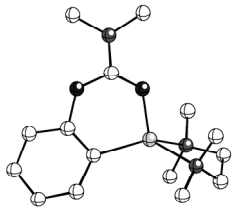


A64
G° = -561.595229
See pg S86

Atom	X	Y	Z	Atom	X	Y	Z
C	3.790035	-0.041585	-0.006320	O	-1.356695	1.637312	0.011185
C	3.016530	1.121400	-0.014112	N	-2.592207	-0.269410	-0.043252
C	1.601876	1.132757	-0.008075	C	-2.715847	-1.720422	-0.013640
C	1.056460	-0.148588	0.005755	H	-3.428983	-2.039224	-0.783036
C	1.771190	-1.350273	0.014858	H	-1.751448	-2.182654	-0.206952
C	3.161664	-1.290054	0.008692	H	-3.088084	-2.060434	0.962559
H	4.876698	0.020014	-0.011502	C	-3.838503	0.479112	0.017974
H	1.248318	-2.303197	0.026760	H	-4.488113	0.191704	-0.817892
H	3.744164	-2.208010	0.015206	H	-4.369996	0.268119	0.955964
Li	0.199109	2.528045	0.003236	H	-3.623700	1.543905	-0.040775
O	-0.366462	-0.440995	0.014470	H	3.547095	2.074987	-0.025197
C	-1.398833	0.388651	-0.003020				

Table 5 (Continued).

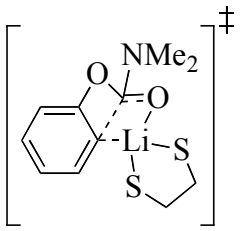


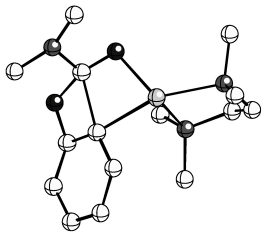


A65
G° = -909.173538
See pg S86
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.582750	3.878130	0.105214	C	3.596549	0.124750	-0.602088
C	-0.516082	2.978851	0.202327	H	4.504173	-0.205959	-1.140064
C	-0.648392	1.569016	0.166974	H	3.743096	1.184253	-0.368508
C	-1.974742	1.175708	0.024248	C	3.468388	-0.674841	0.700250
C	-3.089283	2.013452	-0.082744	H	4.404071	-0.570041	1.280045
C	-2.884154	3.390443	-0.042150	H	3.364407	-1.739842	0.467117
H	-1.406014	4.952261	0.143005	C	2.326697	-1.267885	-2.148557
H	-4.087179	1.594893	-0.191279	H	2.343255	-2.096005	-1.435691
H	-3.730132	4.069222	-0.121470	H	1.383617	-1.327591	-2.698016
Li	0.758317	0.087216	-0.001984	H	3.163708	-1.396990	-2.858829
O	-2.410290	-0.208533	0.008921	C	2.310306	1.124607	-2.404917
C	-1.662924	-1.299177	-0.102659	H	1.383829	1.033739	-2.978788
O	-0.435988	-1.355028	-0.283391	H	2.278223	2.076898	-1.868586
N	-2.418031	-2.440343	0.008382	H	3.161347	1.136352	-3.109587
C	-3.870039	-2.427077	0.110662	C	1.899246	-1.315364	2.440641
H	-4.188195	-3.238251	0.775617	H	0.992551	-0.998484	2.964519
H	-4.207350	-1.478013	0.520463	H	1.675864	-2.242453	1.904294
H	-4.345129	-2.580606	-0.869555	H	2.683163	-1.518833	3.192427
C	-1.805424	-3.732056	-0.250395	C	2.493268	1.001887	2.182872
H	-2.097554	-4.445706	0.529669	H	2.742529	1.791553	1.469895
H	-2.125602	-4.136248	-1.222173	H	1.562276	1.292783	2.675322
H	-0.723016	-3.620233	-0.252335	H	3.300418	0.938569	2.935384
N	2.394390	0.017535	-1.445055	H	0.483361	3.409159	0.316646
N	2.291010	-0.274371	1.485834				

Table 5 (Continued).





A66
$G°$ = -909.141316
See pg S86
S = NMe_2

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.448578	-2.277210	2.067056	C	3.463366	0.083532	0.533780
C	-1.101838	-0.918720	1.905402	H	4.488426	0.488194	0.607991
C	-1.298986	-0.304907	0.668333	H	3.375178	-0.690101	1.303467
C	-1.872493	-1.060859	-0.354317	C	3.266980	-0.545668	-0.850238
C	-2.235676	-2.398180	-0.246221	H	4.060922	-1.295181	-1.019809
C	-2.002753	-2.996421	1.004949	H	3.390430	0.219641	-1.623628
H	-1.295046	-2.767490	3.026042	C	2.738338	2.378877	0.119417
H	-2.692310	-2.948087	-1.064483	H	2.758463	2.213663	-0.960195
H	-2.272077	-4.040374	1.149646	H	1.940227	3.096817	0.324188
Li	0.696961	0.358962	-0.113771	H	3.703434	2.814749	0.431605
O	-2.020237	-0.219422	-1.420186	C	2.360136	1.370839	2.272980
C	-1.451288	1.010326	-0.766129	H	1.578499	2.112709	2.462259
O	-0.328792	1.411828	-1.196318	H	2.089195	0.446536	2.792170
N	-2.474042	1.946662	-0.554288	H	3.307050	1.748339	2.696673
C	-3.741722	1.488710	-0.007971	C	1.555878	-1.268217	-2.424818
H	-4.481472	2.288232	-0.121106	H	0.532198	-1.644397	-2.492326
H	-4.088148	0.616256	-0.561312	H	1.581075	-0.289348	-2.910484
H	-3.667400	1.226976	1.060999	H	2.228852	-1.959410	-2.961605
C	-2.024683	3.218165	-0.010030	C	1.795607	-2.421540	-0.322060
H	-2.823951	3.958000	-0.123676	H	2.026368	-2.318718	0.741540
H	-1.773393	3.146846	1.065292	H	0.763269	-2.770803	-0.403233
H	-1.144478	3.554262	-0.556823	H	2.469408	-3.182471	-0.754438
N	2.453734	1.120717	0.828686	H	-0.686577	-0.374457	2.754704
N	1.923093	-1.127218	-1.007383				

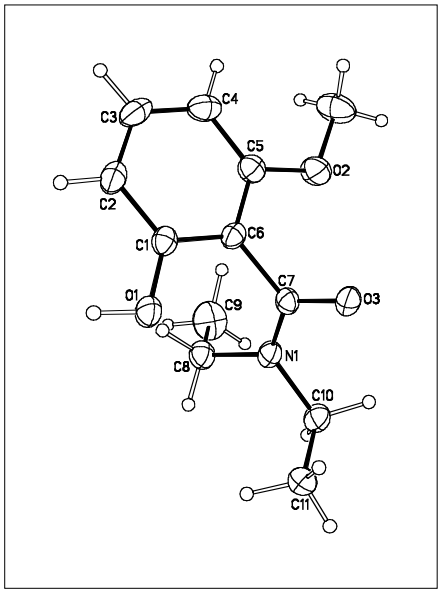


Figure 79. The key structural data for the crystal structure of **5b** have been archived in the Cambridge Crystallographic Database (CCDC 684578).

Figure 79 (Continued).

Table 1. Crystal data and structure refinement for **5b**.

Identification code	**5b**	
Empirical formula	C12 H17 N O3	
Formula weight	223.27	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.2430(4) Å	α= 90°.
	b = 17.1827(10) Å	β= 95.266(2)°.
	c = 9.5958(4) Å	γ = 90°.
Volume	1189.20(11) $Å^3$	
Z	4	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	480	
Crystal size	0.60 x 0.35 x 0.20 mm^3	
Theta range for data collection	2.37 to 27.88°.	
Index ranges	-9<=h<=9, -22<=k<=22, -12<=l<=12	
Reflections collected	10590	
Independent reflections	2837 [R(int) = 0.0420]	
Completeness to theta = 27.88°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9823 and 0.9483	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2837 / 0 / 213	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0433, wR2 = 0.0943	
R indices (all data)	R1 = 0.0656, wR2 = 0.1033	
Largest diff. peak and hole	0.209 and -0.200 $e.Å^{-3}$	

Figure 79 (Continued).

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1295(1)	2499(1)	6177(1)	28(1)
O(2)	3685(1)	199(1)	8203(1)	33(1)
O(3)	4370(1)	1909(1)	8979(1)	28(1)
N(1)	1301(1)	1826(1)	9267(1)	24(1)
C(1)	1724(1)	1738(1)	5973(1)	23(1)
C(2)	1462(2)	1377(1)	4673(1)	28(1)
C(3)	1955(2)	609(1)	4563(1)	33(1)
C(4)	2728(2)	190(1)	5699(1)	32(1)
C(5)	2970(2)	550(1)	6992(1)	26(1)
C(6)	2450(1)	1326(1)	7143(1)	22(1)
C(7)	2764(2)	1715(1)	8543(1)	22(1)
C(8)	-610(2)	1642(1)	8712(1)	28(1)
C(9)	-1214(2)	844(1)	9116(2)	46(1)
C(10)	1510(2)	2228(1)	10620(1)	29(1)
C(11)	1472(2)	3102(1)	10445(1)	34(1)
C(12)	4277(2)	-590(1)	8124(2)	44(1)

Figure 79 (Continued).

Table 3. Bond lengths [Å] and angles [°] for **5b**.

O(1)-C(1)	1.3617(13)
O(2)-C(5)	1.3682(13)
O(2)-C(12)	1.4272(15)
O(3)-C(7)	1.2449(13)
N(1)-C(7)	1.3330(14)
N(1)-C(10)	1.4660(14)
N(1)-C(8)	1.4712(14)
C(1)-C(6)	1.3896(14)
C(1)-C(2)	1.3904(15)
C(2)-C(3)	1.3745(17)
C(3)-C(4)	1.3807(17)
C(4)-C(5)	1.3831(16)
C(5)-C(6)	1.3952(15)
C(6)-C(7)	1.4995(14)
C(8)-C(9)	1.5011(19)
C(10)-C(11)	1.5109(18)
C(5)-O(2)-C(12)	117.77(9)
C(7)-N(1)-C(10)	120.45(9)
C(7)-N(1)-C(8)	123.12(9)
C(10)-N(1)-C(8)	116.07(9)
O(1)-C(1)-C(6)	116.60(9)
O(1)-C(1)-C(2)	122.89(10)
C(6)-C(1)-C(2)	120.51(10)
C(3)-C(2)-C(1)	118.82(10)
C(2)-C(3)-C(4)	121.94(11)
C(3)-C(4)-C(5)	118.96(11)
O(2)-C(5)-C(4)	124.86(10)
O(2)-C(5)-C(6)	114.69(9)
C(4)-C(5)-C(6)	120.44(10)
C(1)-C(6)-C(5)	119.28(9)
C(1)-C(6)-C(7)	120.73(10)

Figure 79 (Continued).

C(5)-C(6)-C(7)	119.92(9)
O(3)-C(7)-N(1)	123.32(10)
O(3)-C(7)-C(6)	118.70(10)
N(1)-C(7)-C(6)	117.98(9)
N(1)-C(8)-C(9)	112.93(10)
N(1)-C(10)-C(11)	111.74(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	34(1)	27(1)	22(1)	2(1)	-4(1)	3(1)
O(2)	42(1)	25(1)	32(1)	3(1)	1(1)	8(1)
O(3)	23(1)	34(1)	24(1)	-5(1)	-3(1)	0(1)
N(1)	25(1)	29(1)	19(1)	-1(1)	0(1)	1(1)
C(1)	19(1)	27(1)	22(1)	0(1)	1(1)	-3(1)
C(2)	25(1)	39(1)	21(1)	-1(1)	-1(1)	-3(1)
C(3)	31(1)	41(1)	26(1)	-13(1)	5(1)	-7(1)
C(4)	32(1)	28(1)	38(1)	-9(1)	7(1)	-2(1)
C(5)	23(1)	27(1)	28(1)	0(1)	3(1)	-1(1)
C(6)	20(1)	25(1)	20(1)	-2(1)	1(1)	-3(1)
C(7)	25(1)	20(1)	20(1)	3(1)	-2(1)	2(1)
C(8)	23(1)	35(1)	26(1)	0(1)	3(1)	1(1)
C(9)	37(1)	47(1)	54(1)	7(1)	5(1)	-11(1)
C(10)	29(1)	39(1)	19(1)	-2(1)	2(1)	4(1)
C(11)	28(1)	38(1)	36(1)	-10(1)	-2(1)	8(1)
C(12)	55(1)	30(1)	48(1)	8(1)	14(1)	14(1)

Figure 79 (Continued).

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5b**.

	x	y	z	U(eq)
H(10B)	2705(17)	2063(7)	11123(12)	31(3)
H(10A)	491(17)	2070(7)	11144(12)	30(3)
H(8B)	-714(18)	1687(7)	7670(13)	37(3)
H(3)	1736(17)	356(7)	3673(13)	37(3)
H(12C)	5260(20)	-636(8)	7470(14)	49(4)
H(11C)	1422(19)	3351(8)	11358(14)	45(4)
H(11B)	327(19)	3263(7)	9840(13)	38(4)
H(8A)	-1441(17)	2025(7)	9083(12)	28(3)
H(4)	3061(18)	-335(8)	5610(13)	37(3)
H(2)	880(18)	1666(7)	3871(13)	39(4)
H(11A)	2606(19)	3287(7)	10004(13)	38(4)
H(9C)	-400(20)	428(10)	8702(17)	75(5)
H(12B)	4789(19)	-725(8)	9083(14)	46(4)
H(12A)	3180(20)	-929(8)	7846(15)	58(4)
H(9B)	-2520(20)	756(9)	8764(15)	59(4)
H(9A)	-1120(20)	806(8)	10126(15)	54(4)
H(1O)	570(20)	2674(8)	5384(15)	54(4)

REFERENCES

1. Briggs, T. F.; Winemiller, M. D.; Collum, D. B.; Parsons, R. L., Jr.; Davulcu, A. K.; Harris, G. D.; Fortunak, J. D.; Confalone, P. N. *J. Am. Chem. Soc.* **2004**, *126*, 5427.

2. Zhao, P.; Lucht, B. L.; Kenkre, S. L.; Collum, D. B. *J. OrG°. Chem.* **2004**, *69*, 242.

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

4. GaussView, Version 3.09, Dennington II, R.; Keith, T.; Millam, J.; Eppinnett, K.; Hovell, W. L.; Gilliland, R.; Semichem, Inc., Shawnee Mission, KS, 2003.