Lithium Enolates Derived from Pyroglutaminol:
Aggregation, Solvation, and Atropisomerism

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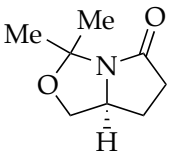
Part 1: NMR Spectroscopic Studies

Part 2: Derivation for Job Plot with relative integration vs intended mole fraction and Matlab code

Part 3: Density Functional Theory Calculations of Ground State and Transition State

Part 1: NMR Spectroscopic Studies

Chart 1



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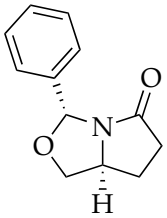

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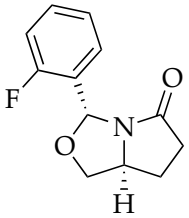

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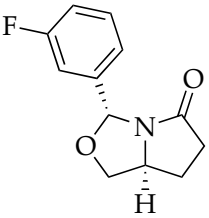

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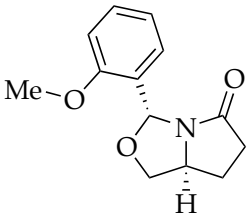

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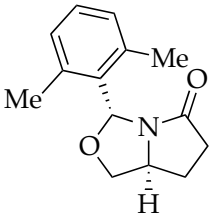

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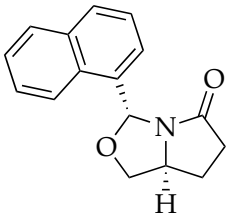

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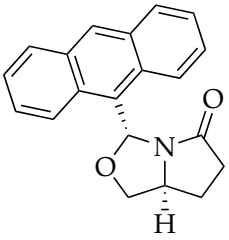

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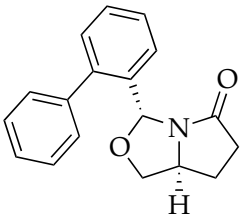

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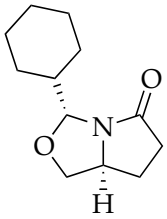

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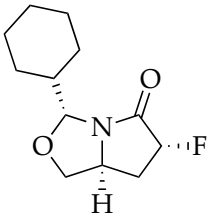

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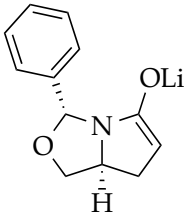
Chart 2



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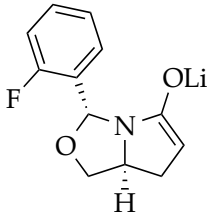

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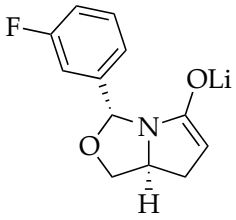

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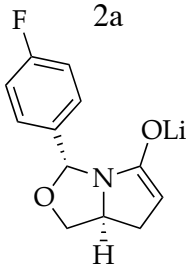

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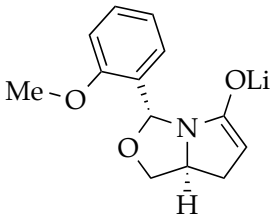

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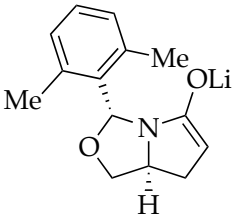

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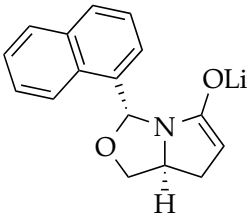

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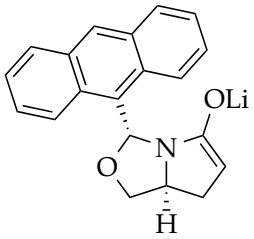

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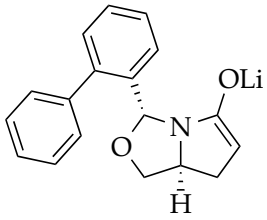

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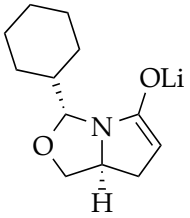

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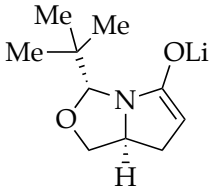

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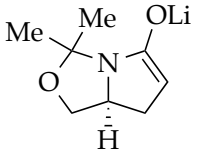

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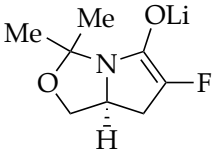

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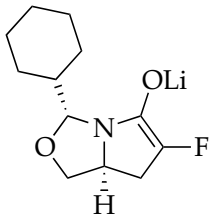

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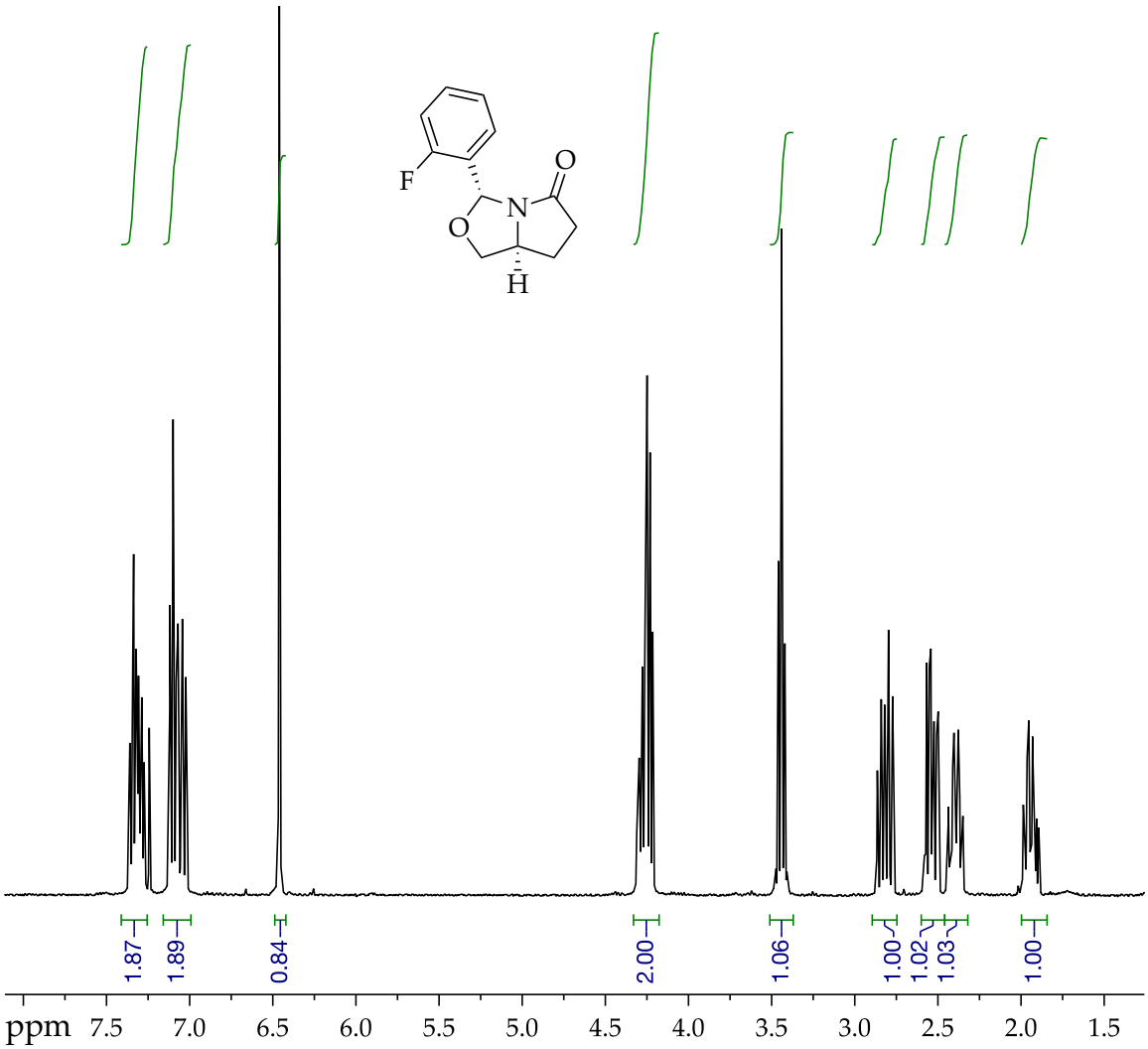


Figure 1. ^{1}H NMR of **1c** in $CDCl_3$.

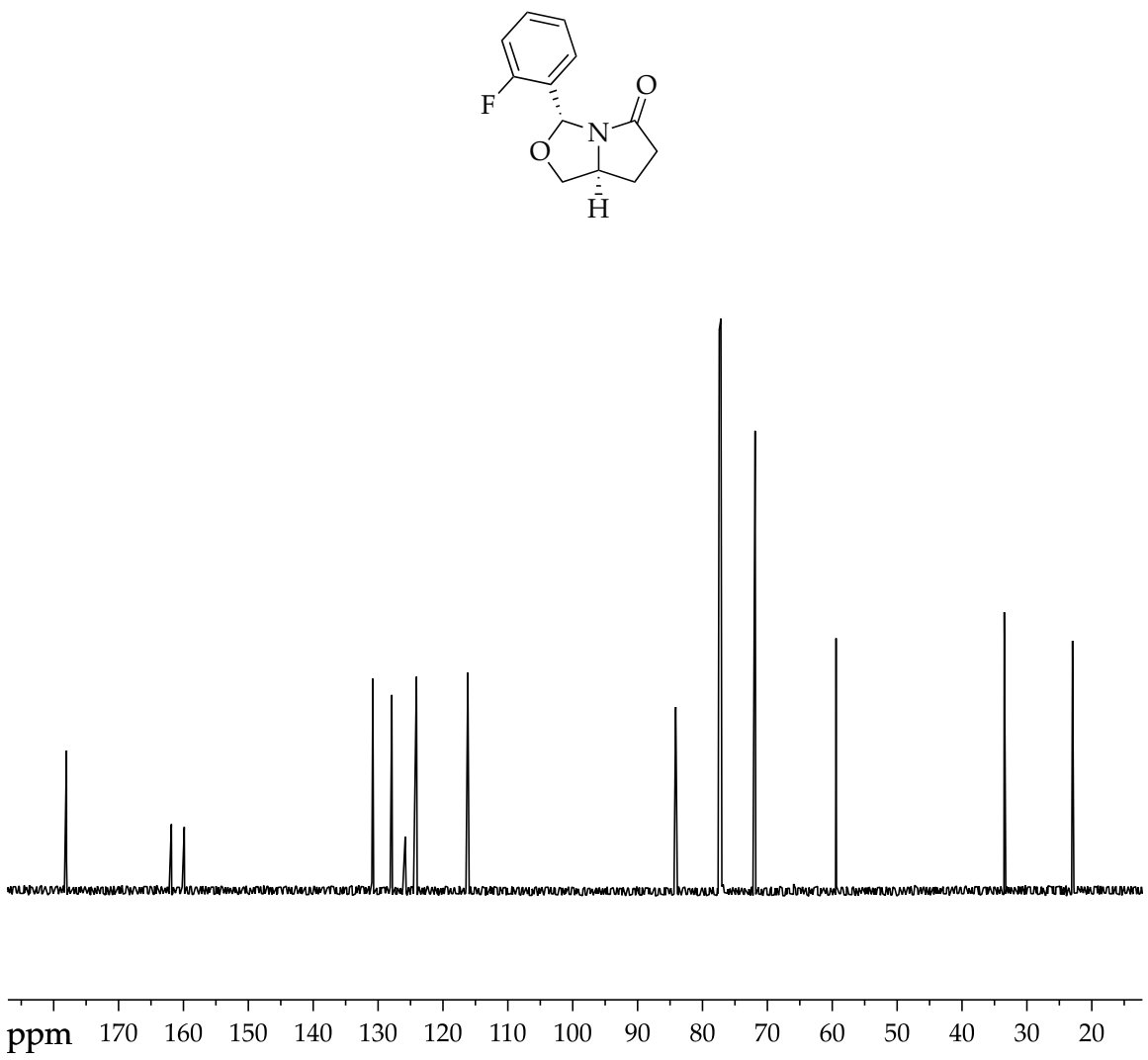


Figure 2. ^{13}C NMR of **1c** in $CDCl_3$.

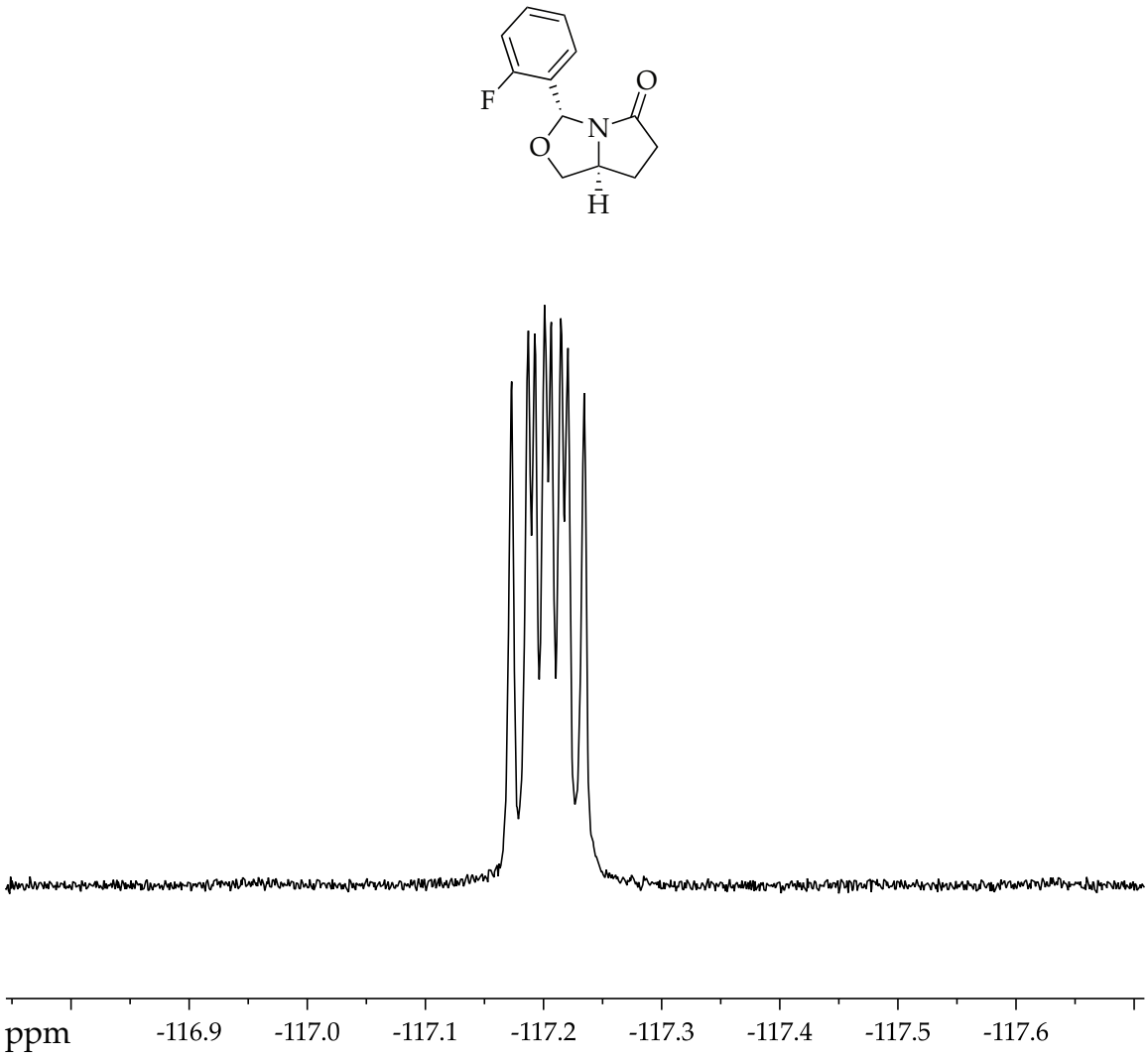


Figure 3. ^{19}F NMR of **1c** in $CDCl_3$.

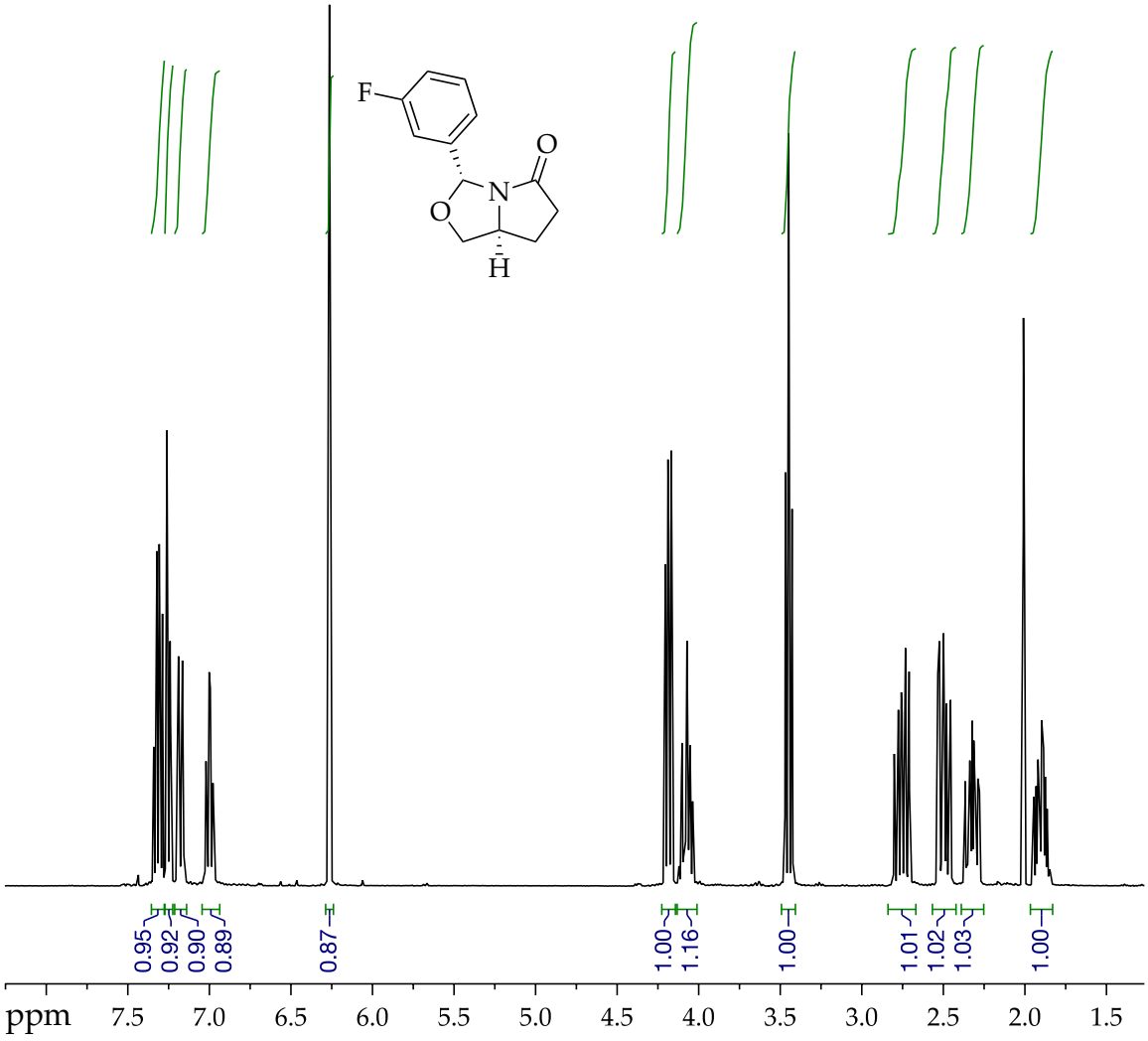


Figure 4. ^{1}H NMR of **1d** in $CDCl_3$.

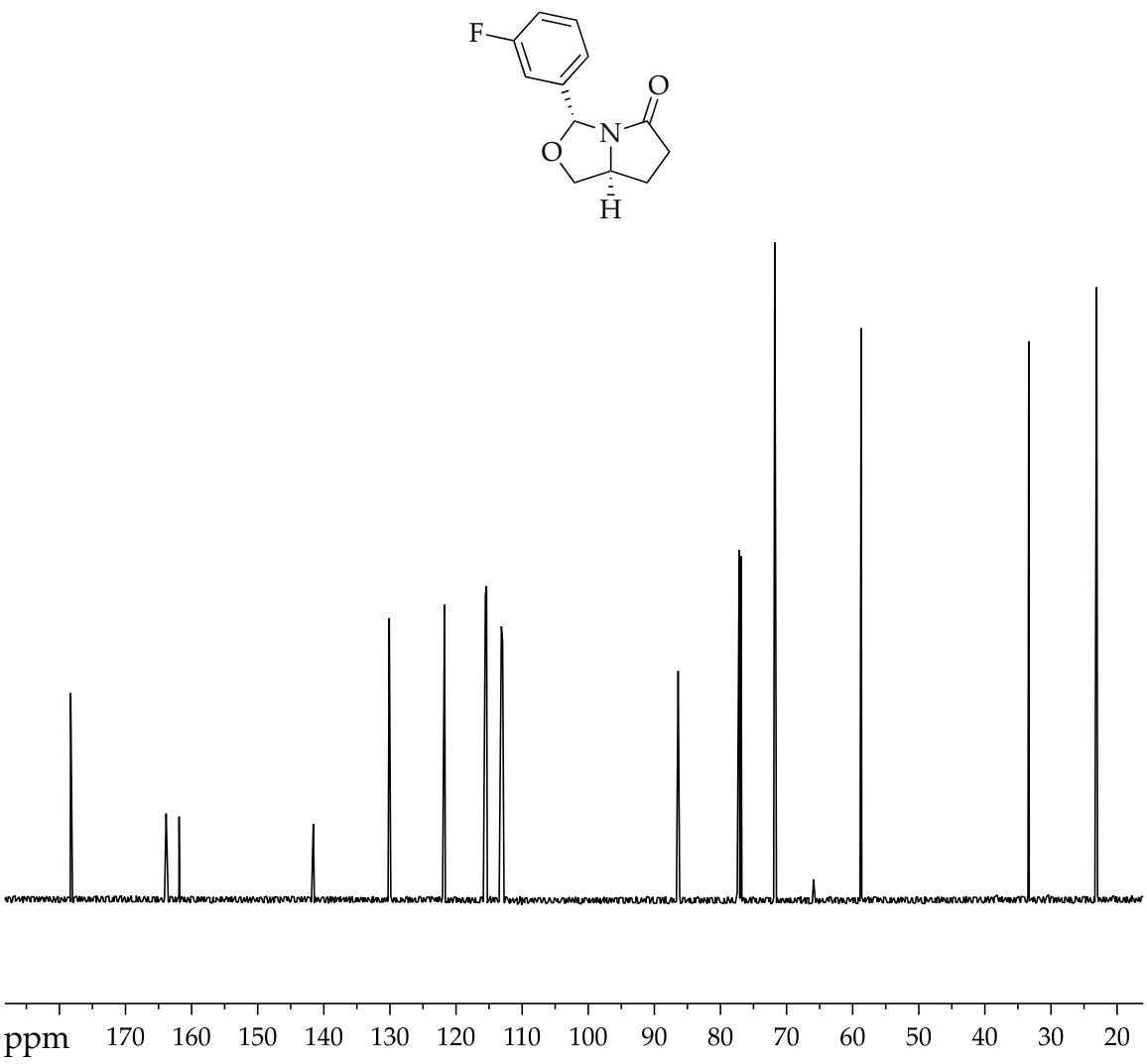


Figure 5. ^{13}C NMR of **1d** in $CDCl_3$.

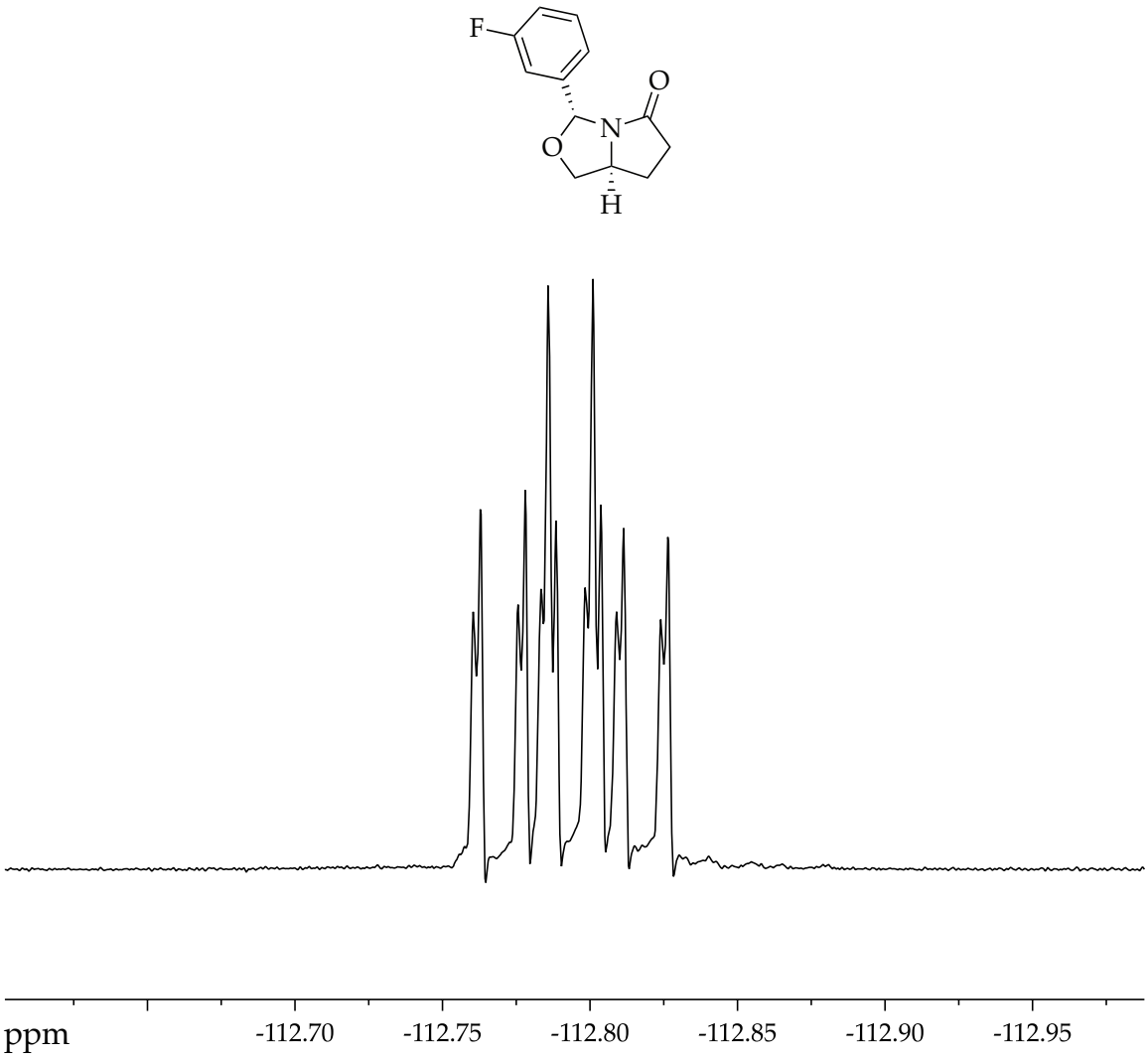


Figure 6. ^{19}F NMR of **1d** in $CDCl_3$.

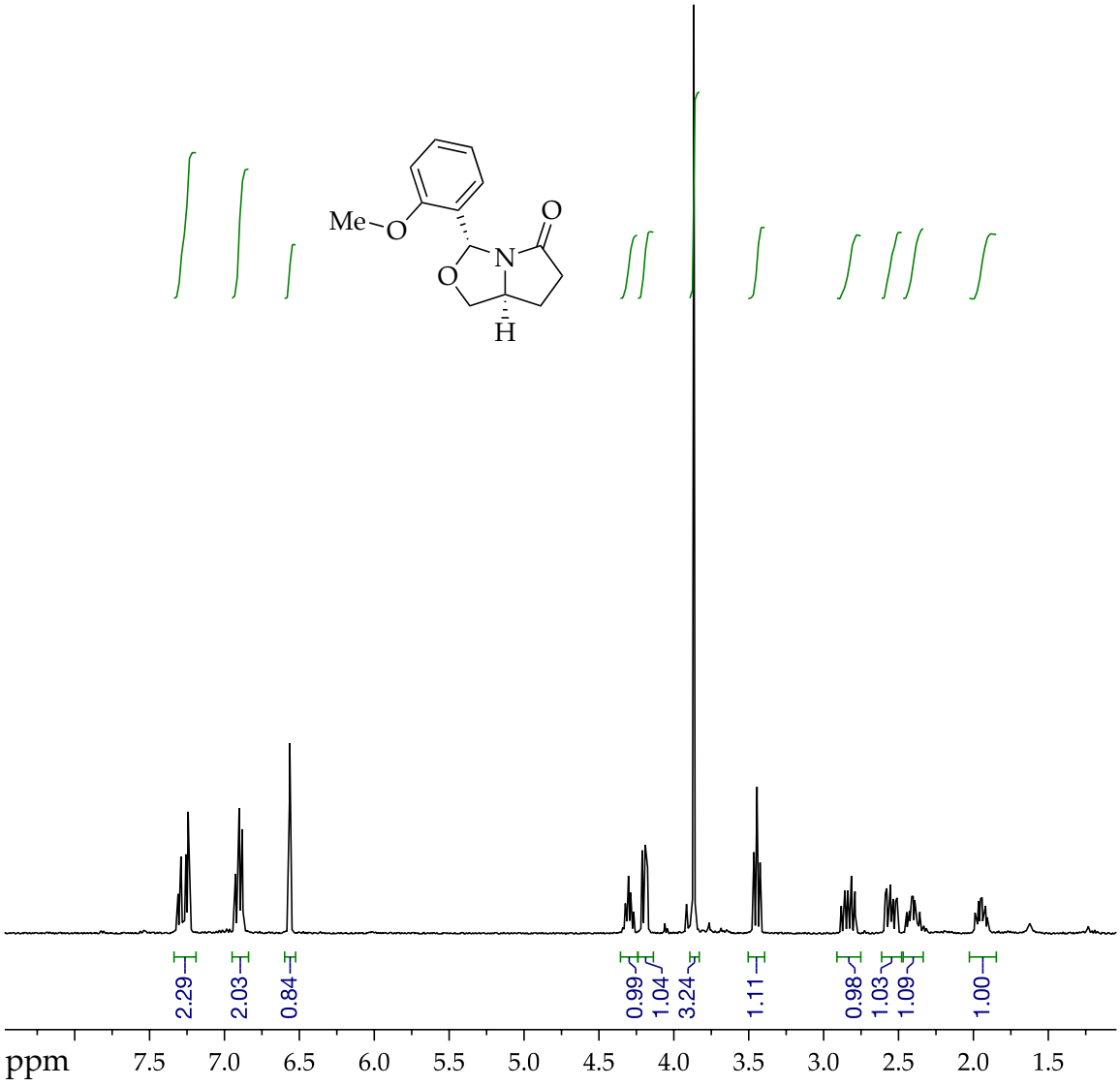


Figure 7. ^{1}H NMR of **1e** in $CDCl_3$.

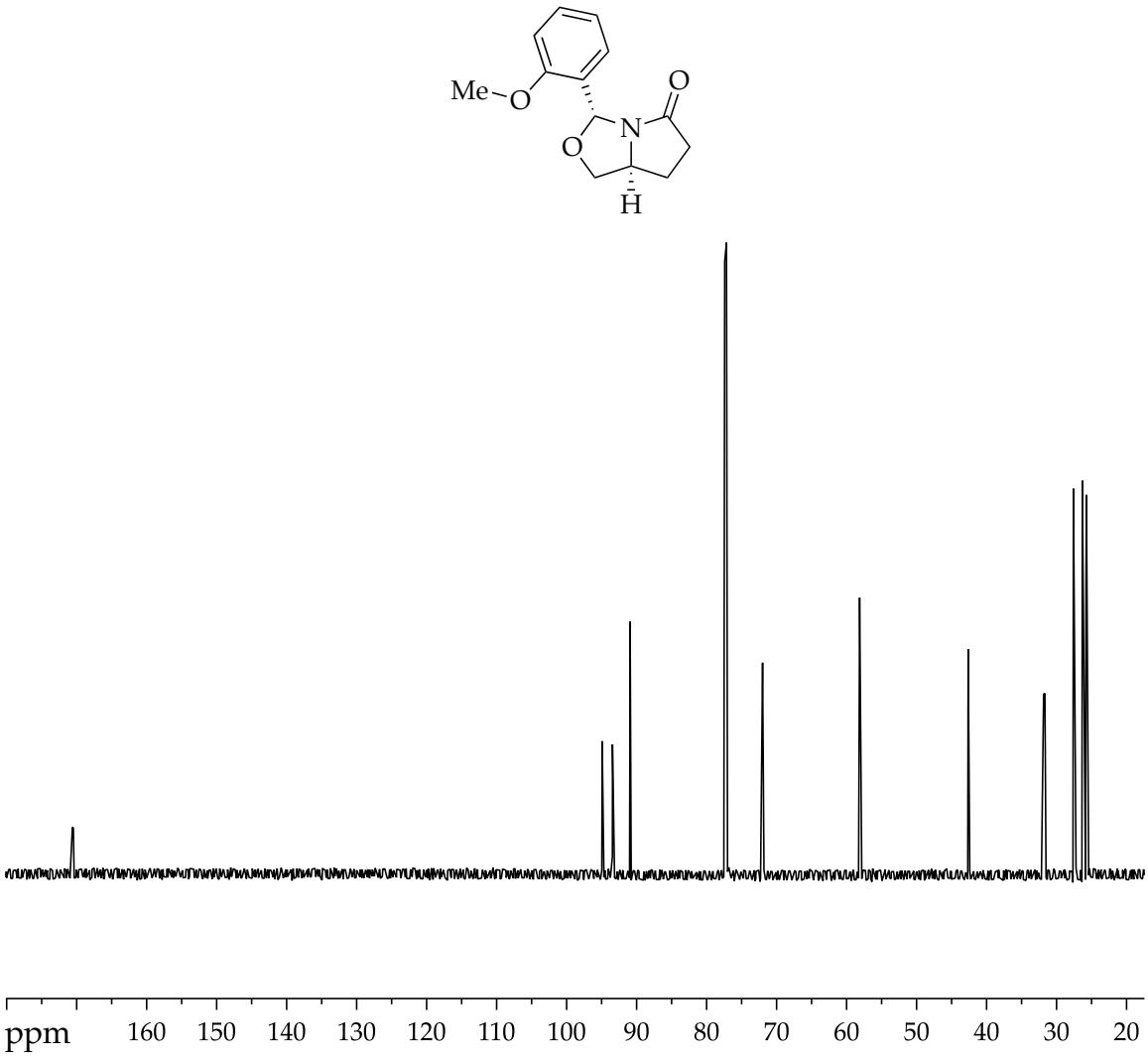


Figure 8. ^{13}C NMR of **1e** in $CDCl_3$.

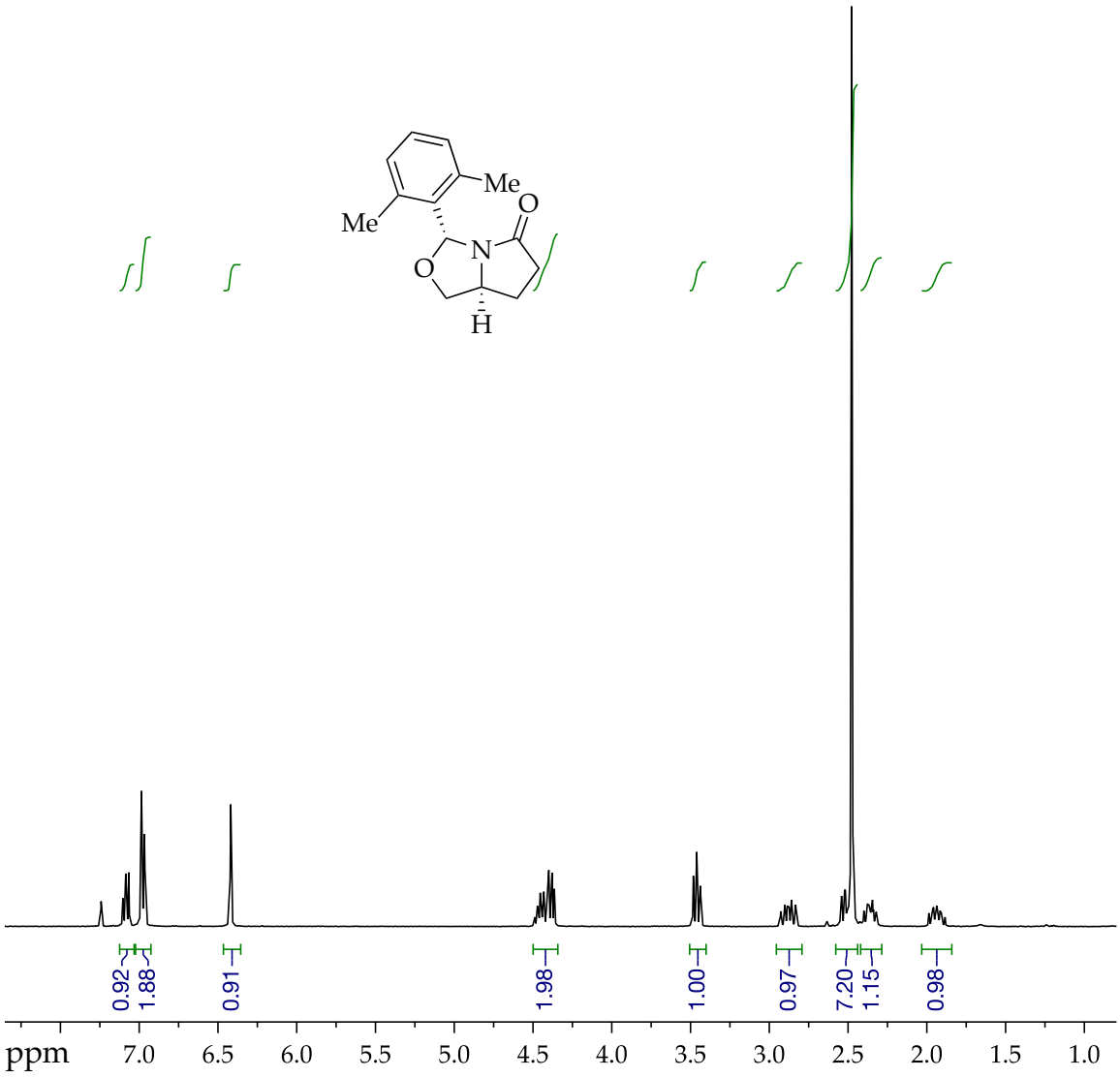


Figure 9. ^{1}H NMR of **1f** in $CDCl_3$.

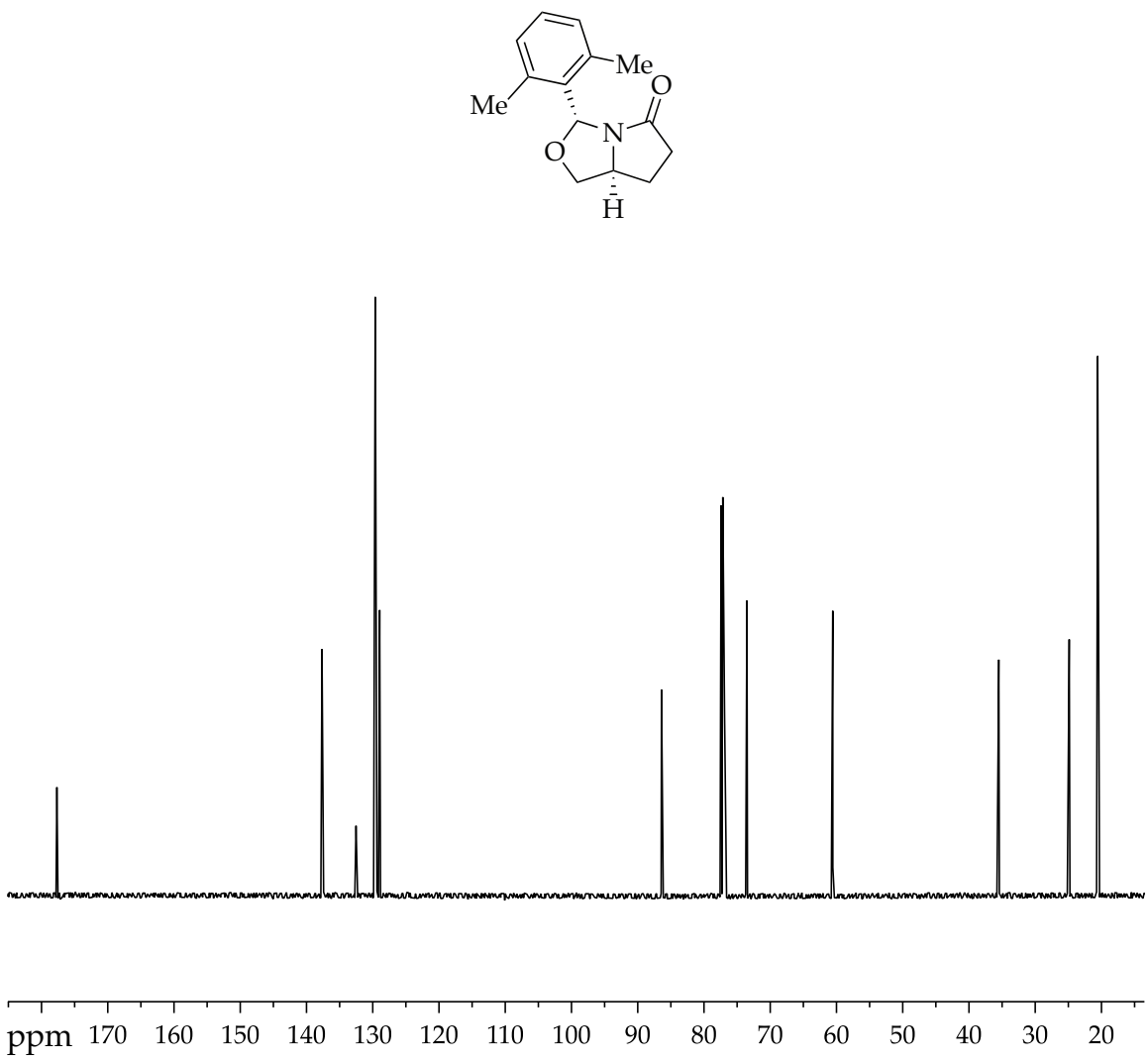


Figure 10. ^{13}C NMR of **1f** in $CDCl_3$.

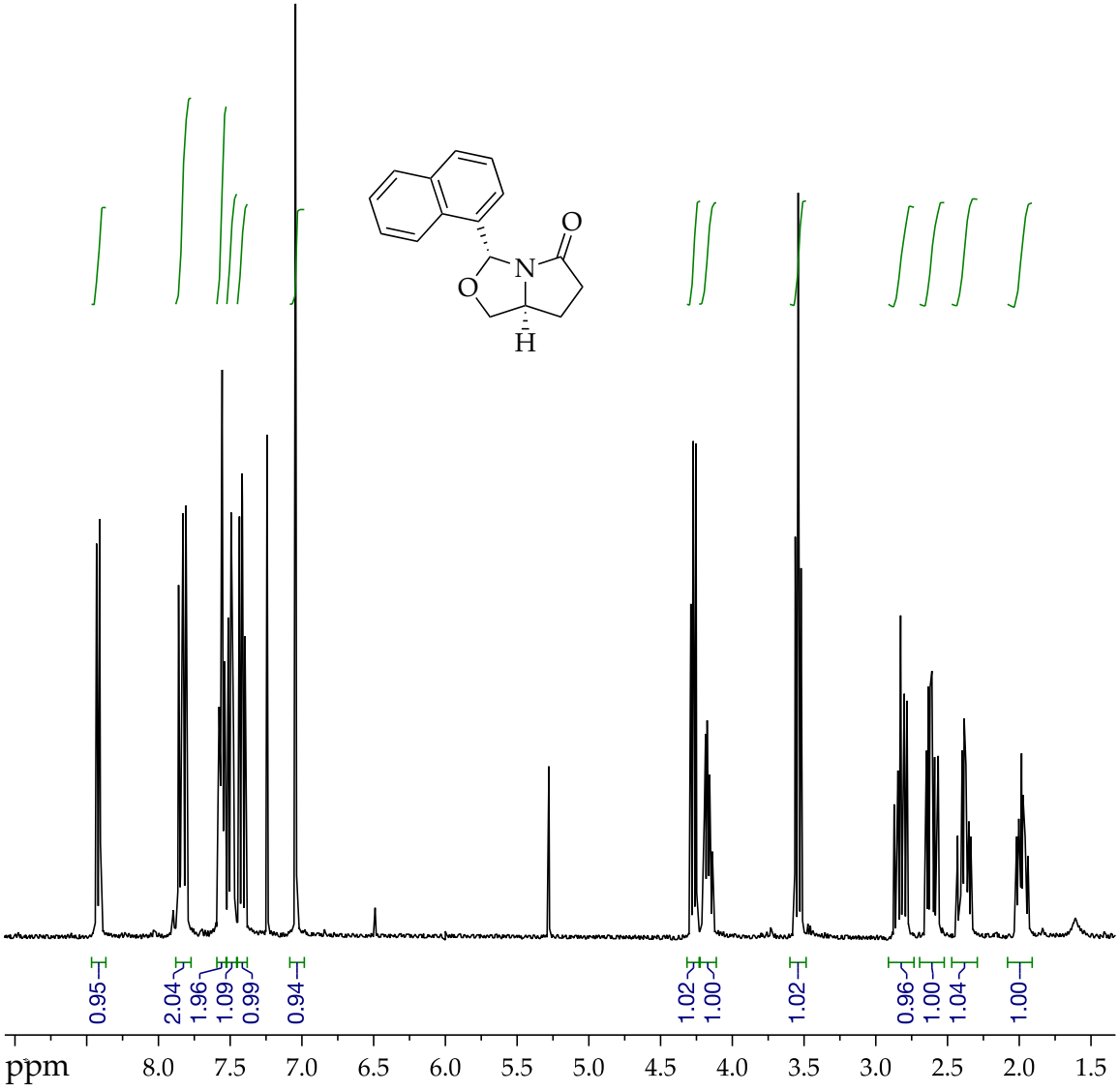


Figure 11. ^{1}H NMR of **1g** in $CDCl_3$.

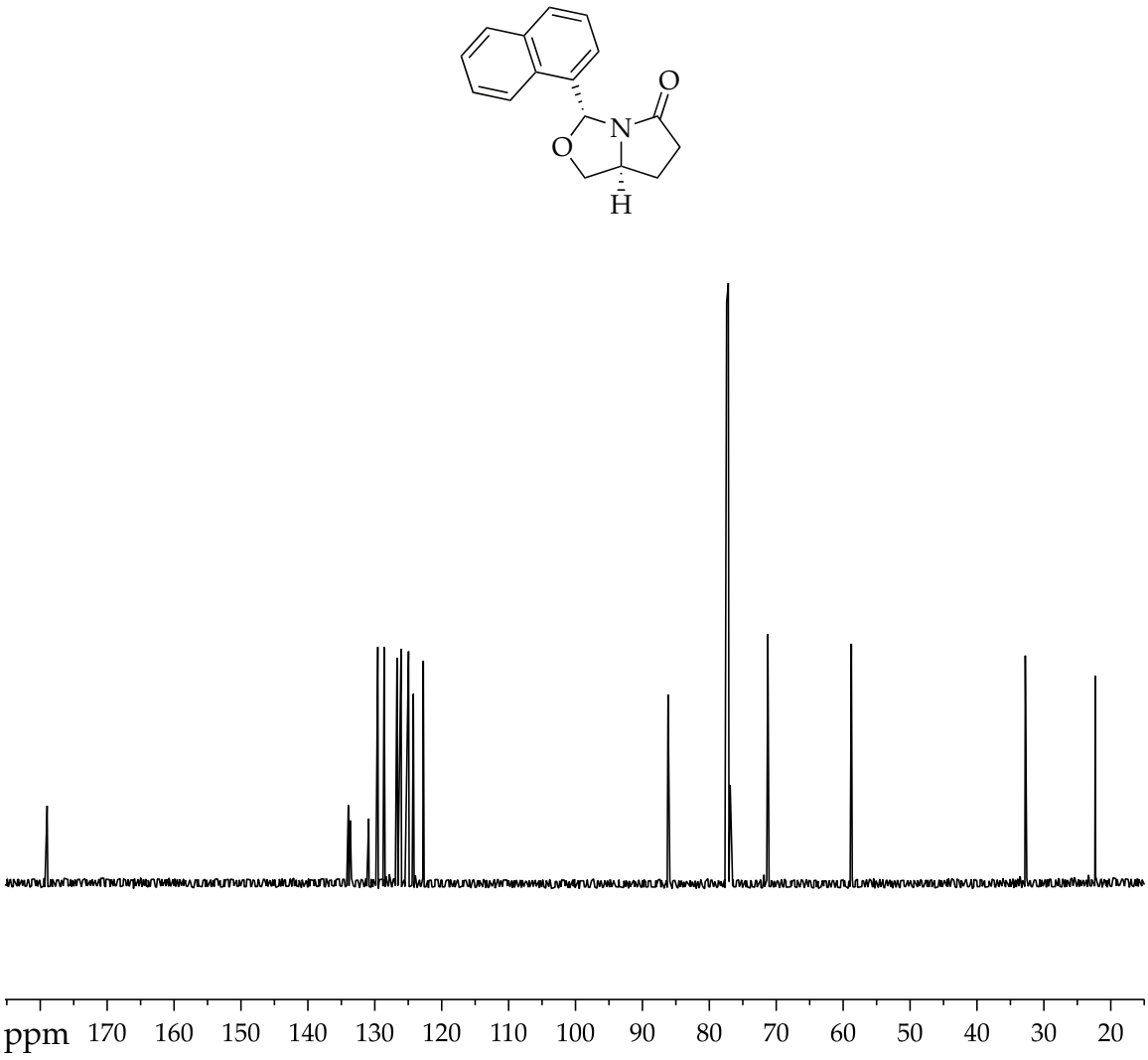


Figure 12. ^{13}C NMR of **1g** in $CDCl_3$.

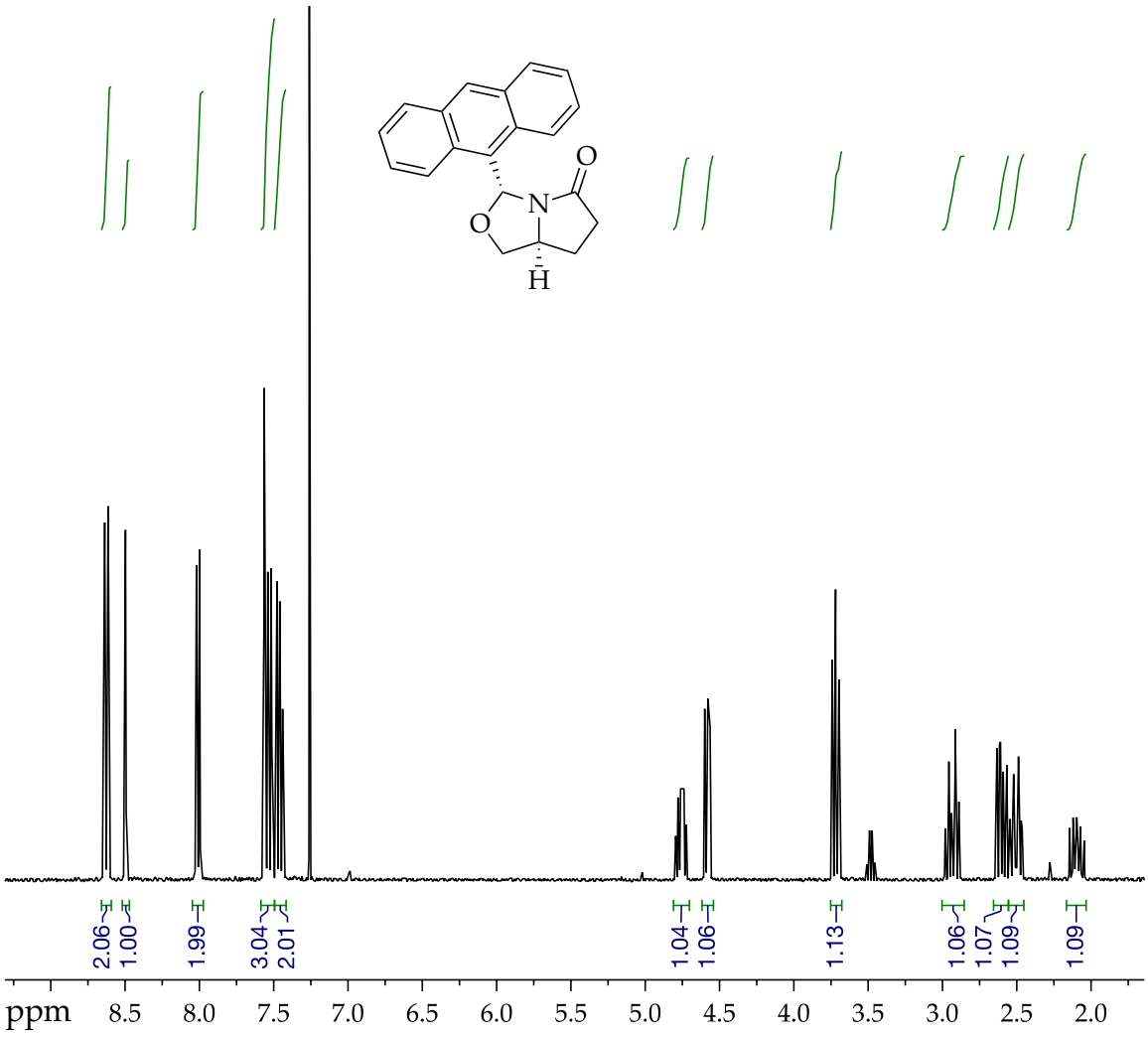


Figure 13. ^{1}H NMR of **1h** in $CDCl_3$.

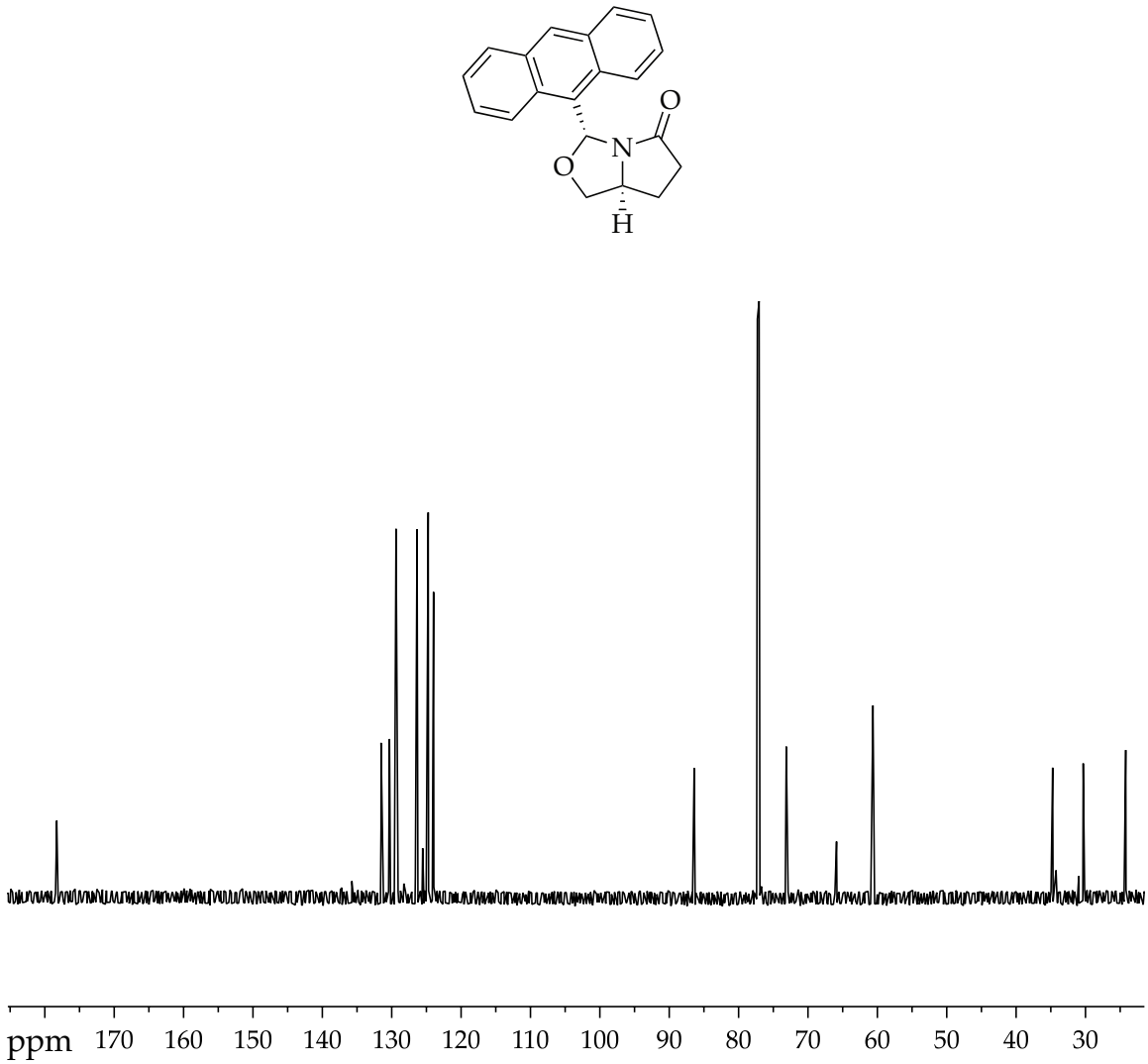


Figure 14. ^{13}C NMR of **1h** in $CDCl_3$.

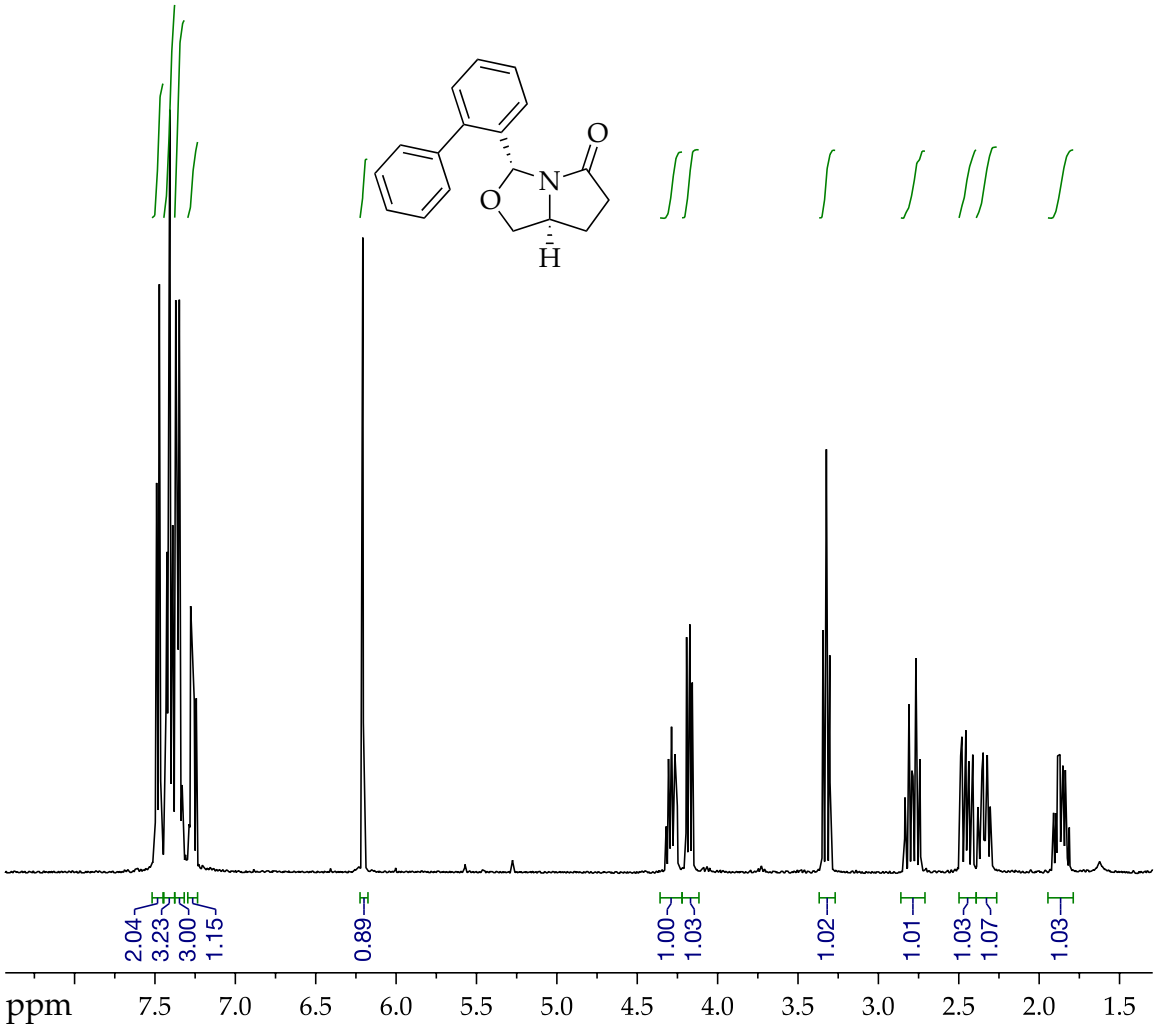


Figure 15. ^{1}H NMR of **1i** in $CDCl_3$.

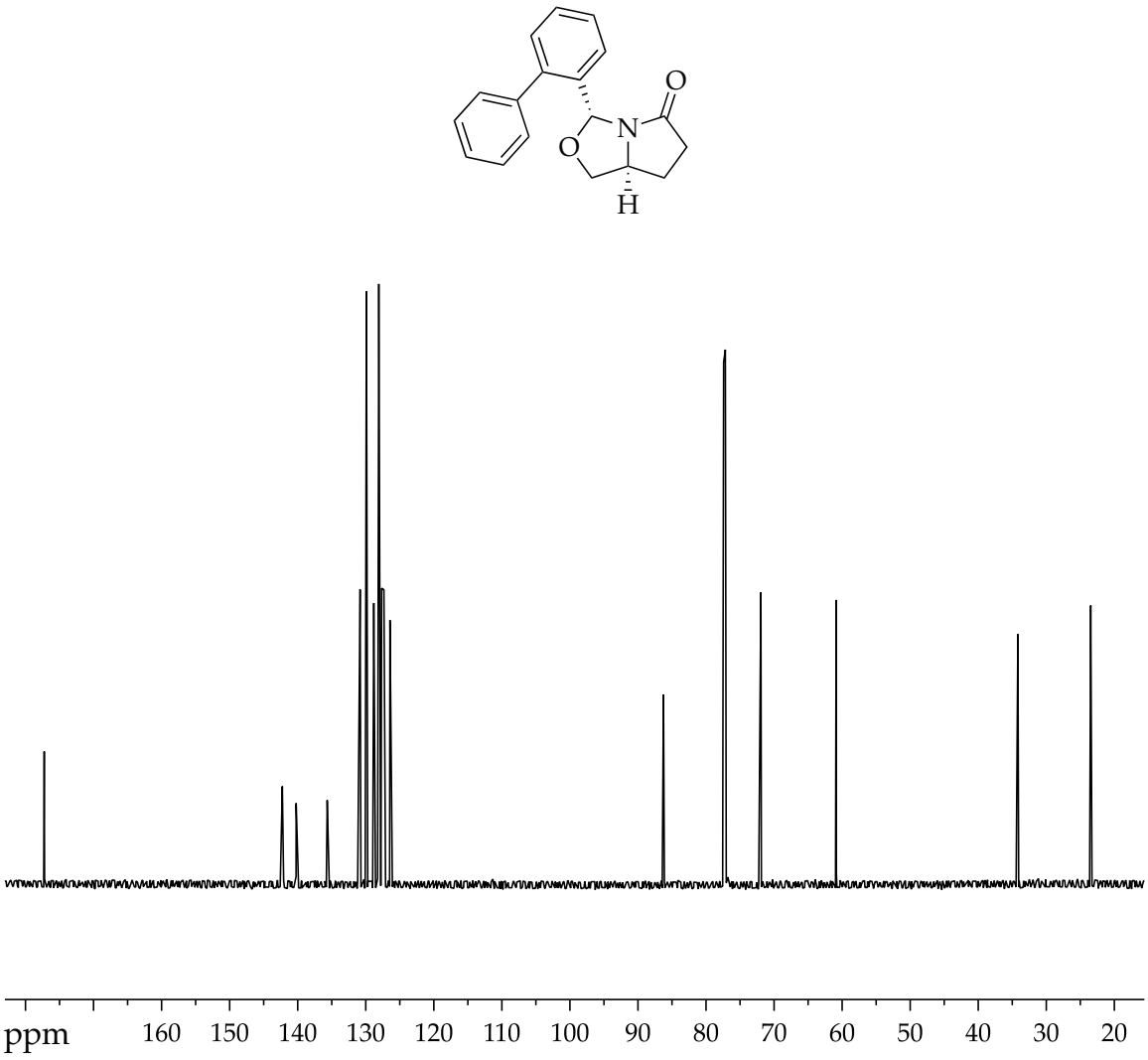


Figure 16. ^{13}C NMR of **1i** in $CDCl_3$.

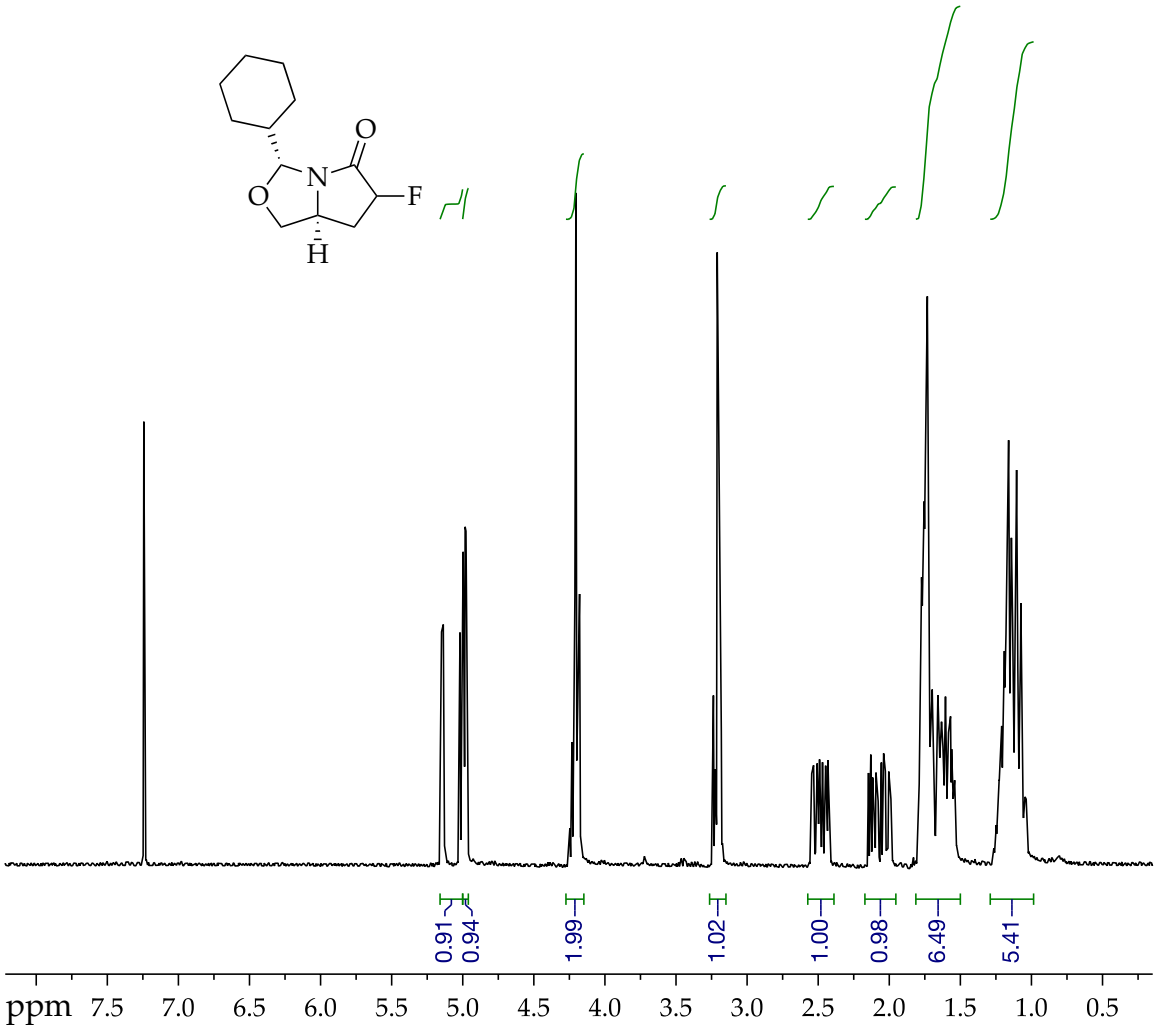


Figure 17. ^{1}H NMR of **1k** in $CDCl_3$.

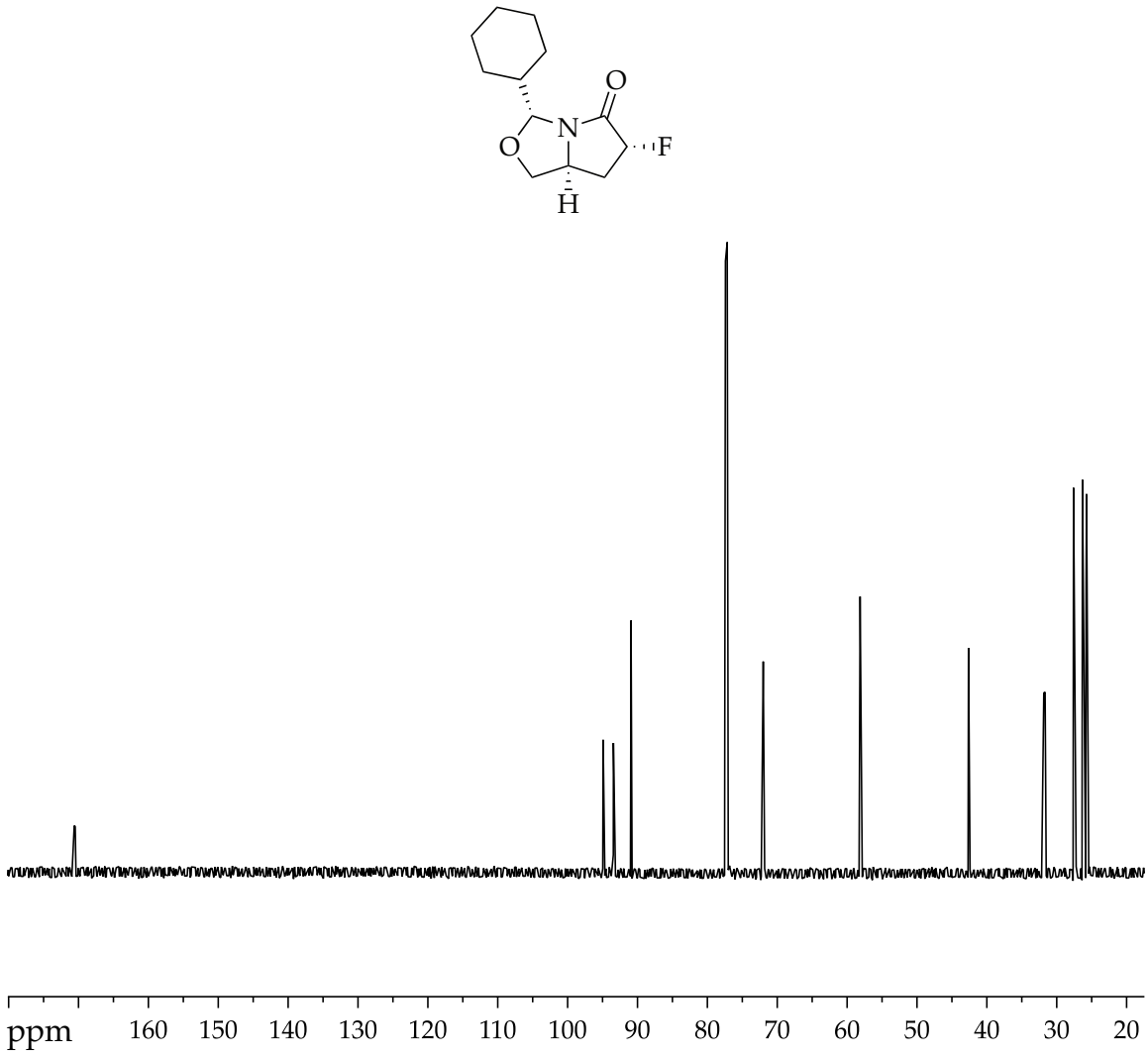


Figure 18. ^{13}C NMR of **1k** in $CDCl_3$.

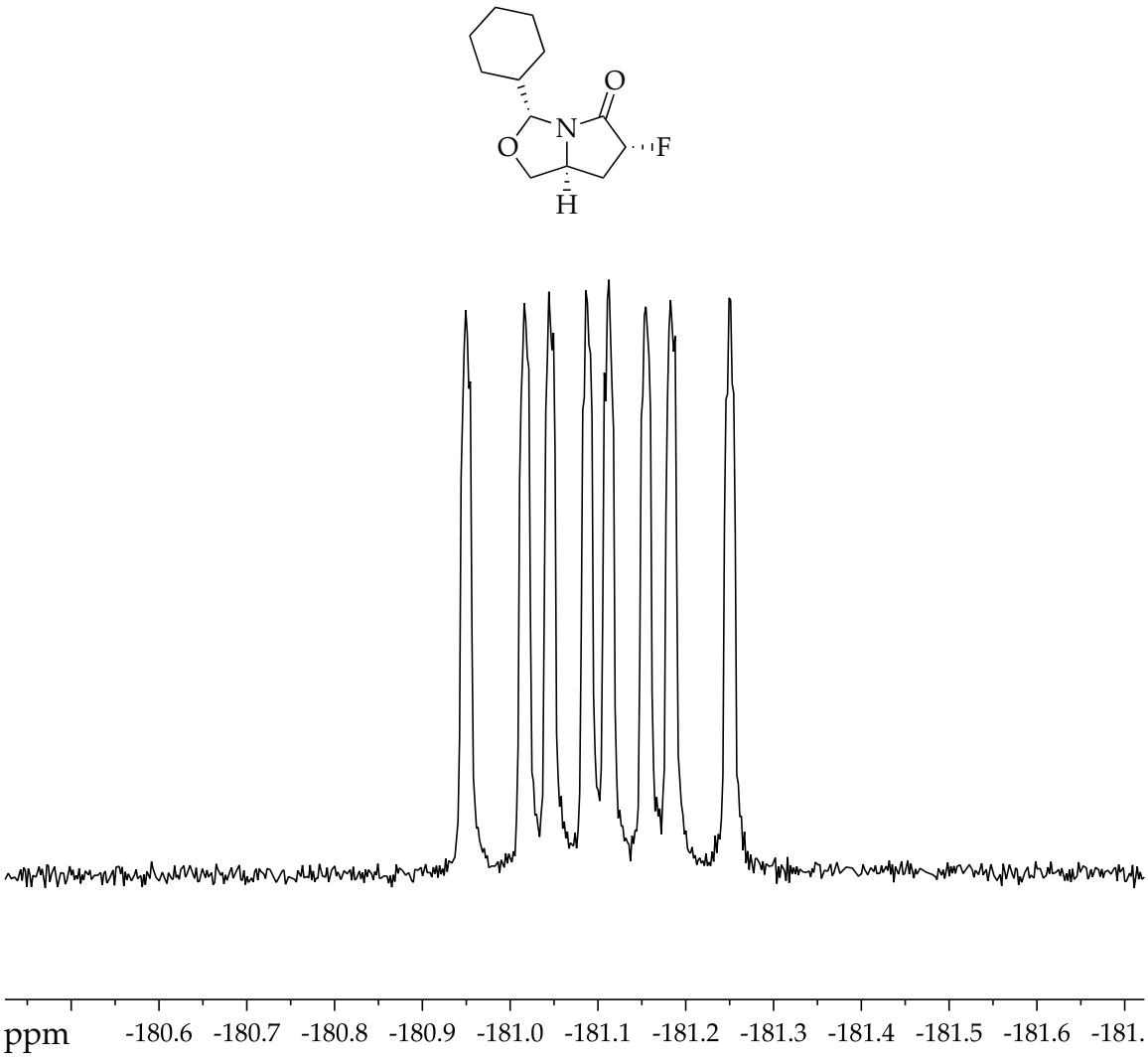


Figure 19. ^{19}F NMR of **1k** in $CDCl_3$.

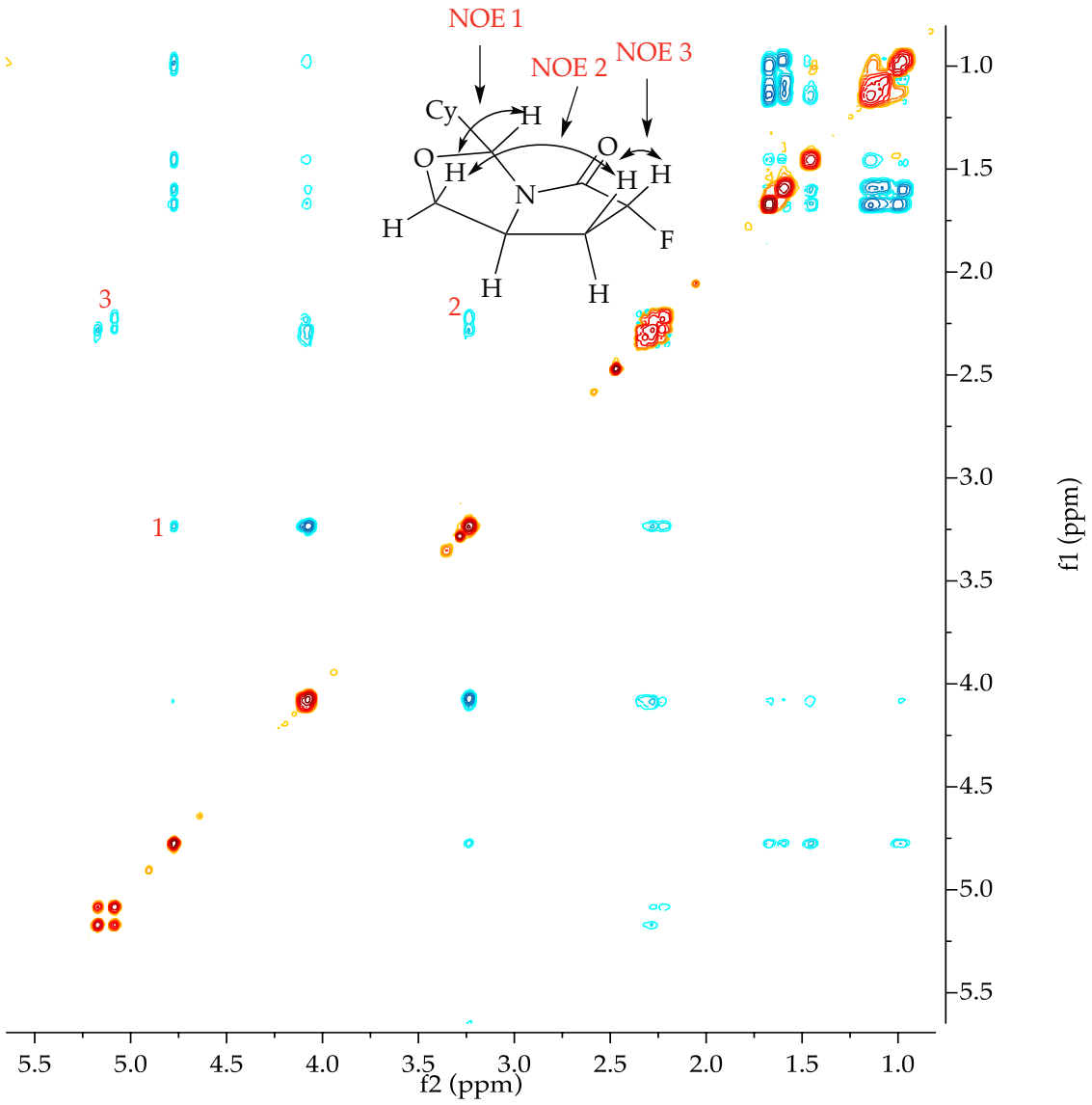


Figure 20. NOESY of **1k** in DMSO-d_6.

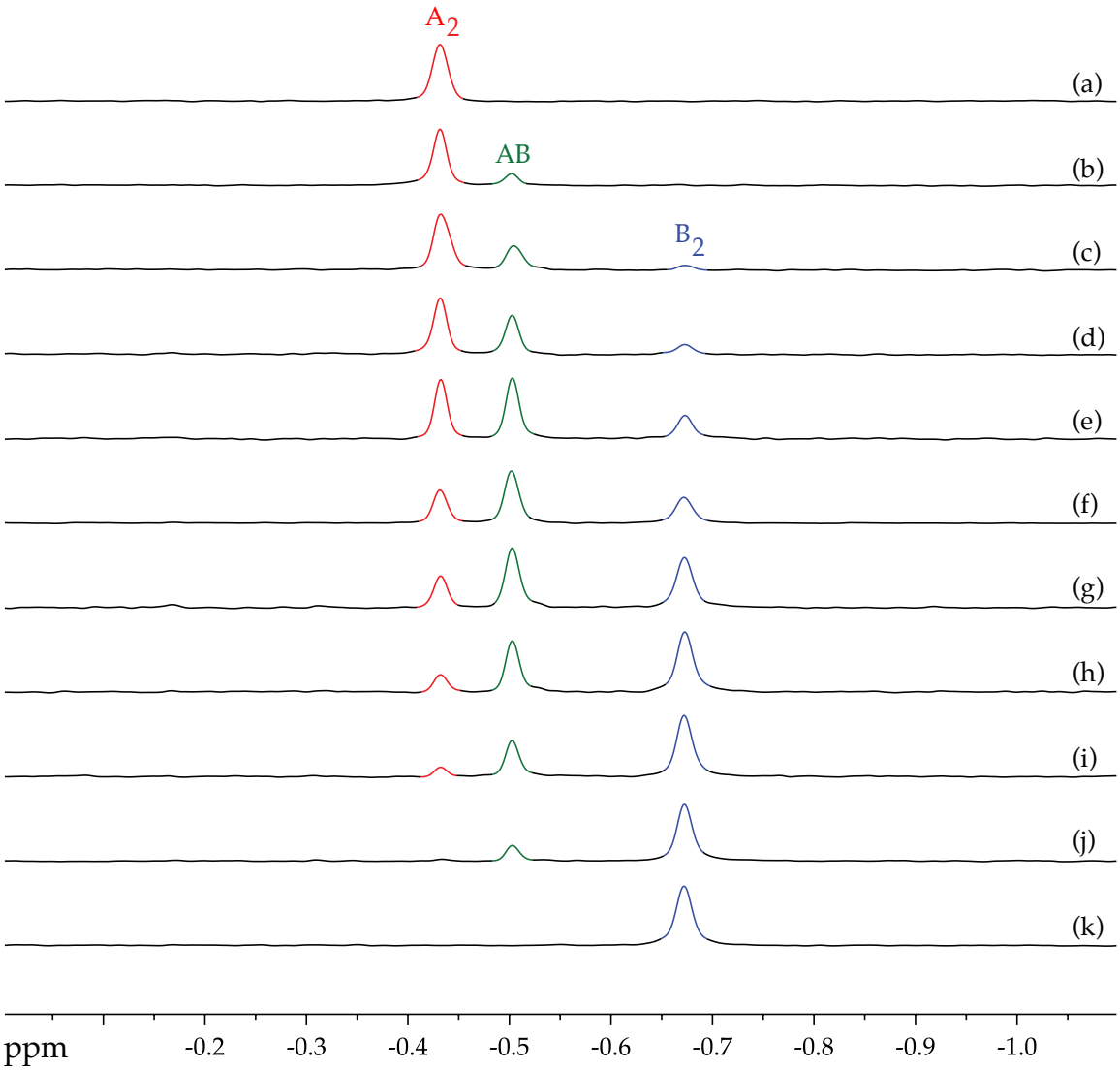


Figure 21. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** (**A**) and [^{6}Li]**2i** (**B**) in 1.0 M TMEDA/toluene at –50 °C with 0.103 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.088, 0.21, 0.31, 0.42, 0.51, 0.60, 0.70, 0.77, 0.89, and 1.00, respectively.

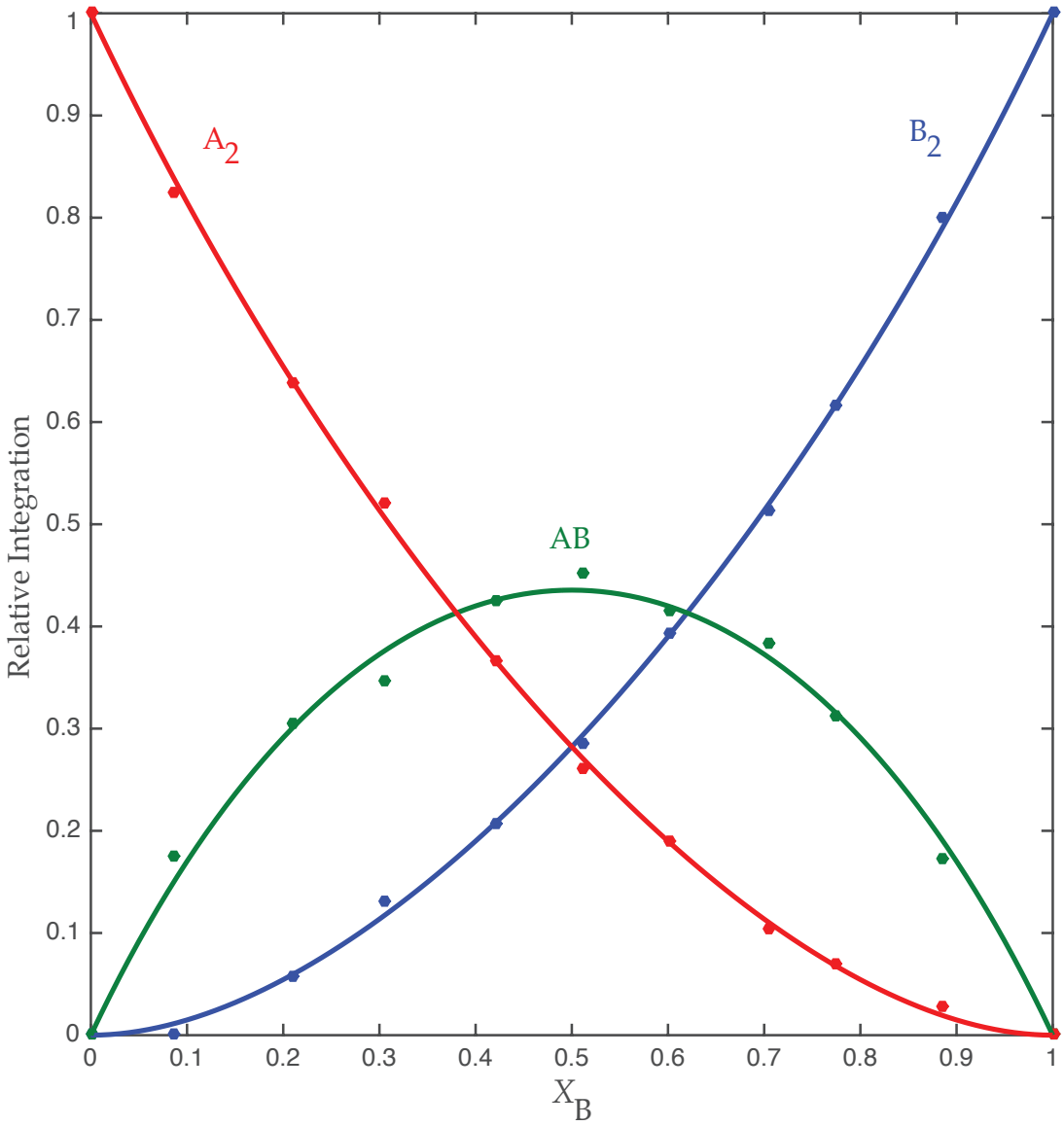


Figure 22. Job plot showing the relative integrations versus the measured mole fraction of **2i** for 0.10 M mixtures of [^{6}Li]**2j** (**A**) and [^{6}Li]**2i** (**B**) in 1.0 M TMEDA and toluene at –50 °C.

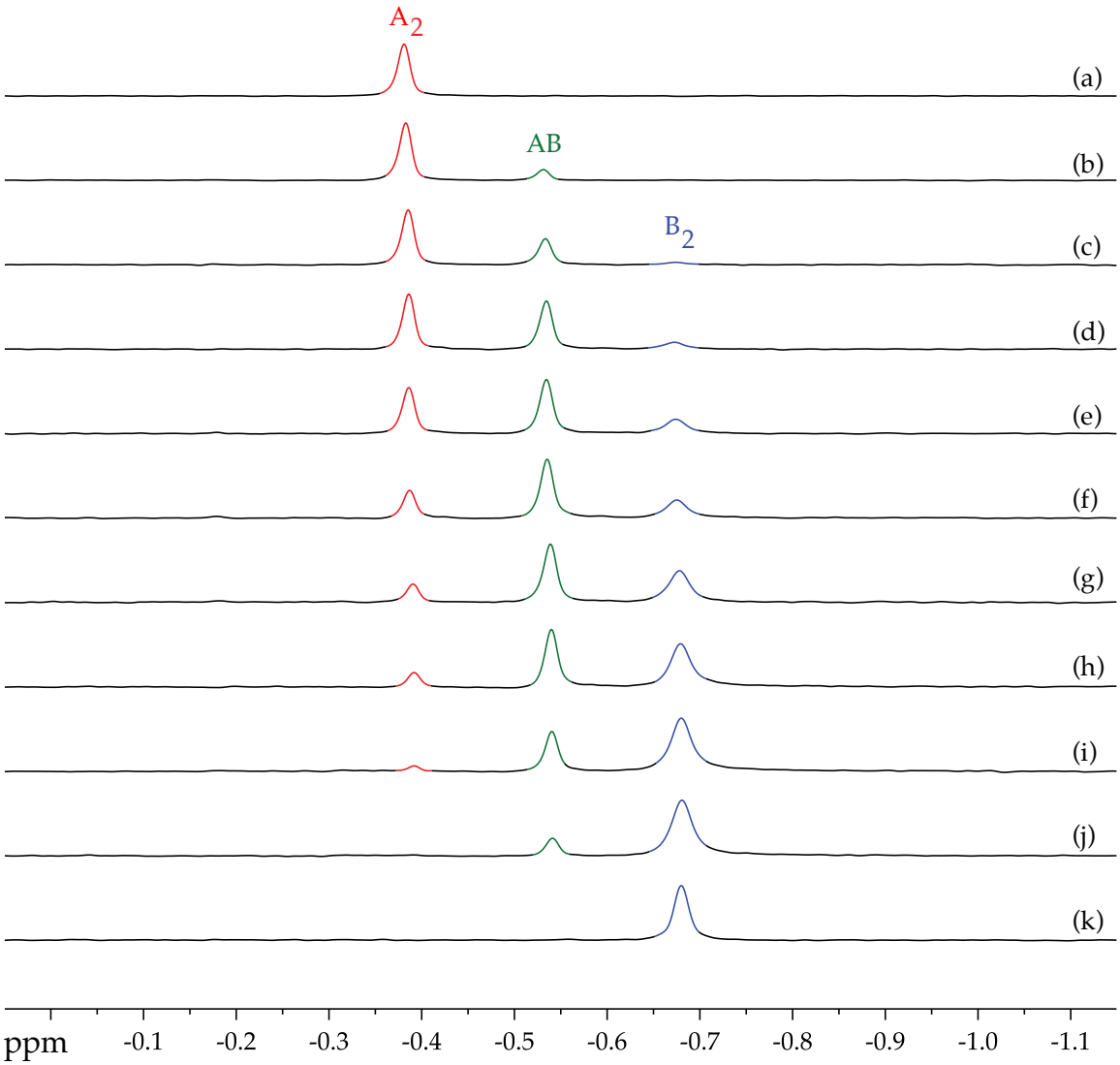


Figure 23. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**3** (**A**) and [^{6}Li]**2i** (**B**) in 1.0 M TMEDA and toluene at –80 °C with 0.103 M [^{6}Li]LDA. The measured mole fractions, X_{B}, in (a)–(k) are 0.00, 0.087, 0.23, 0.34, 0.43, 0.51, 0.64, 0.70, 0.82, 0.92, and 1.00, respectively.

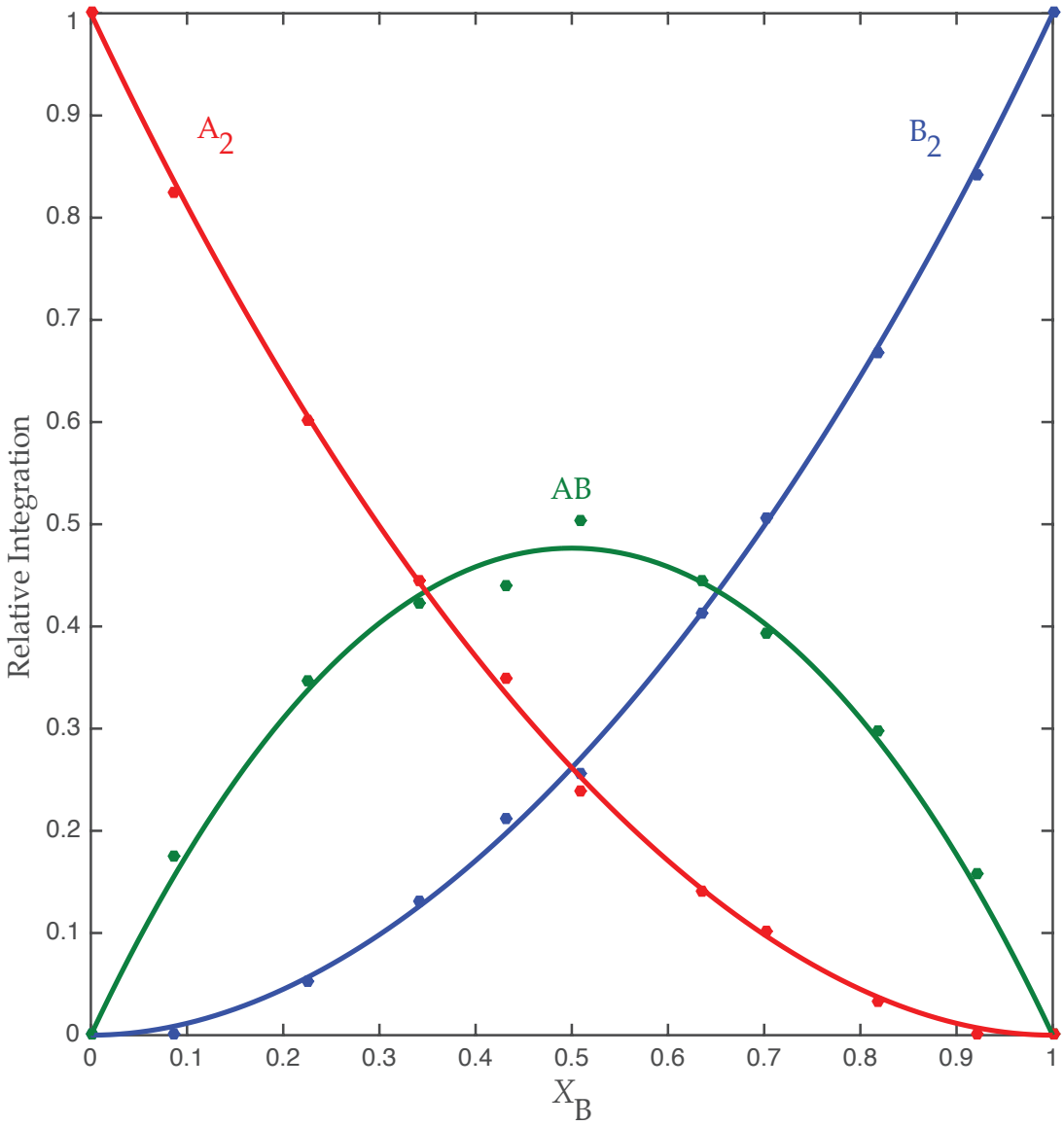


Figure 24. Job plot showing the relative integrations versus the measured mole fraction of **2i** for 0.10 M mixtures of [^{6}Li]**3** (**A**) and [^{6}Li]**2i** (**B**) in 1.0 M TMEDA and toluene at –80 °C.

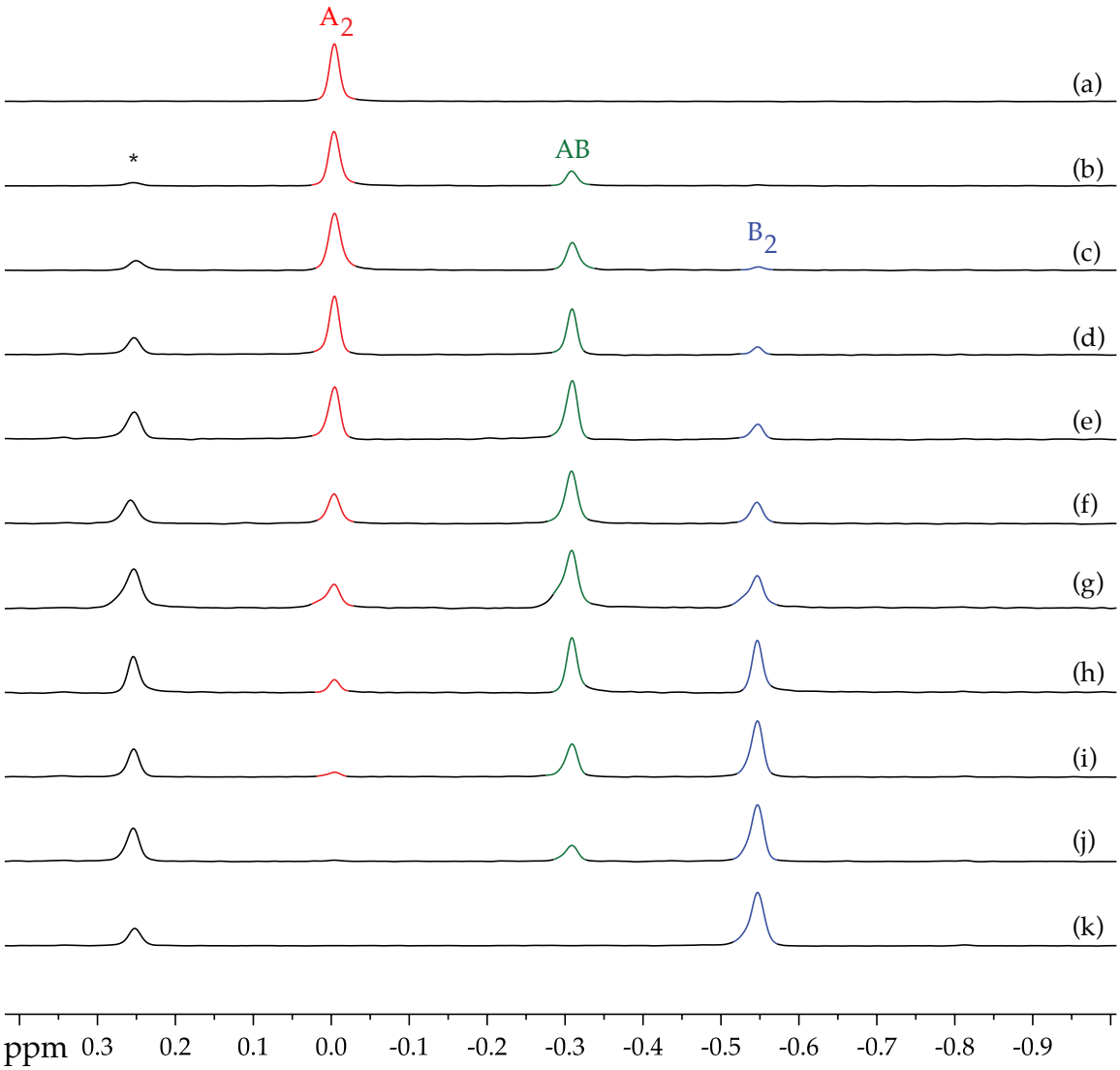


Figure 25. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2a** (**A**) and [^{6}Li]**2i** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.14, 0.24, 0.34, 0.46, 0.54, 0.64, 0.73, 0.81, 0.88, and 1.00, respectively.
* denotes a mixed aggregate with [^{6}Li]**2i** (**B**) and [^{6}Li]LDA.

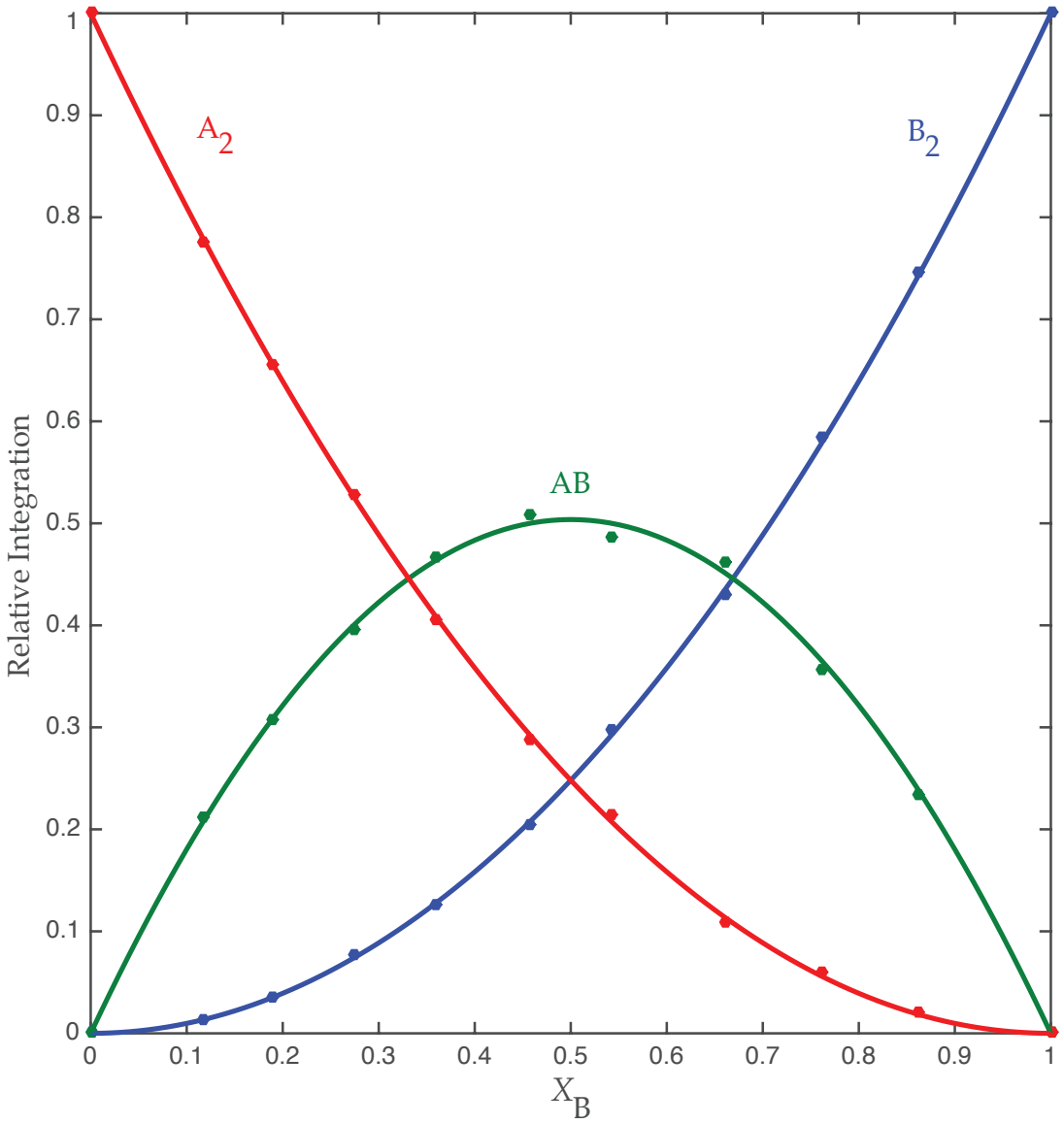


Figure 26. Job plot showing the relative integrations versus the measured mole fraction of **2i** for 0.10 M mixtures of [^{6}Li]**2a** (**A**) and [^{6}Li]**2i** (**B**) in 12.3 M THF at –80 °C.

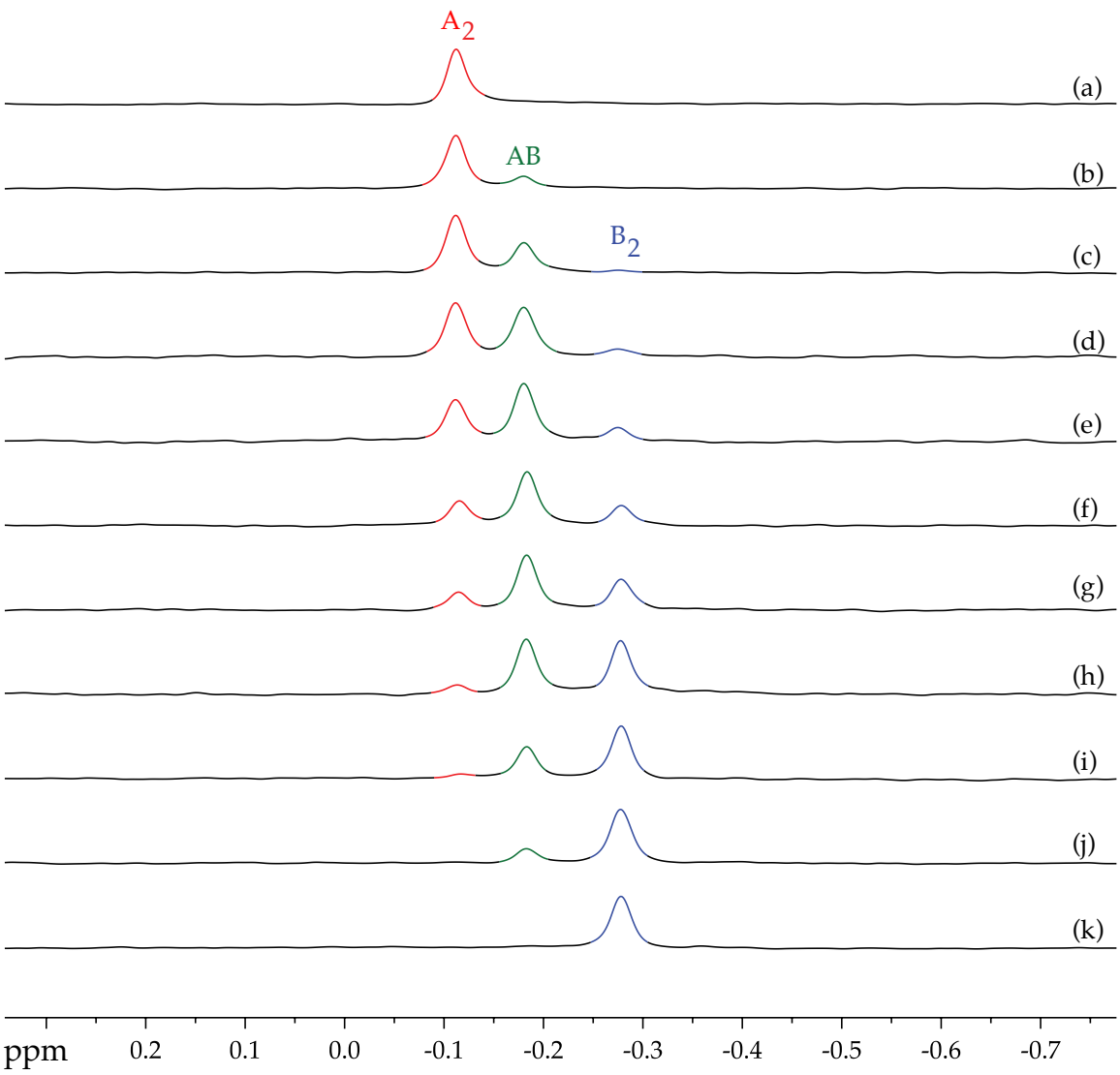


Figure 27. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2b** (**A**) and [^{6}Li]**3** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.11, 0.21, 0.32, 0.39, 0.48, 0.58, 0.69, 0.77, 0.90, and 1.00, respectively.

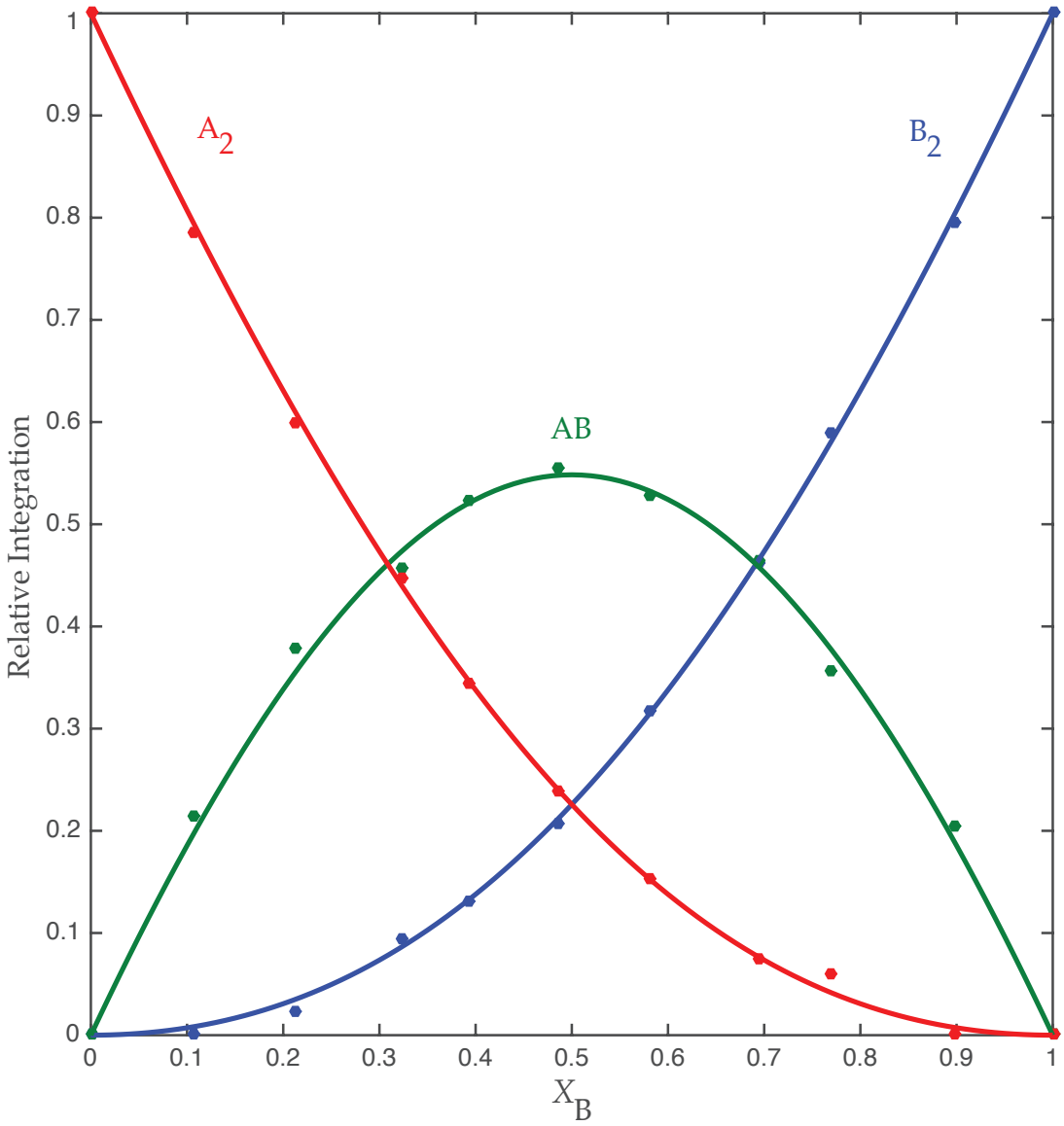


Figure 28. Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [^{6}Li]**2b** (**A**) and [^{6}Li]**3** (**B**) in 12.3 M THF at –80 °C.

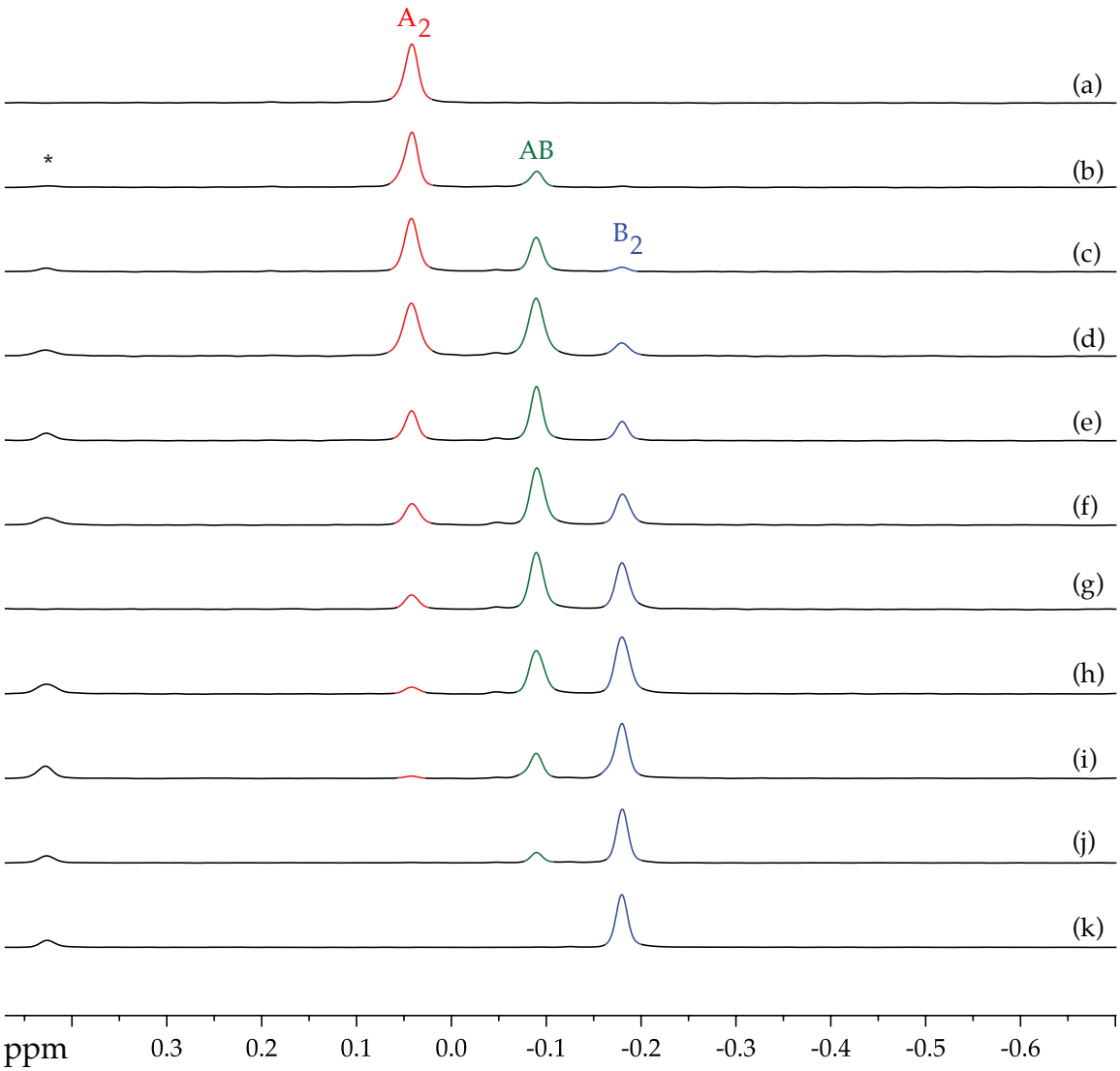


Figure 29. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2g** (**A**) and [^{6}Li]**2j** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.14, 0.24, 0.34, 0.44, 0.53, 0.63, 0.73, 0.82, 0.91, and 1.00, respectively.
* denotes a mixed aggregate with [^{6}Li]**2j** (**B**) and [^{6}Li]LDA.

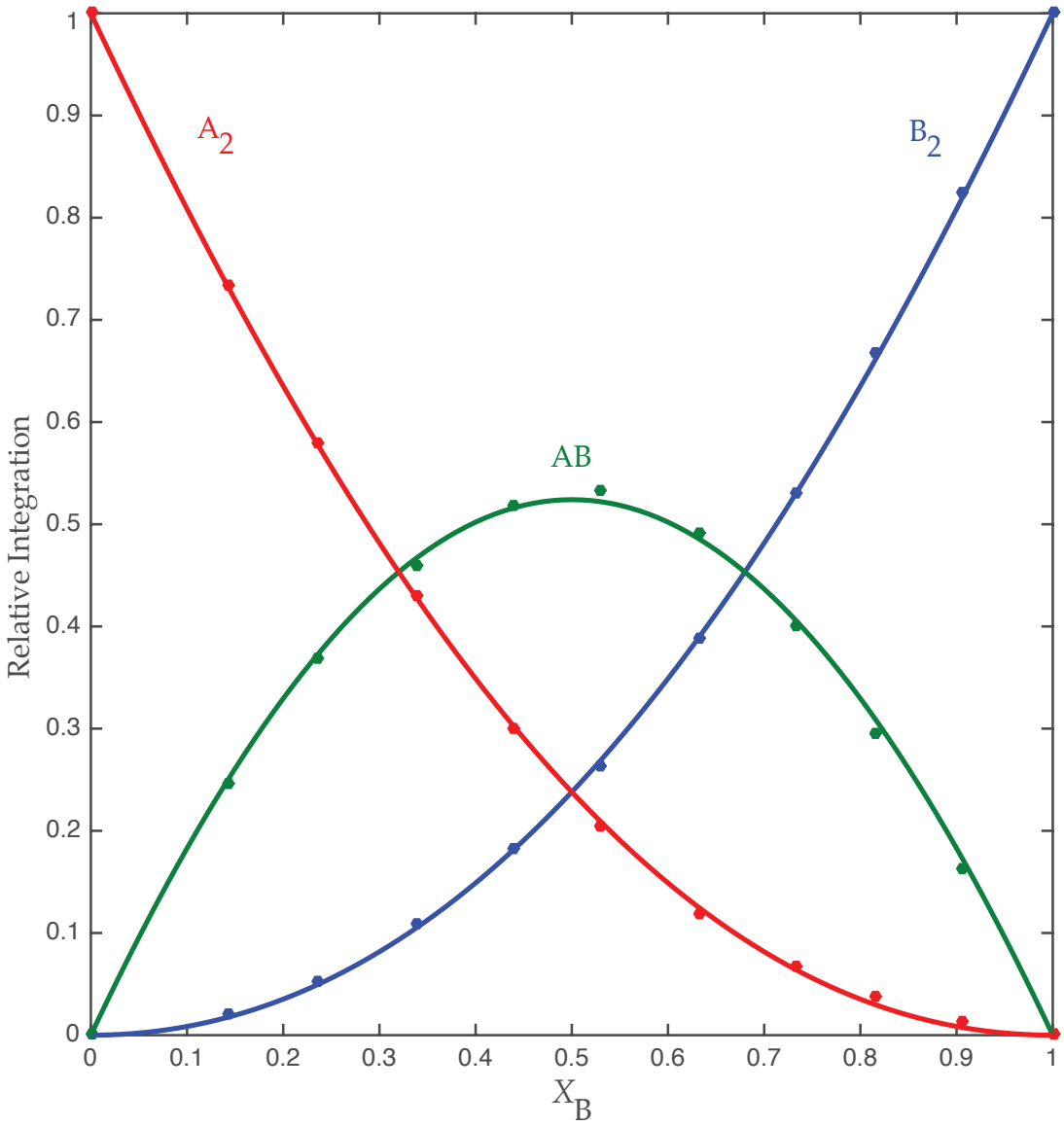


Figure 30. Job plot showing the relative integrations versus the measured mole fraction of **2j** for 0.10 M mixtures of [^{6}Li]**2g** (**A**) and [^{6}Li]**2j** (**B**) in 12.3 M THF at –80 °C.

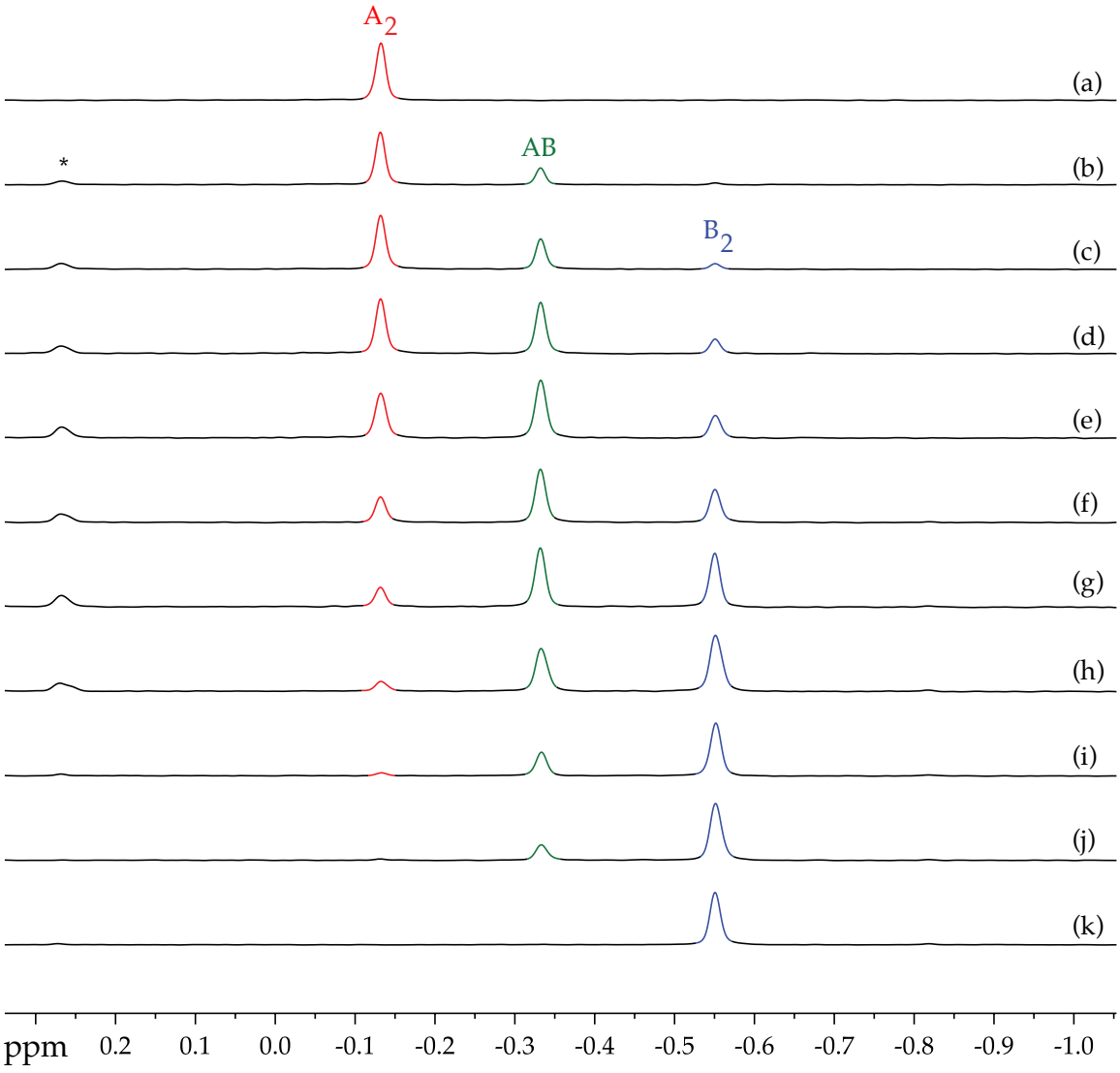


Figure 31. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2h** (**A**) and [^{6}Li]**2i** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.15, 0.23, 0.33, 0.41, 0.53, 0.62, 0.72, 0.81, 0.86, and 1.00, respectively. * denotes a mixed aggregate with [^{6}Li]**2i** (**B**) and [^{6}Li]LDA.

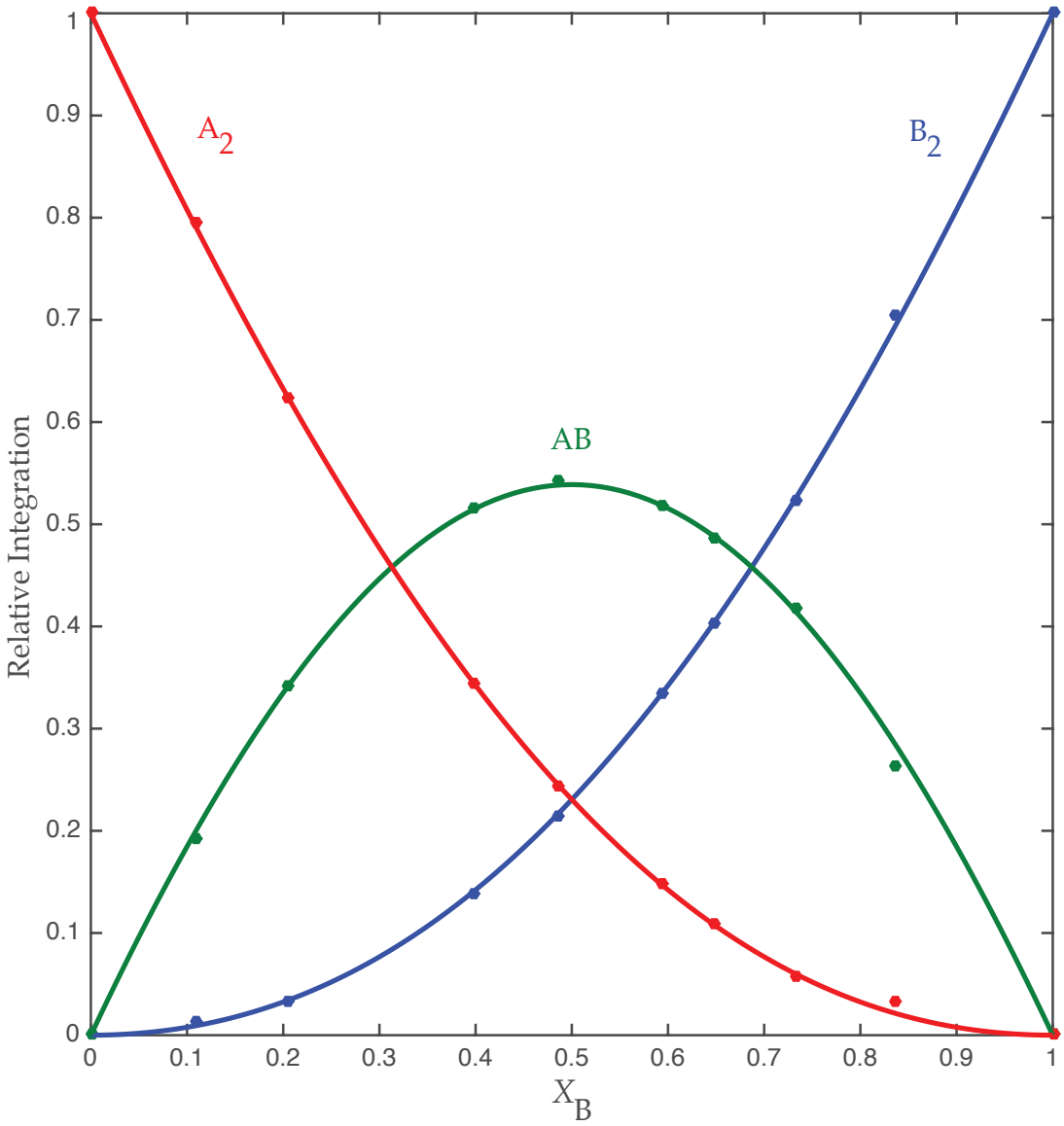


Figure 32. Job plot showing the relative integrations versus the measured mole fraction of **2i** for 0.10 M mixtures of [^{6}Li]**2h** (**A**) and [^{6}Li]**2i** (**B**) in 12.3 M THF at –80 °C.

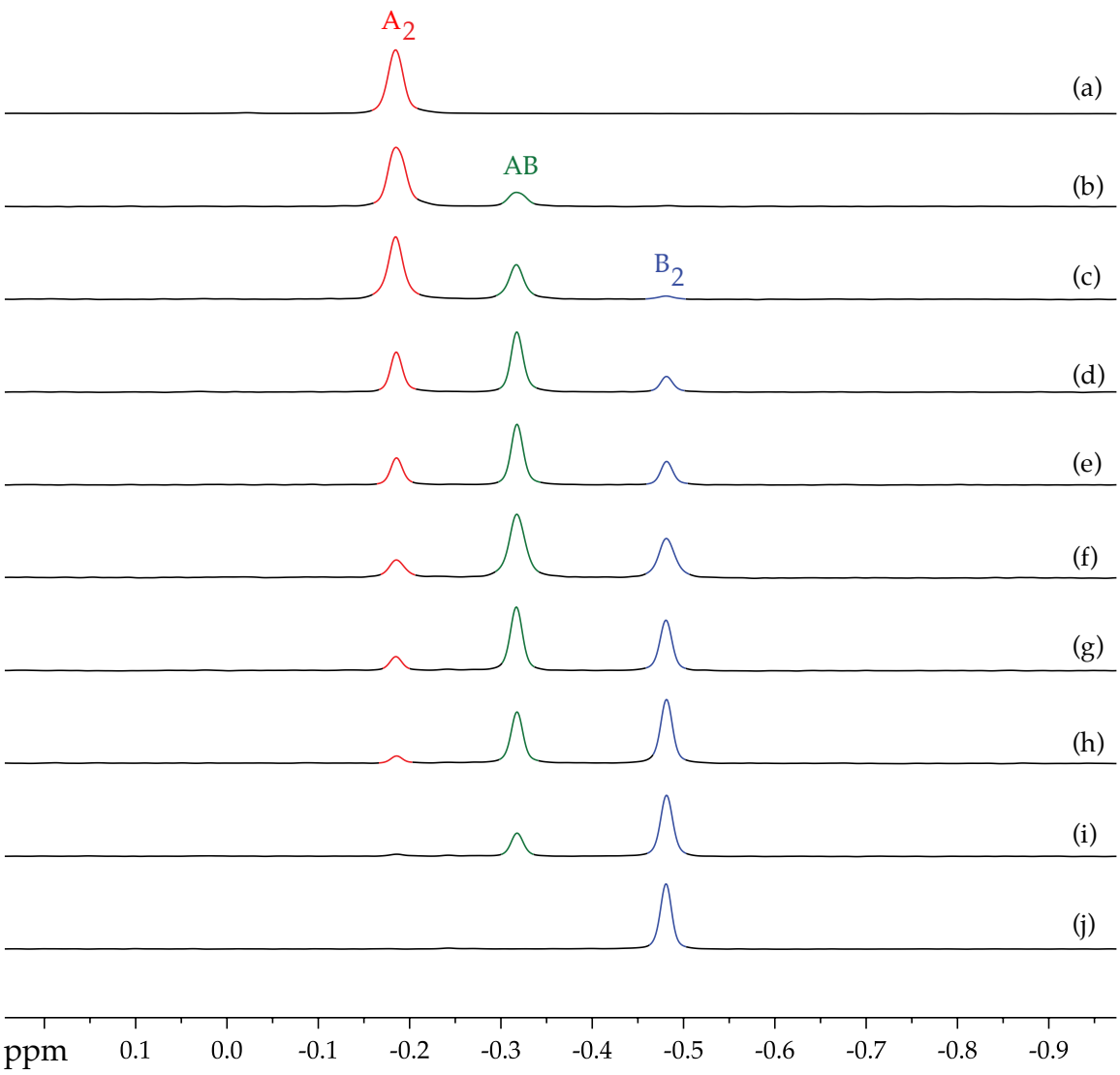


Figure 33. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2e** (**A**) and [^{6}Li]**2f** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(j) are 0.00, 0.11, 0.21, 0.40, 0.49, 0.59, 0.65, 0.73, 0.84, and 1.00, respectively.

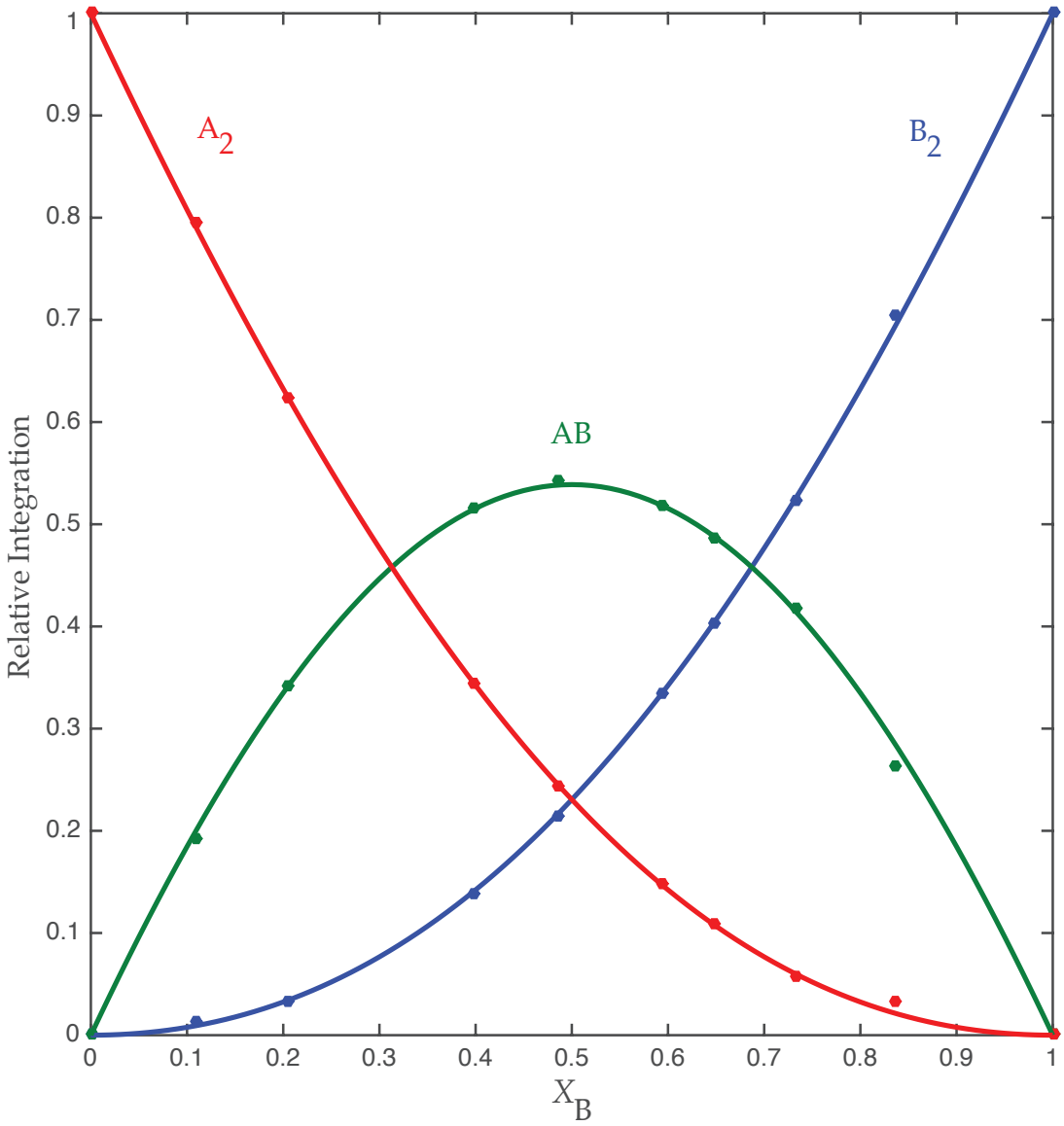


Figure 34. Job plot showing the relative integrations versus the measured mole fraction of **2f** for 0.10 M mixtures of [^{6}Li]**2e** (**A**) and [^{6}Li]**2f** (**B**) in 12.3 M THF at –80 °C.

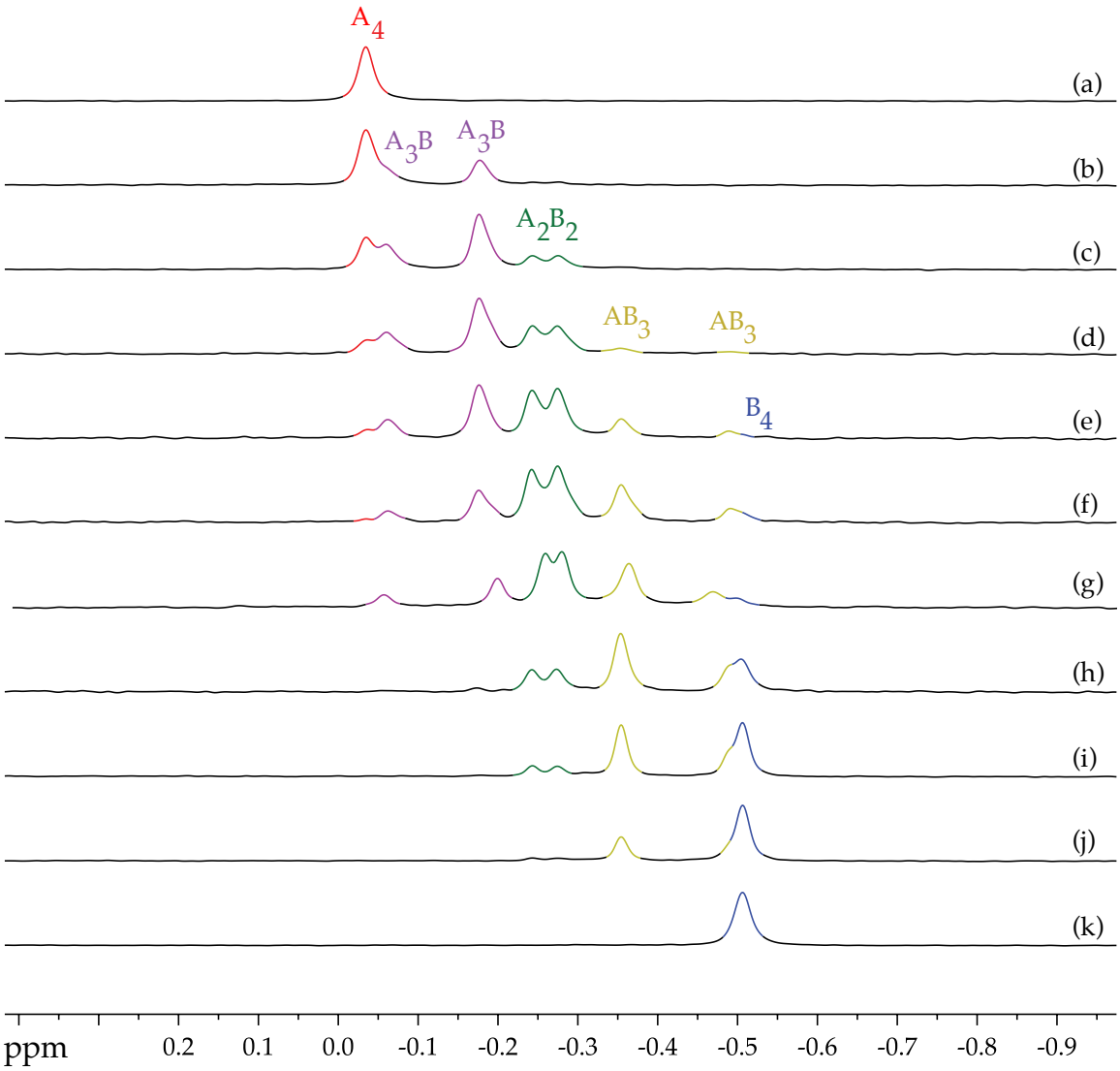


Figure 35. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2b** (**A**) and [^{6}Li]**3** (**B**) in 0.13 M THF at –90 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(j) are 0.00, 0.11, 0.25, 0.35, 0.43, 0.52, 0.73, 0.81, 0.89, and 1.00, respectively.

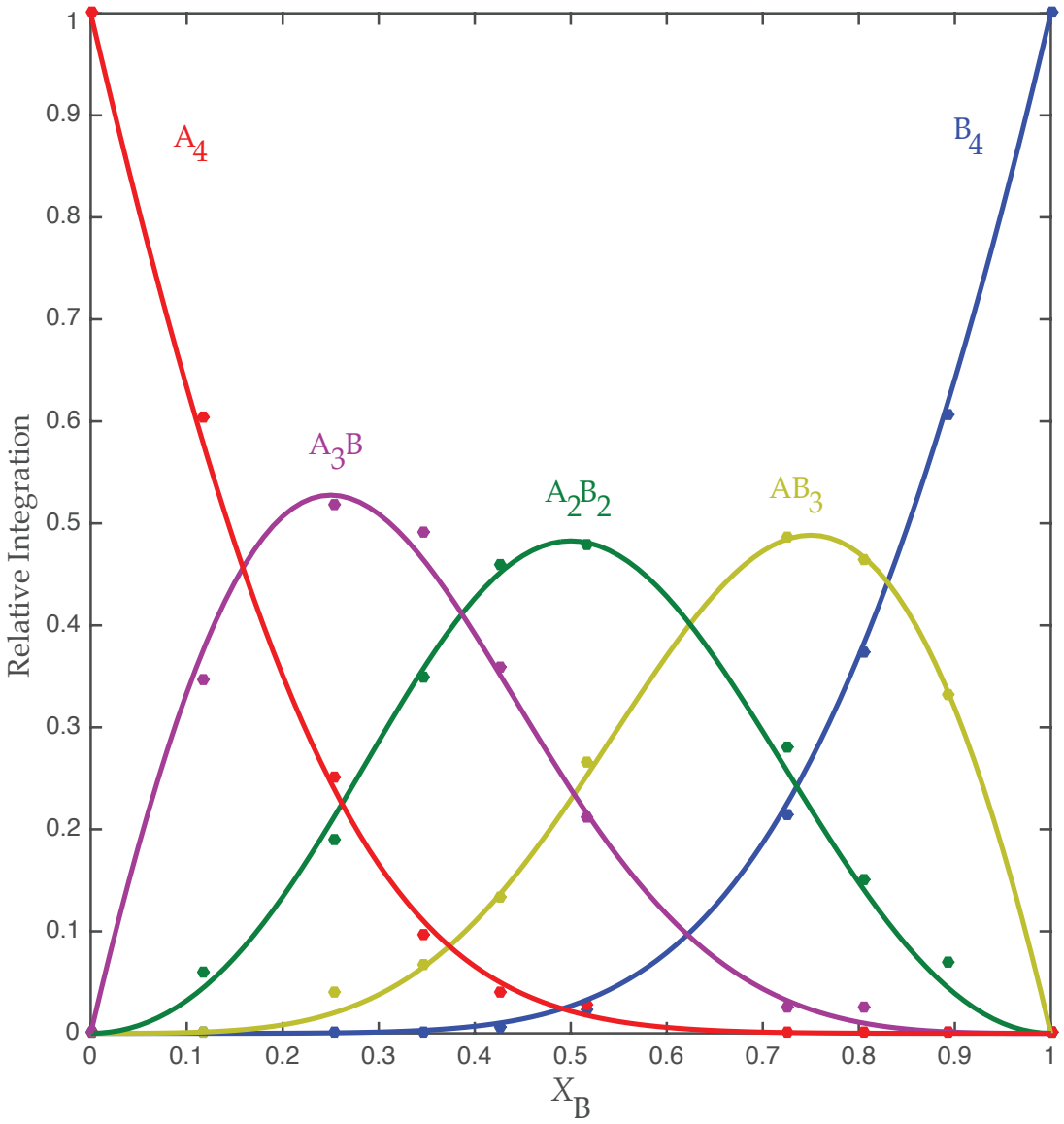


Figure 36. Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [^{6}Li]**2b** (**A**) and [^{6}Li]**3** (**B**) in 0.13 M THF at –90 °C.

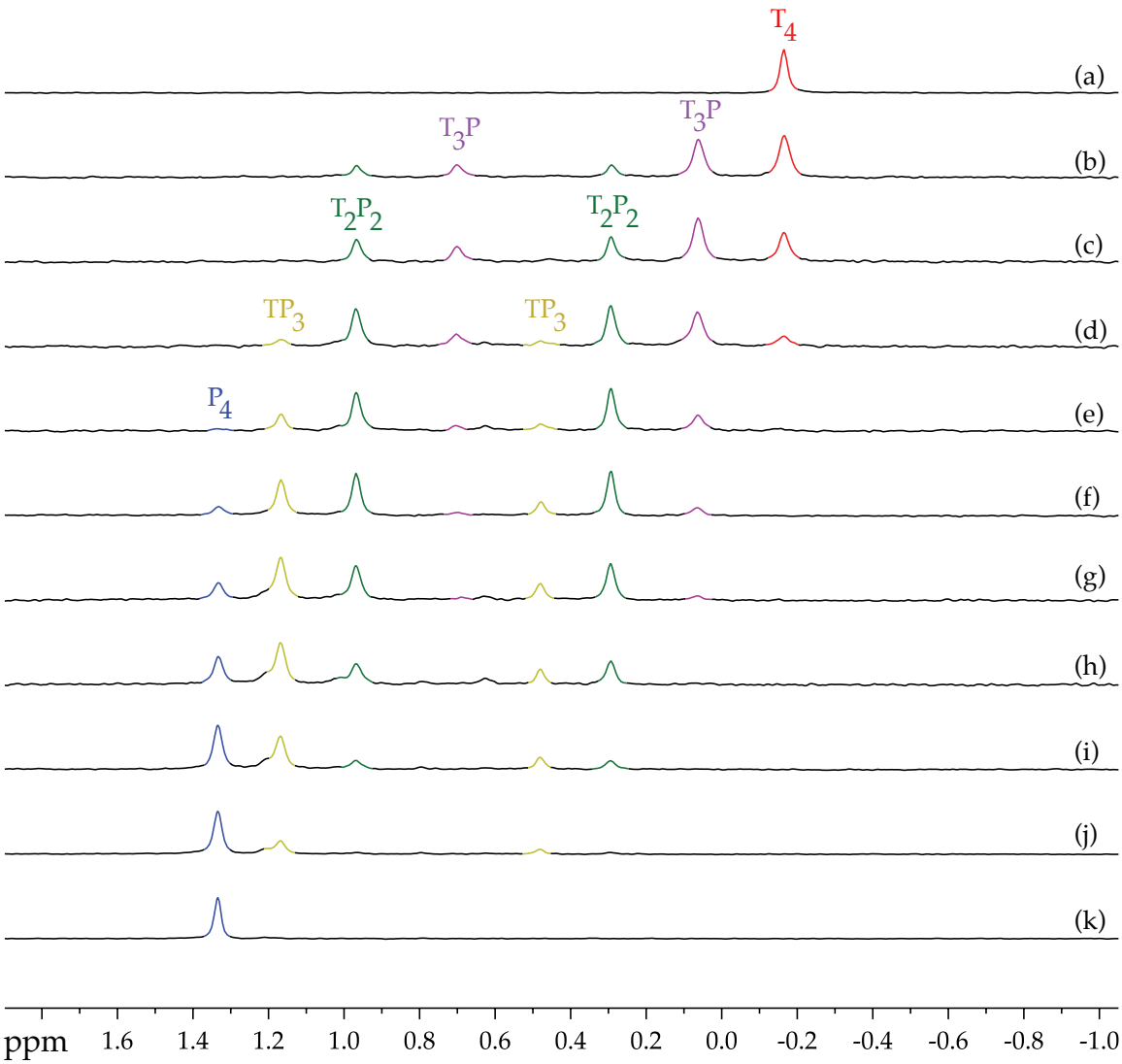


Figure 37. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** in 0.15 M total solvent concentration with varying amounts of THF (**T**) and pyridine (**P**) in toluene at –95 °C with 0.105 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{P}}$, in (a)–(k) are 0.00, 0.21, 0.27, 0.39, 0.49, 0.59, 0.65, 0.72, 0.81, 0.91, and 1.00, respectively.

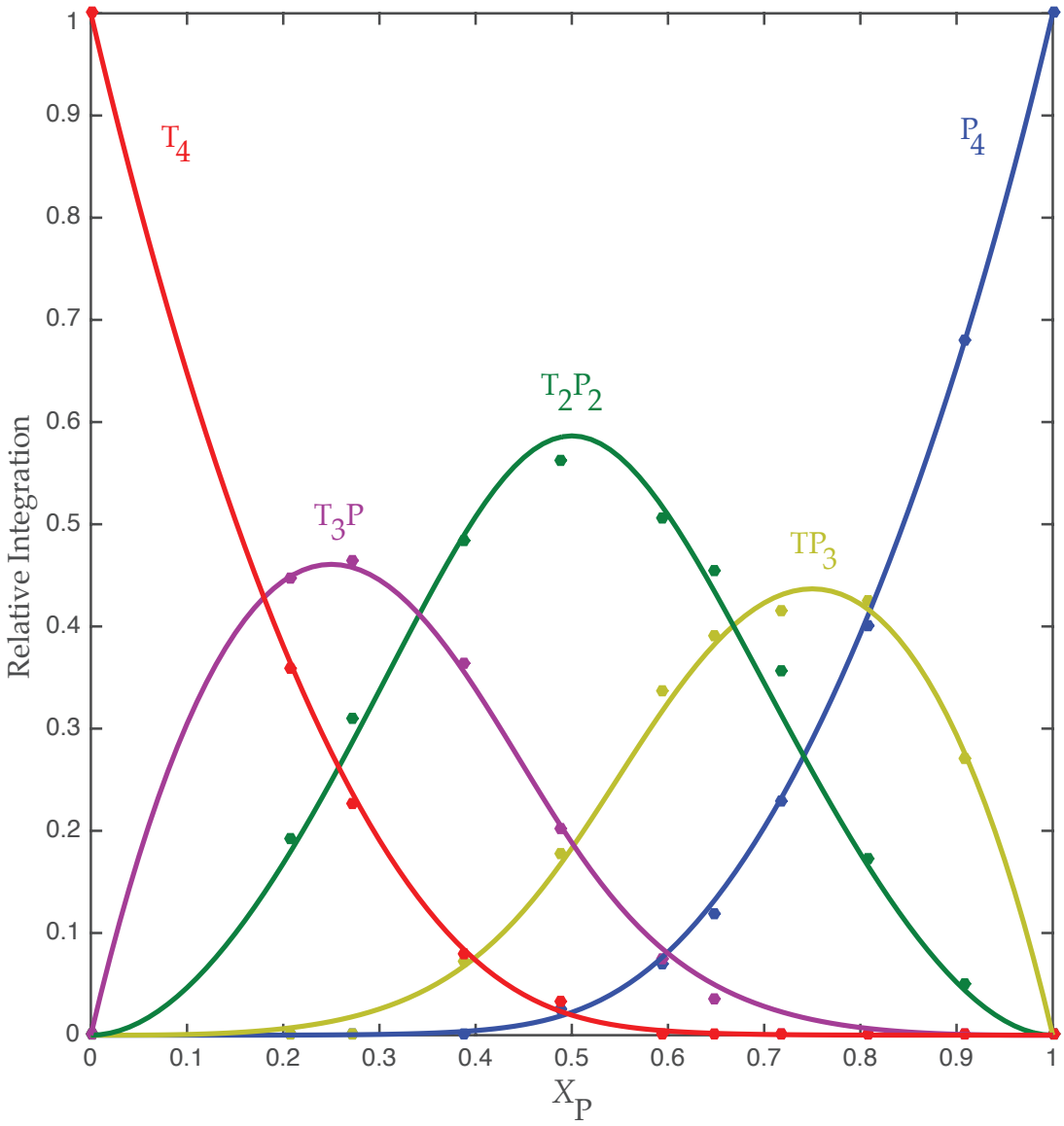


Figure 38. Job plot showing the relative integrations versus the measured mole fraction of pyridine for 0.15 M mixtures of THF (**T**) and pyridine (**P**) with 0.10 M **2j** at –95 °C.

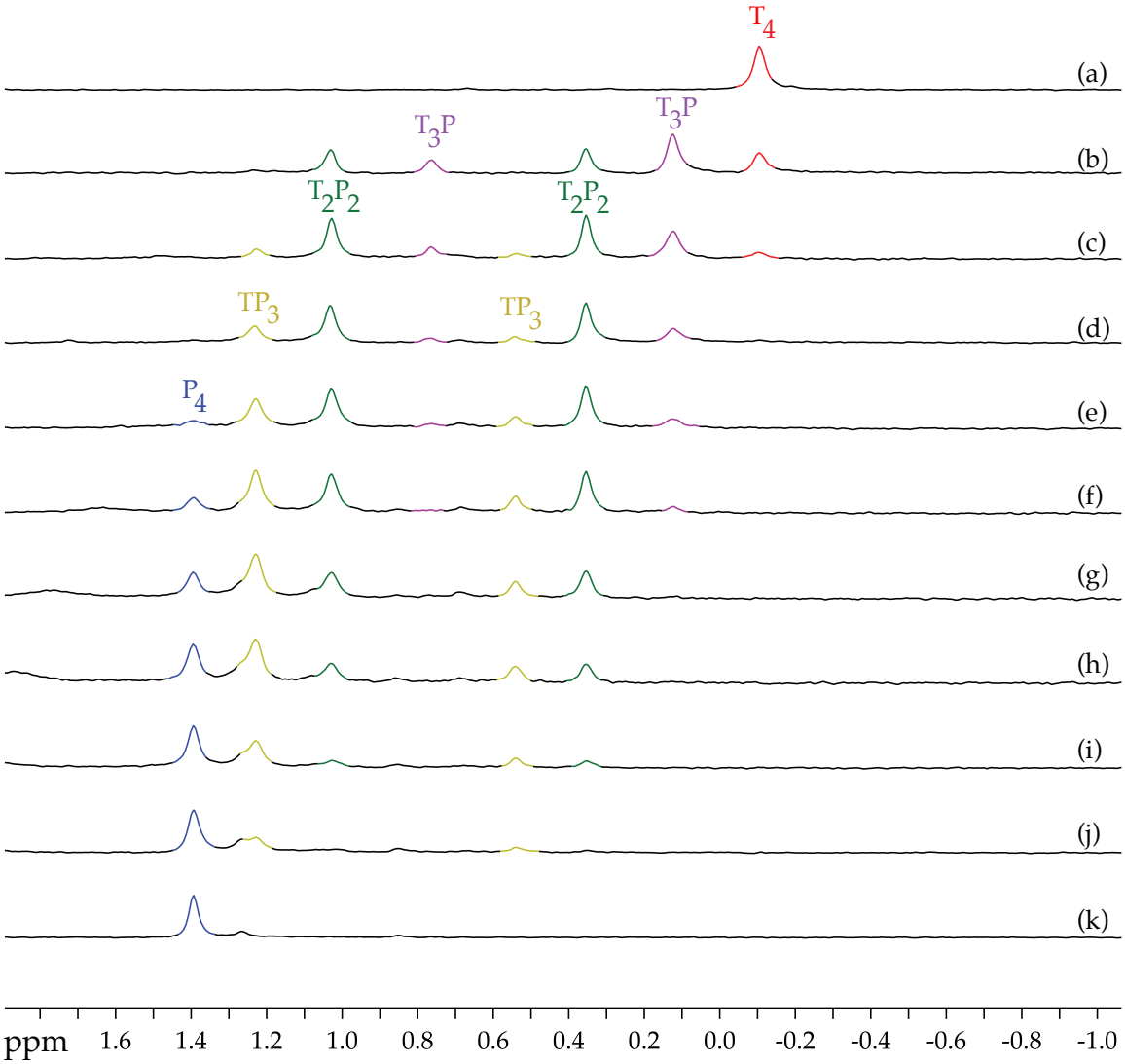


Figure 39. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** in 0.50 M total solvent concentration with varying amounts of THF (**T**) and pyridine (**P**) in toluene at –95 °C with 0.105 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{P}}$, in (a)–(k) are 0.00, 0.28, 0.42, 0.50, 0.58, 0.63, 0.70, 0.75, 0.81, 0.93, and 1.00, respectively.

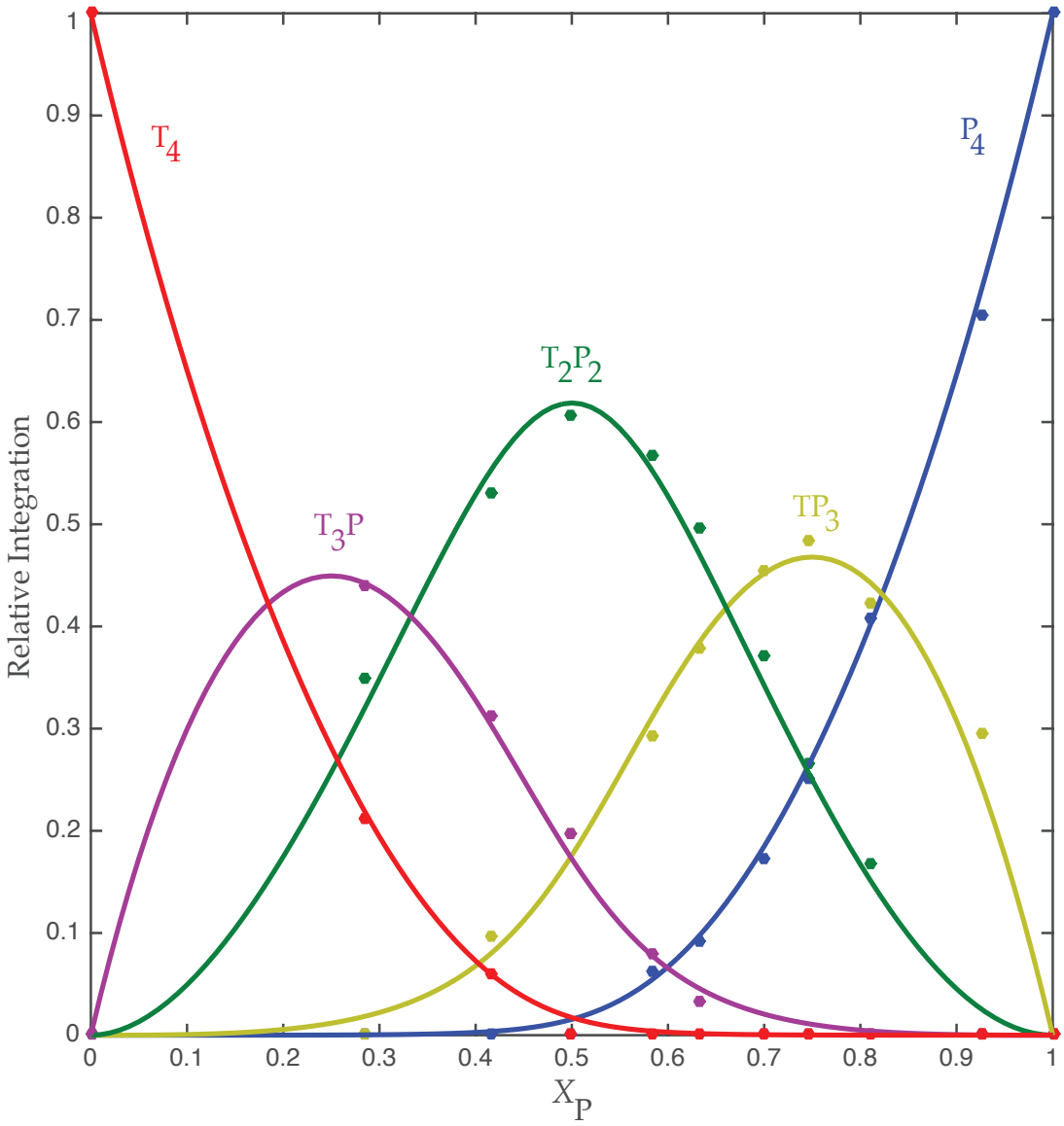


Figure 40. Job plot showing the relative integrations versus the measured mole fraction of pyridine for 0.50 M mixtures of THF (**A**) and pyridine (**B**) in toluene with 0.10 M **2j** at –95 °C.

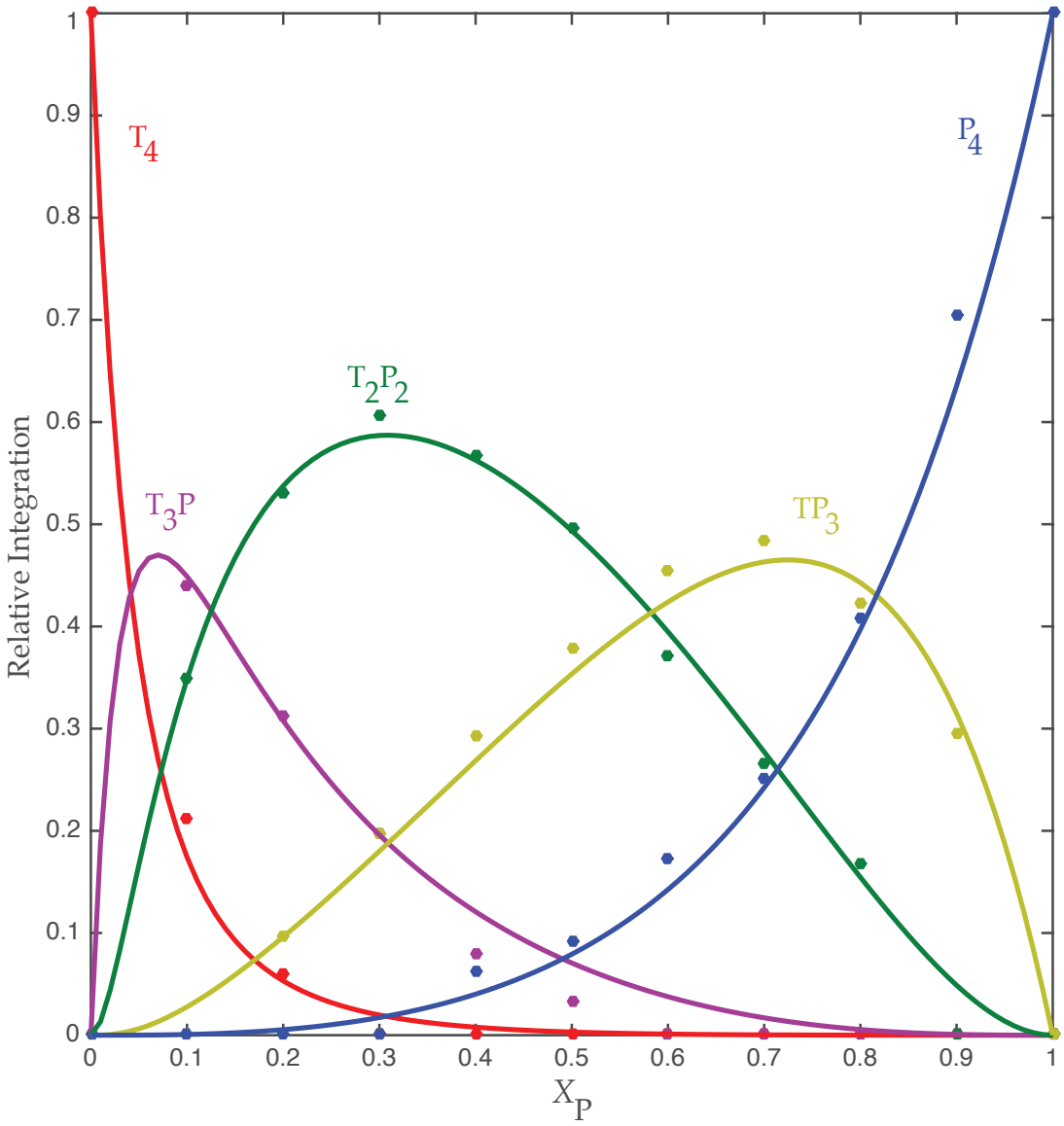


Figure 41. Job plot showing the relative integrations versus the intended mole fraction of pyridine for 0.50 M mixtures of THF (**A**) and pyridine (**B**) in toluene with 0.10 M **2j** at –95 °C.

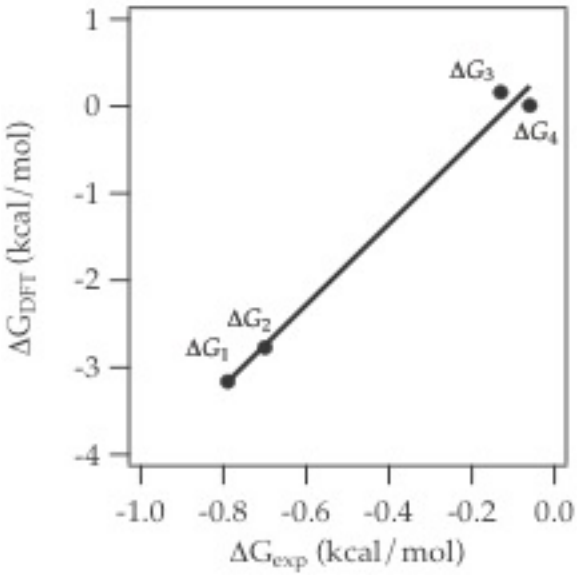


Figure 42. Plot showing the agreement between the measured free energies and calculated free energies per incremental replacement of a THF ligand with a pyridine ligand on a the cube of 2j.

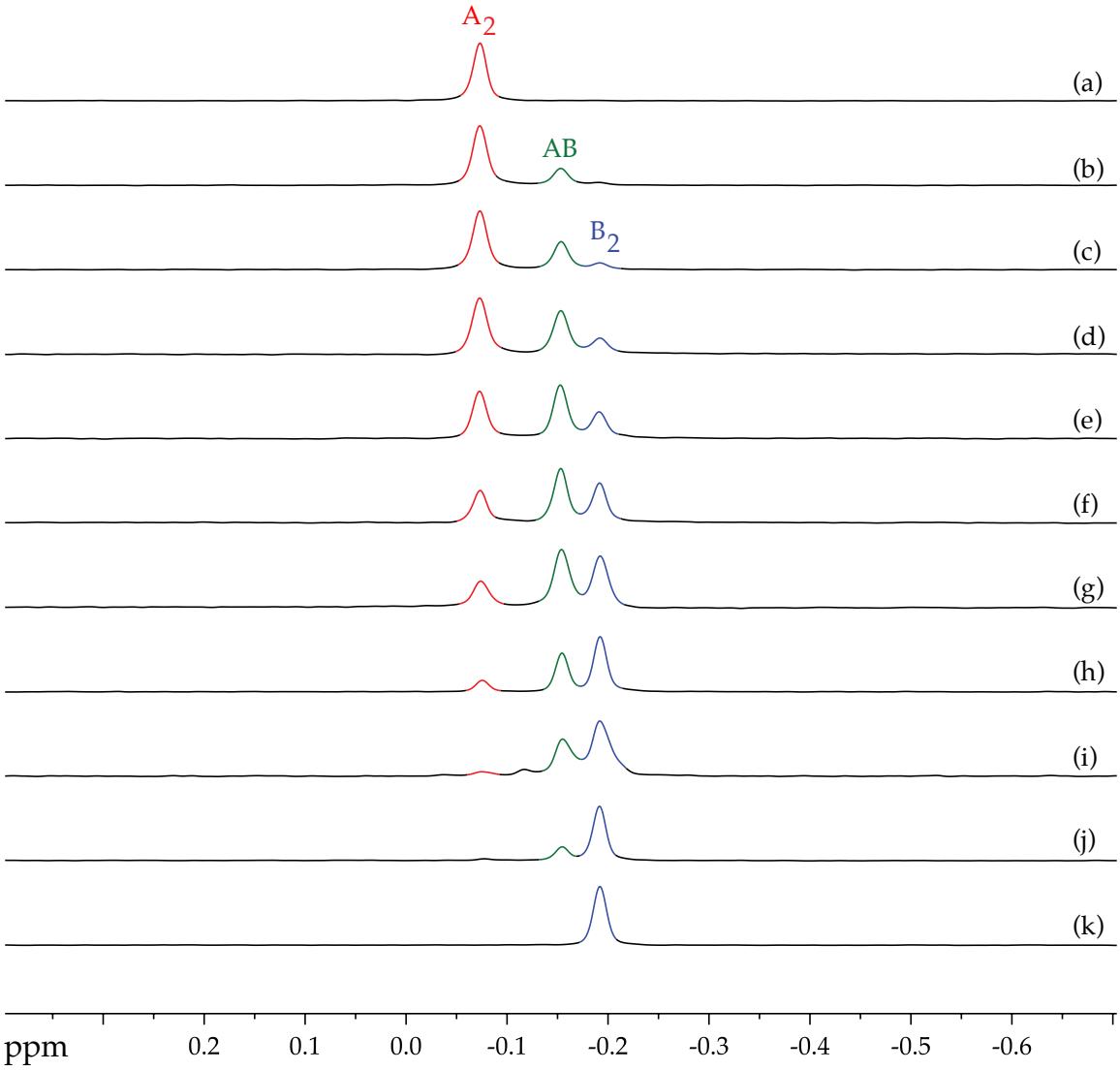


Figure 43. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**5** (**A**) and [^{6}Li]**4** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.13, 0.19, 0.30, 0.43, 0.49, 0.57, 0.68, 0.77, 0.84, and 1.00, respectively.

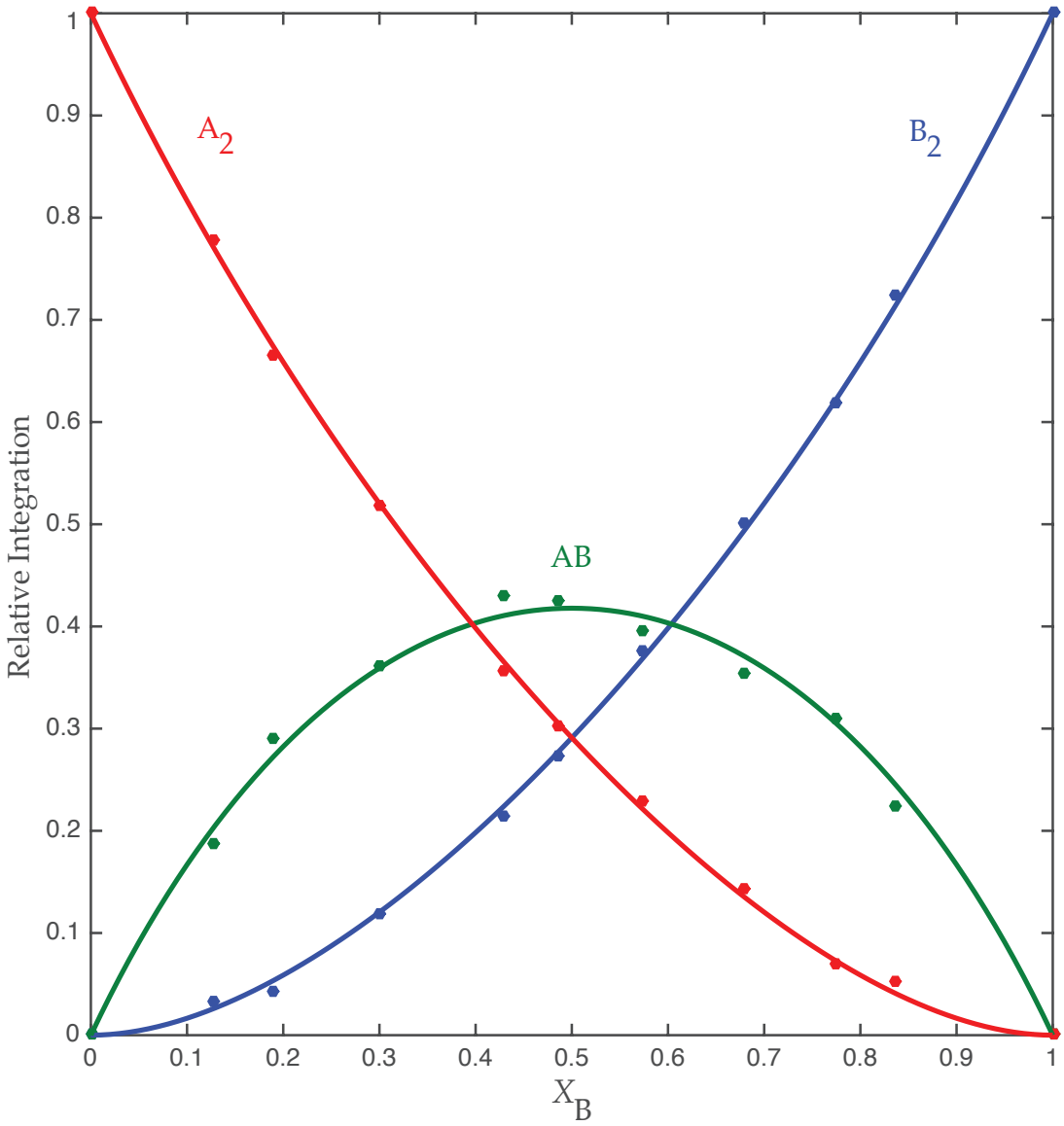


Figure 44. Job plot showing the relative integrations versus the measured mole fraction of **4** for 0.10 M mixtures of [^{6}Li]**5** (**A**) and [^{6}Li]**4** (**B**) in 12.3 M THF at –80 °C.

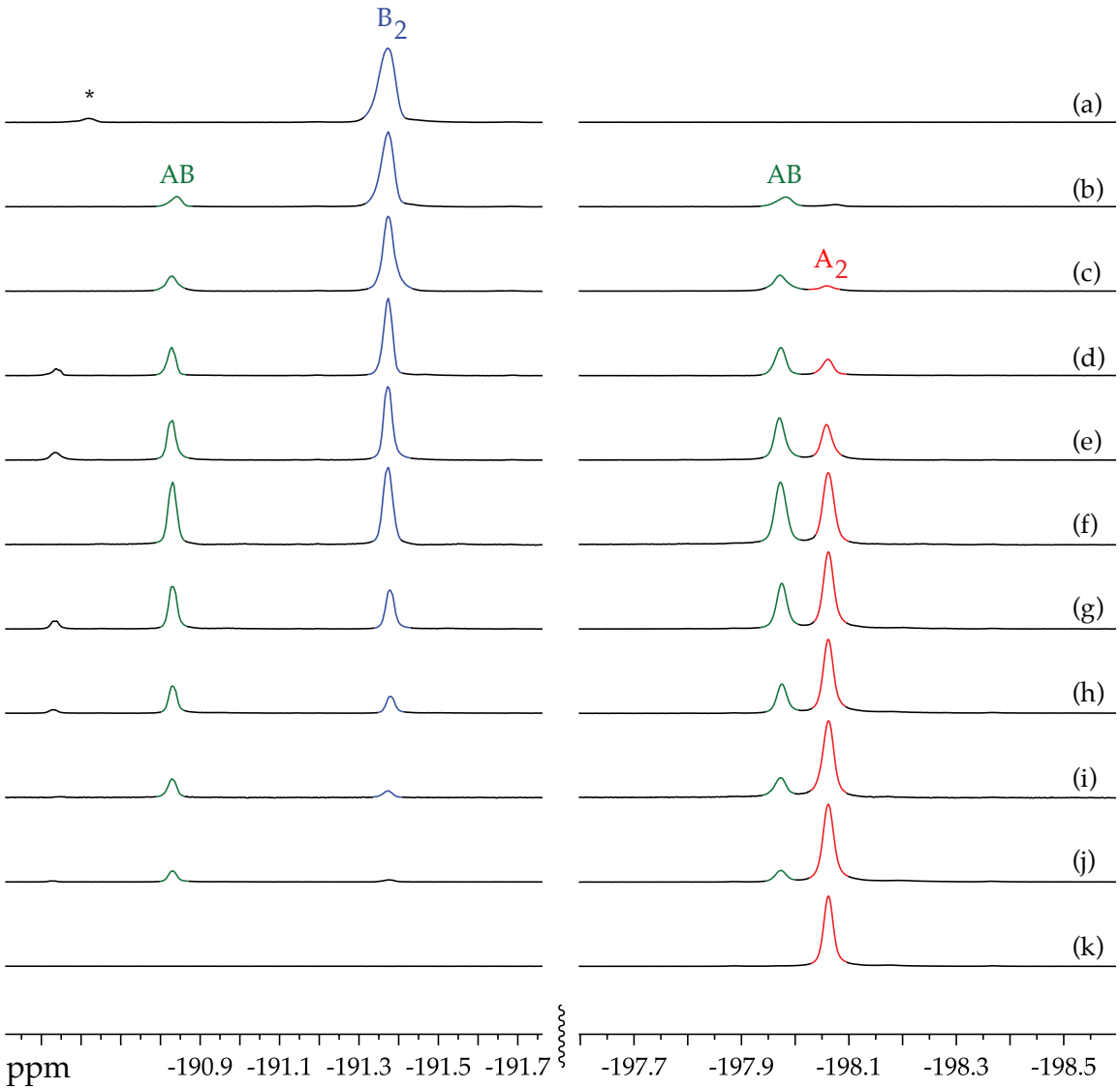


Figure 45. ^{19}F NMR spectra of 0.10 M solutions of [^{6}Li]**5** (**A**) and [^{6}Li]**4** (**B**) in 12.3 M THF at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(k) are 0.00, 0.12, 0.19, 0.29, 0.40, 0.48, 0.59, 0.69, 0.77, 0.87, and 1.00, respectively.
* denotes a mixed aggregate with [^{6}Li]4 (**B**) and [^{6}Li]LDA.

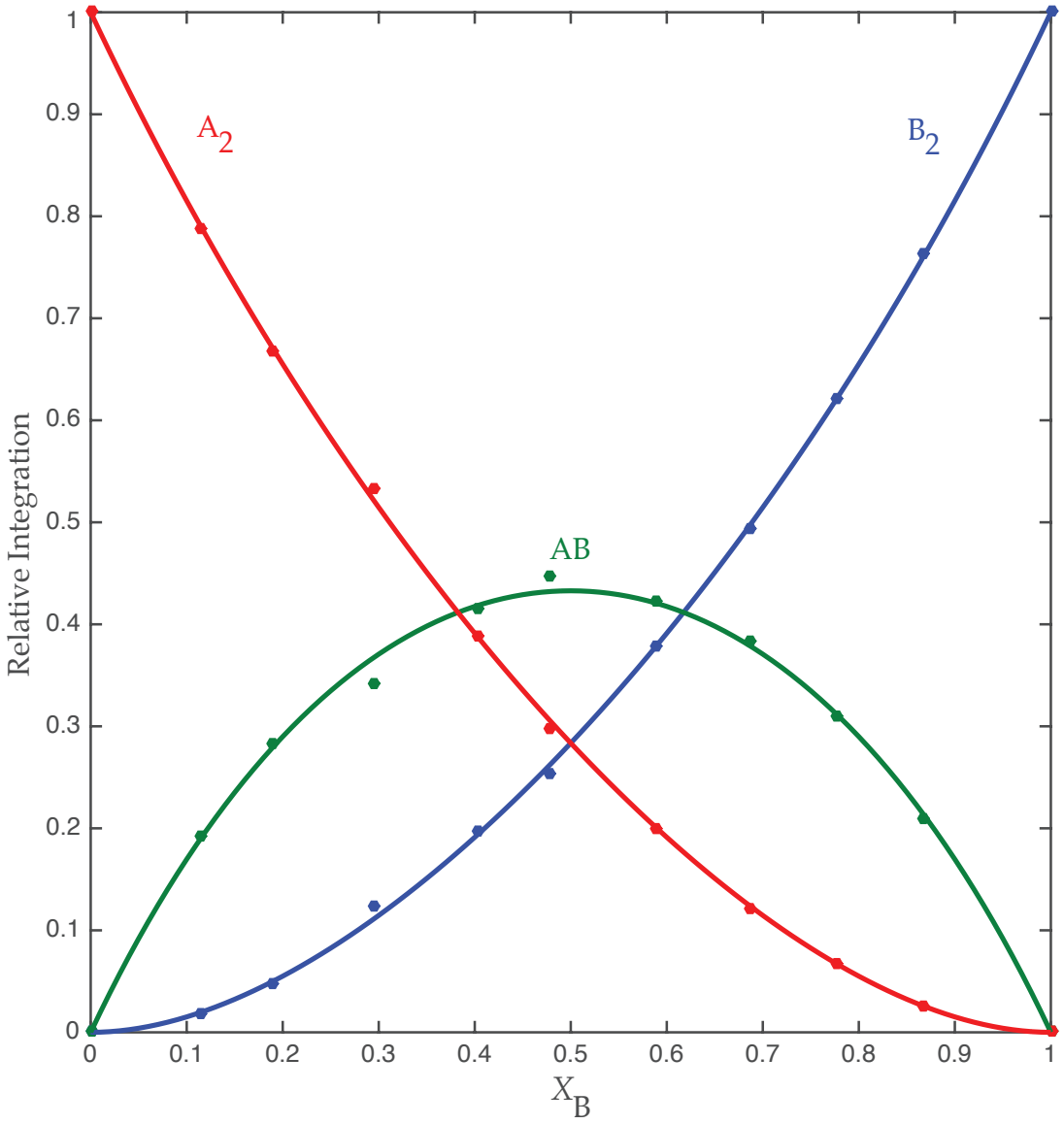


Figure 46. Job plot showing the [^{19}F] relative integrations versus the measured mole fraction of **4** for 0.10 M mixtures of [^{6}Li]**5** (**A**) and [^{6}Li]**4** (**B**) in 12.3 M THF at –80 °C.

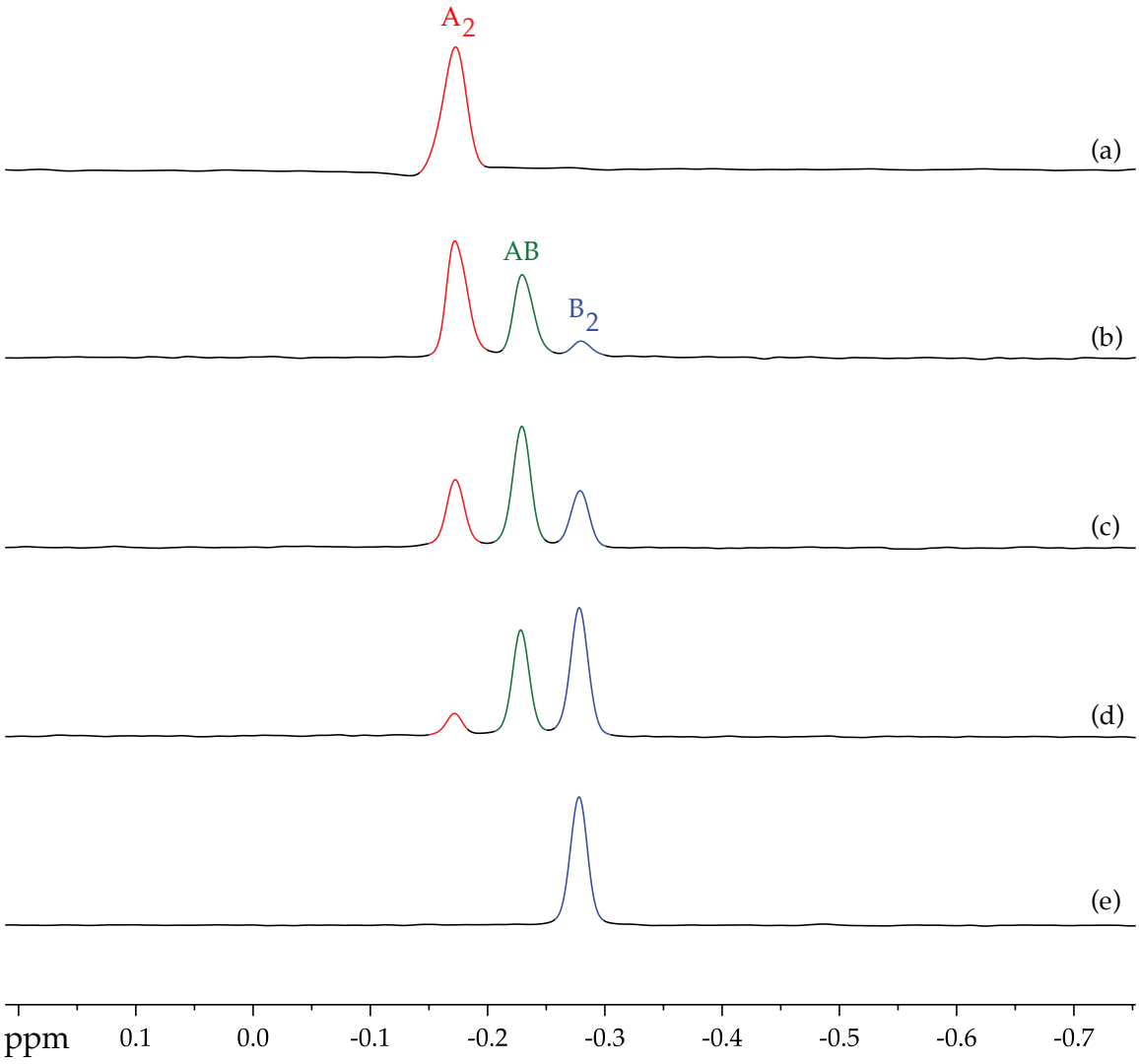


Figure 47. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**4** (**A**) and [^{6}Li]**3** (**B**) in 4.1 M THF and toluene at –80 °C with 0.13 M [^{6}Li]LDA. The measured mole fractions, $X_{\mathbf{B}}$, in (a)–(e) are 0.00, 0.28, 0.47, 0.70, 1.00, respectively.

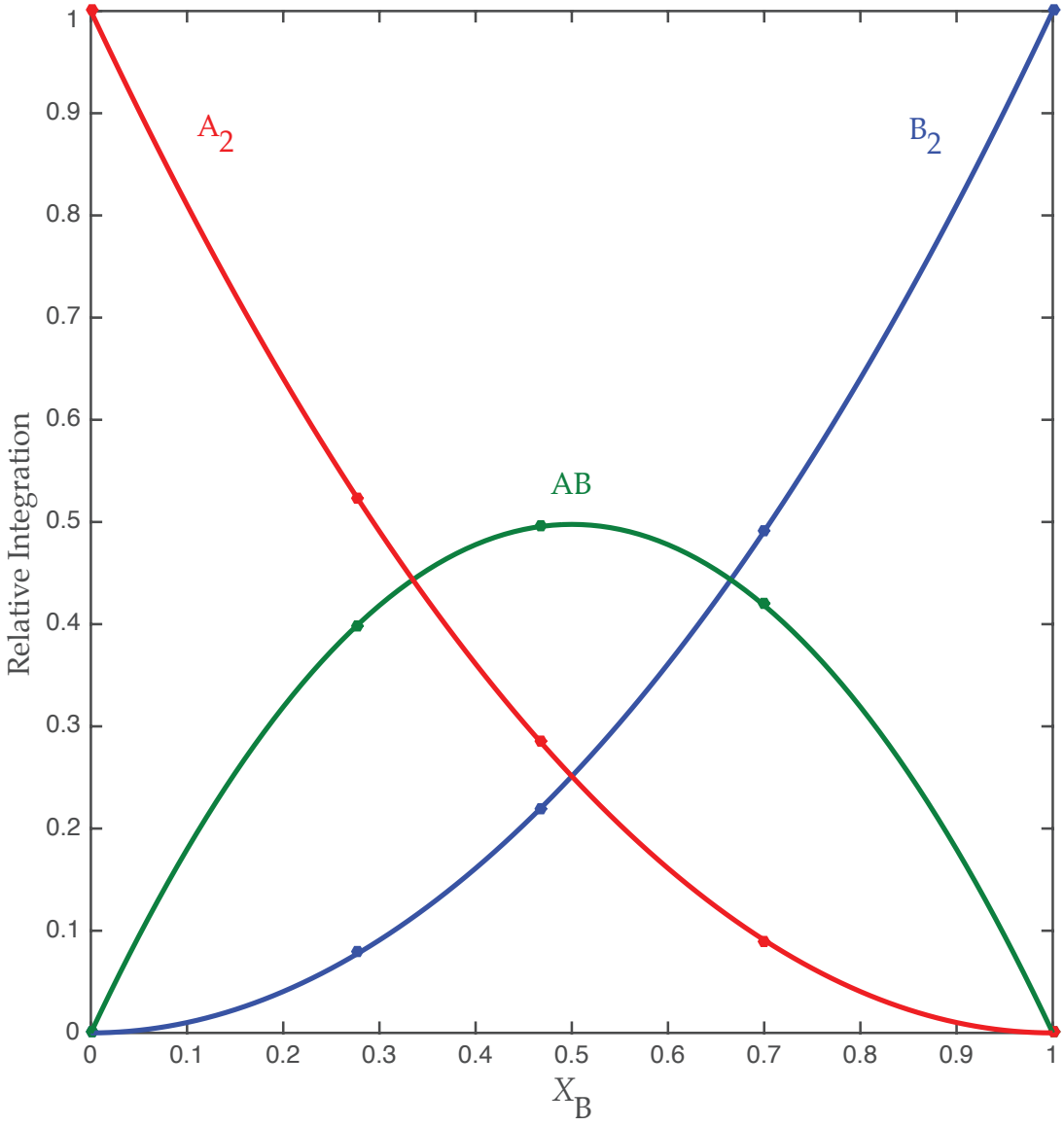


Figure 48. Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [^{6}Li]**4** (**A**) and [^{6}Li]**3** (**B**) in 4.1 M THF and toluene at –80 °C.

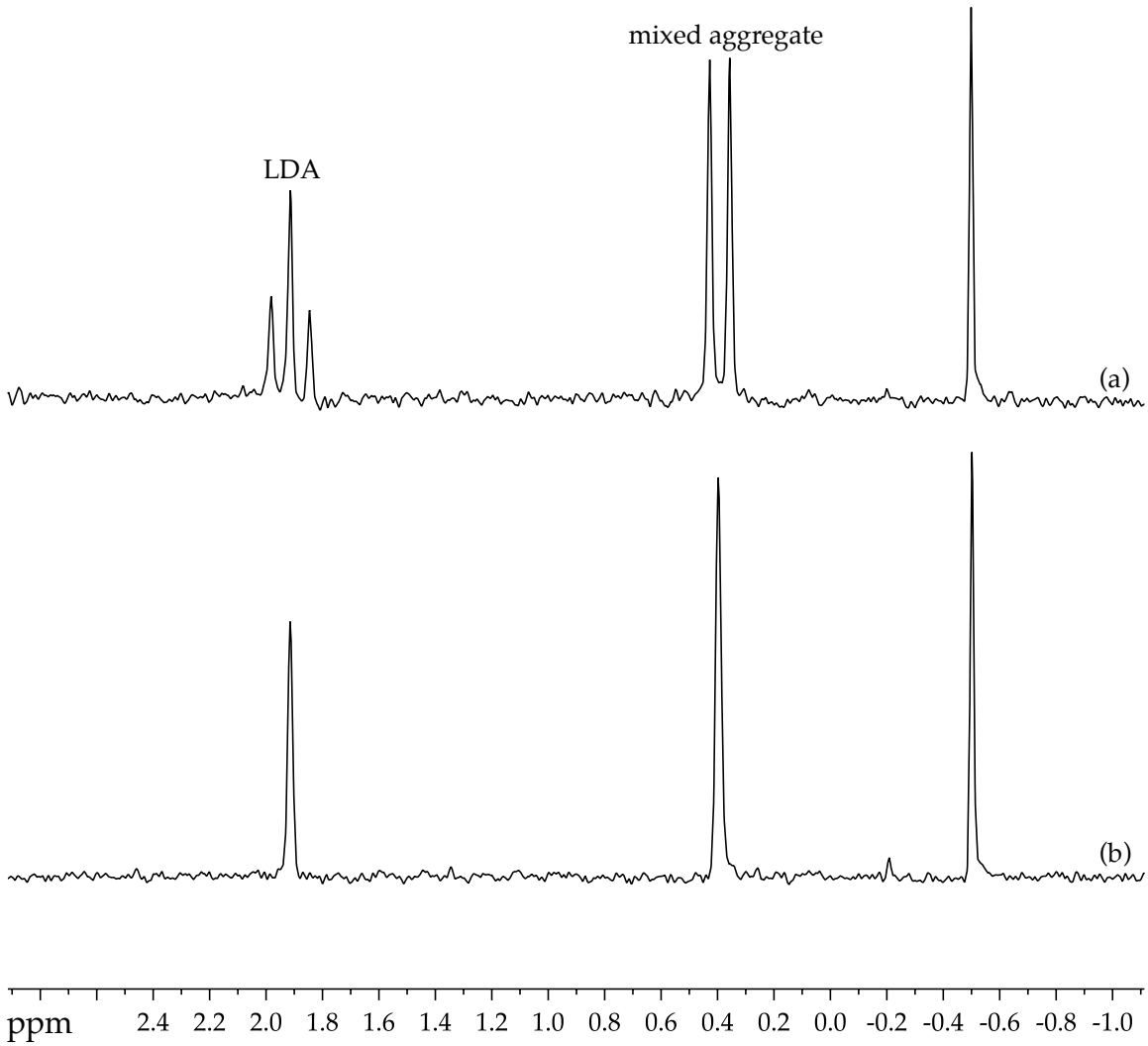


Figure 49. ^{6}Li NMR spectra for a 0.10 M solution of [^{6}Li]**2i** in 3.1 M THF and toluene with 0.15 M [^{6}Li ,^{15}N]LDA at –80 °C: (a) ^{6}Li spectrum; and (b) ^{6}Li{^{15}N} spectrum.

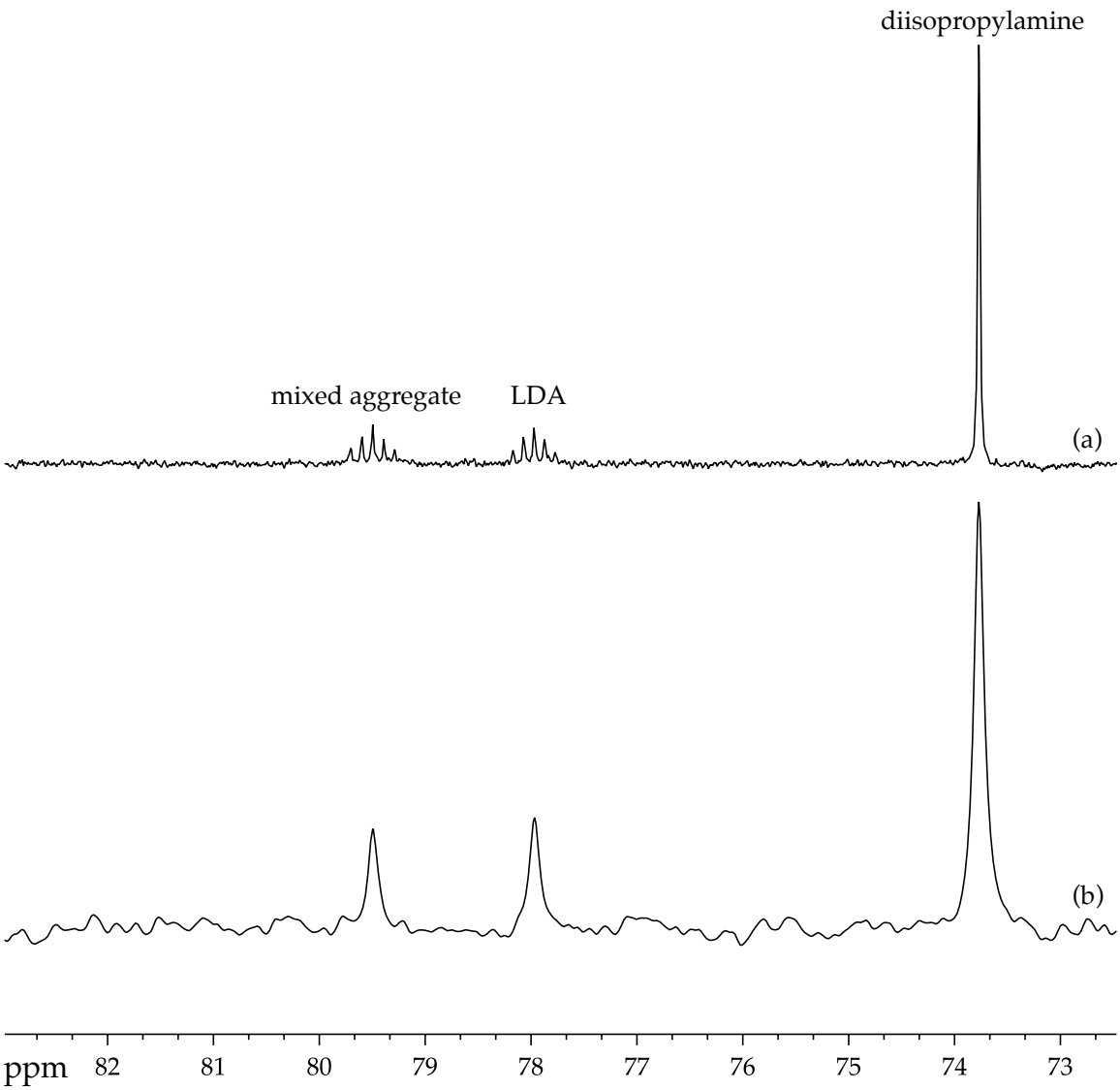


Figure 50. ^{15}N NMR spectra for 0.10 M solution of [^{6}Li]**2i** in 12.3 M THF with 0.20 M [^{6}Li ,^{15}N]LDA at –80 °C: (a) (a) ^{15}N spectrum; and (b) ^{15}N {^{6}Li } spectrum.

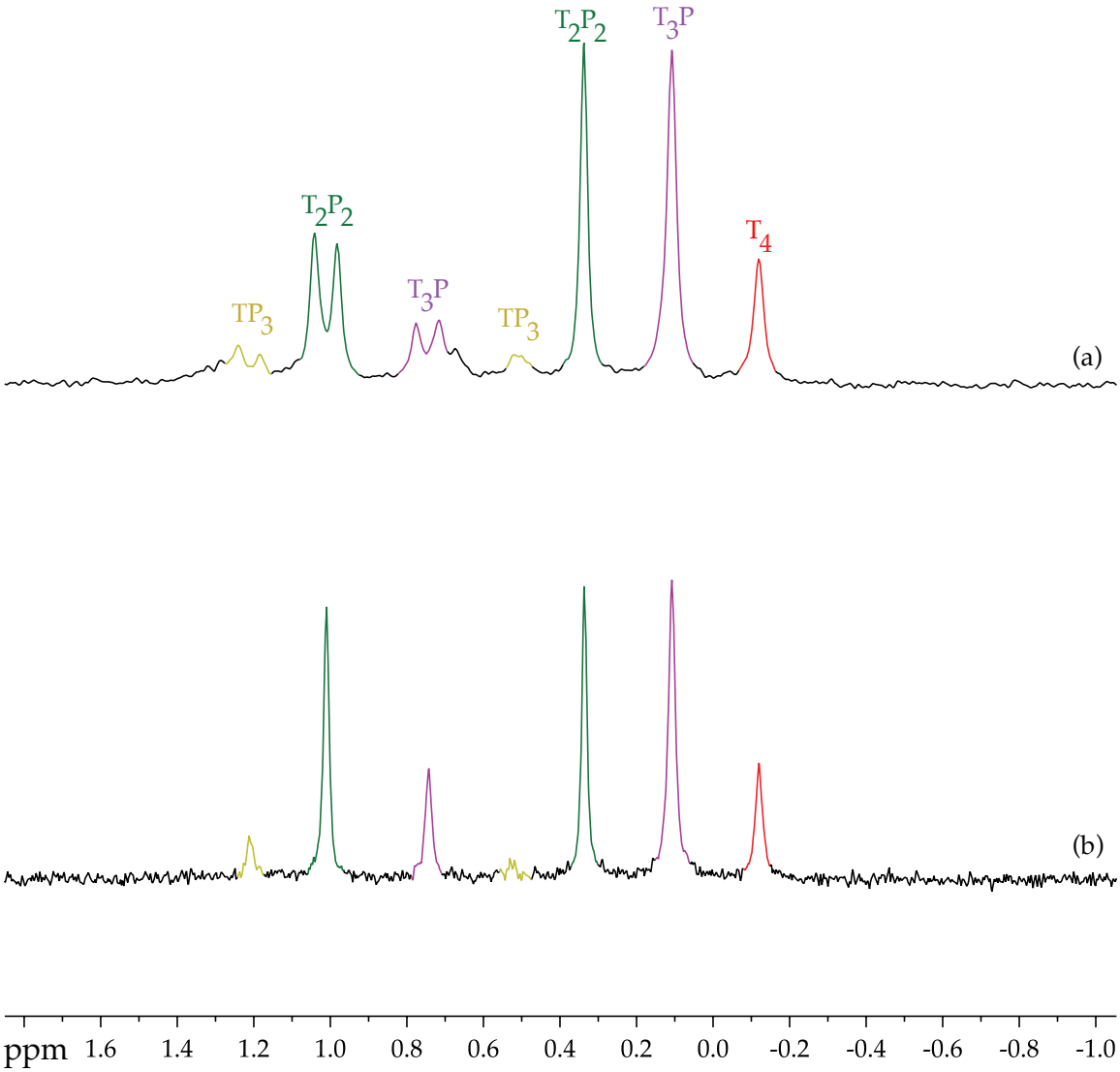


Figure 51. ^{6}Li NMR spectra for 0.10 M solution of [^{6}Li]**2j** in 0.11 M THF and 0.045 M pyridine in toluene with 0.11 M [^{6}Li ,^{15}N]LDA at –95 °C: (a) ^{6}Li spectrum; and (b) ^{6}Li{^{15}N} spectrum.

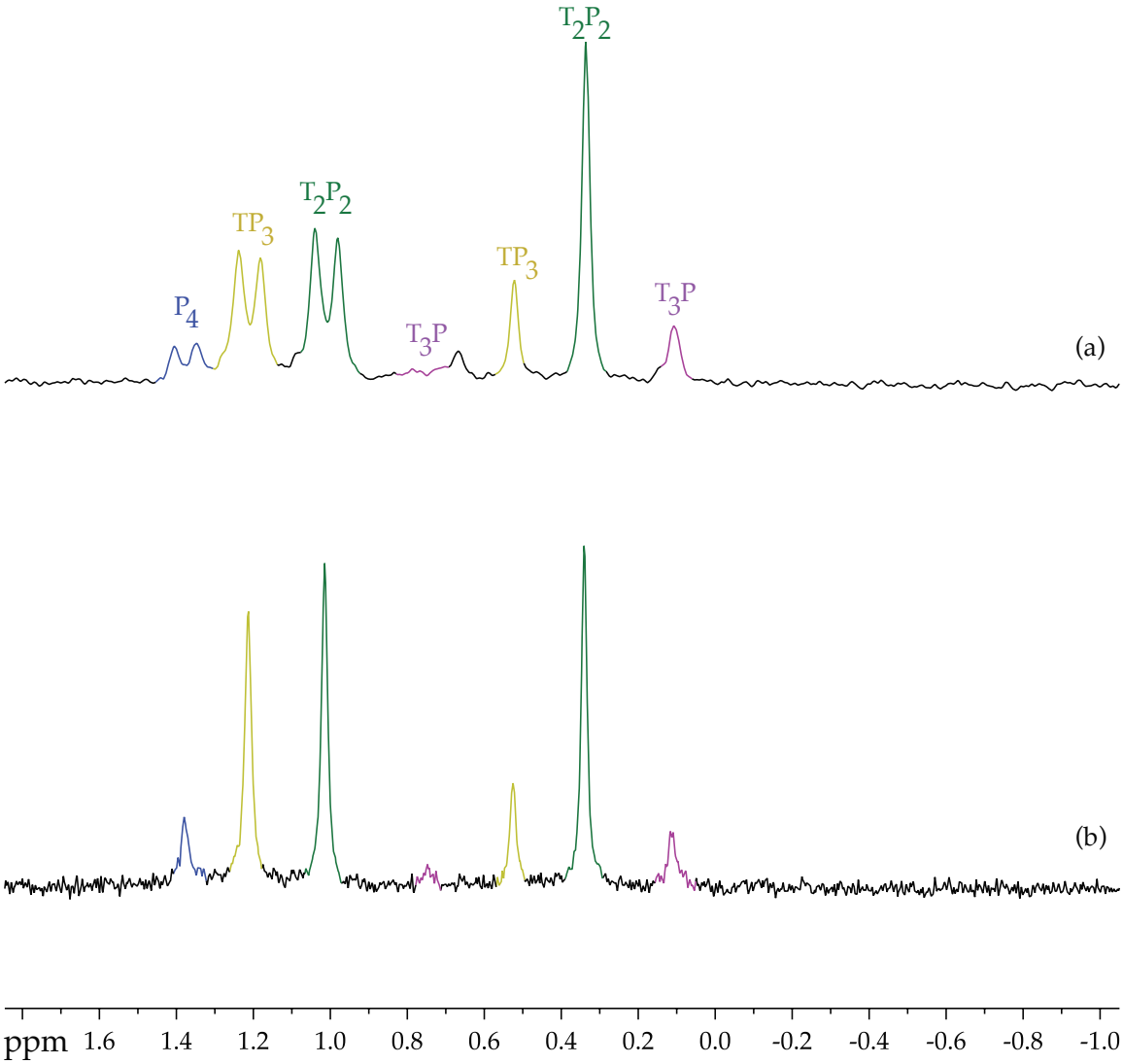


Figure 52. ^{6}Li NMR spectra for 0.10 M solution of [^{6}Li]**2j** in 0.075 M THF and 0.075 M pyridine in toluene with 0.11 M [^{6}Li ,^{15}N]LDA at –95 °C: (a) ^{6}Li spectrum; and (b) ^{6}Li{^{15}N} spectrum.

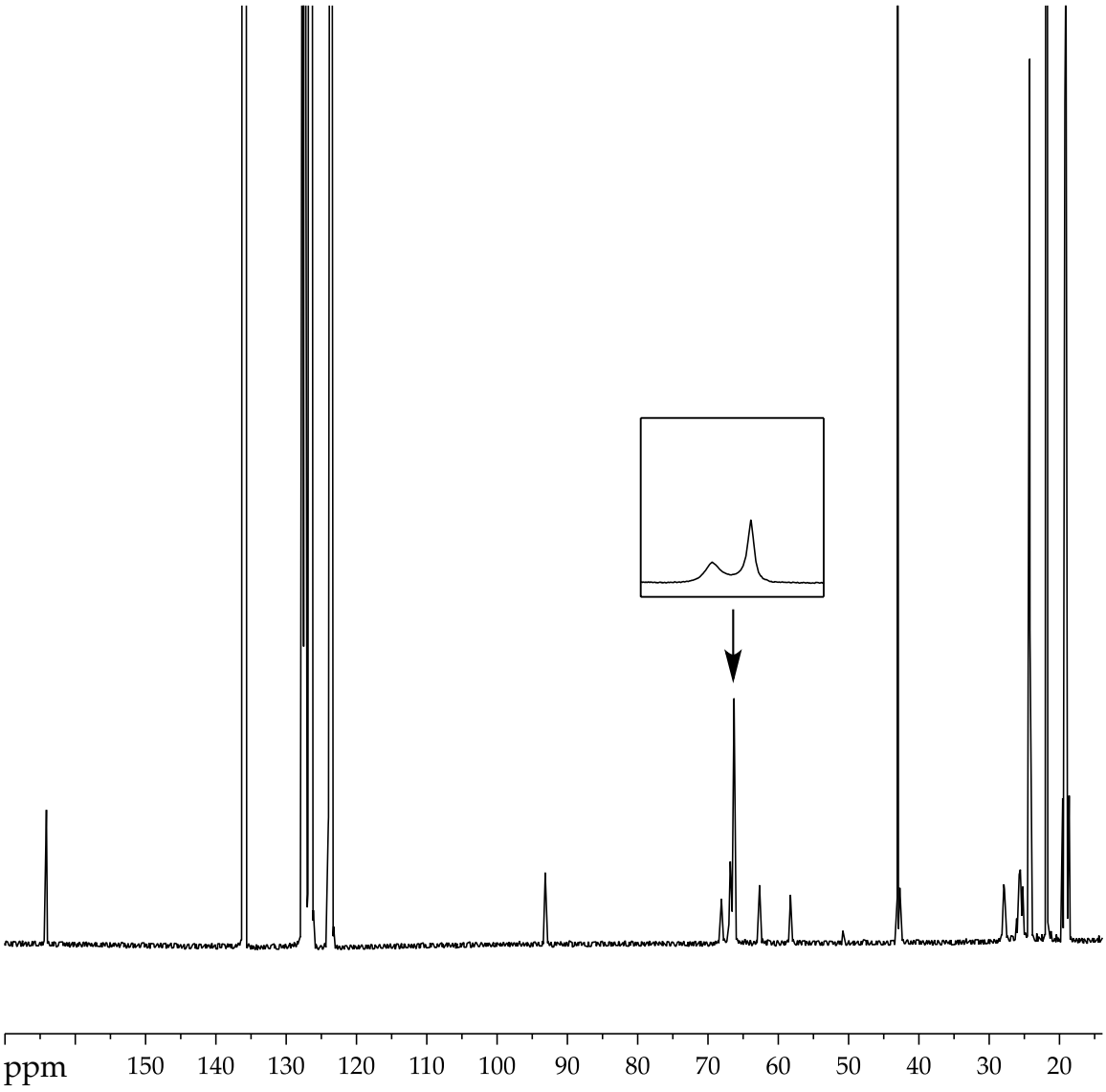


Figure 53. ^{13}C NMR spectrum for a 0.20 M solution of [^{6}Li]**2j** in 0.45 M THF and toluene-d_8 with 0.20 M [^{6}Li]LDA at –85 °C.

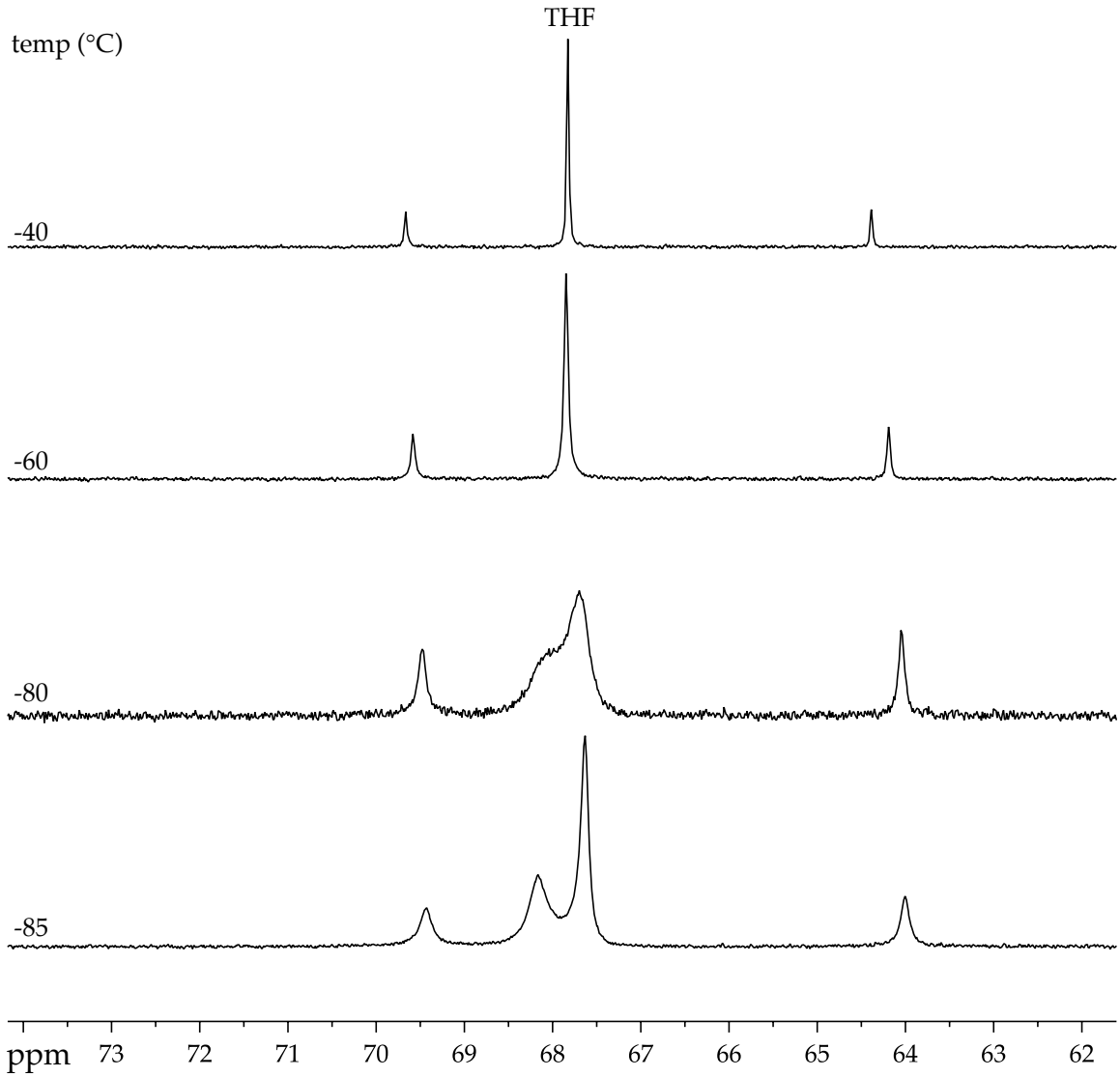


Figure 54. ^{13}C NMR spectrum for a 0.20 M solution of [^{6}Li]**2j** in 0.45 M THF and toluene-d_8 with 0.20 M [^{6}Li]LDA at varying temperatures. The spectra are focused on the THF ^{13}C resonance, exemplifying the slow solvent exchange on the NMR time scale by showing free and bound THF to the [^{6}Li]**2j** tetramer.

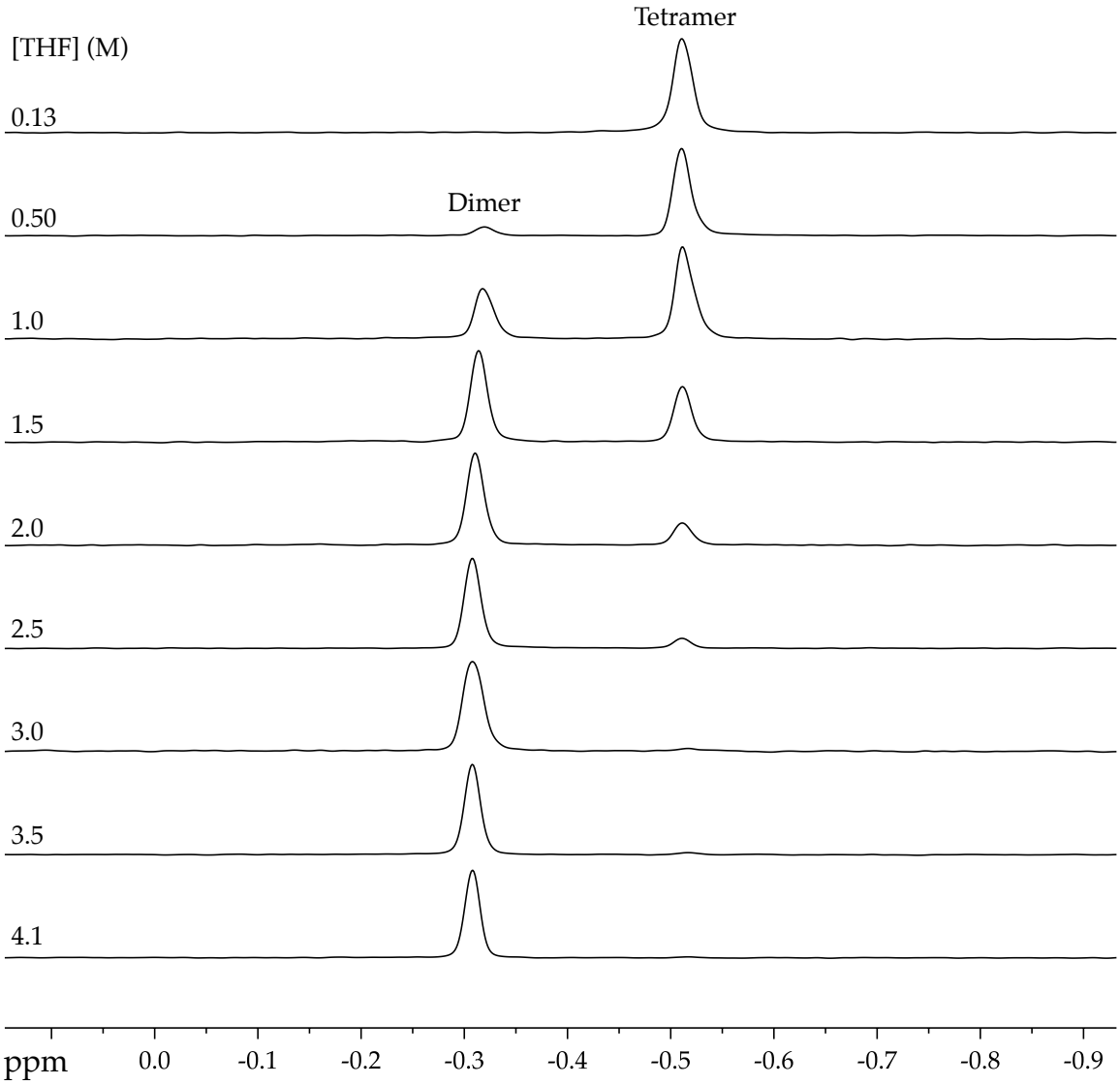


Figure 55. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**3** with varying concentrations of THF and toluene at –80 °C with 0.11 M [^{6}Li]LDA.

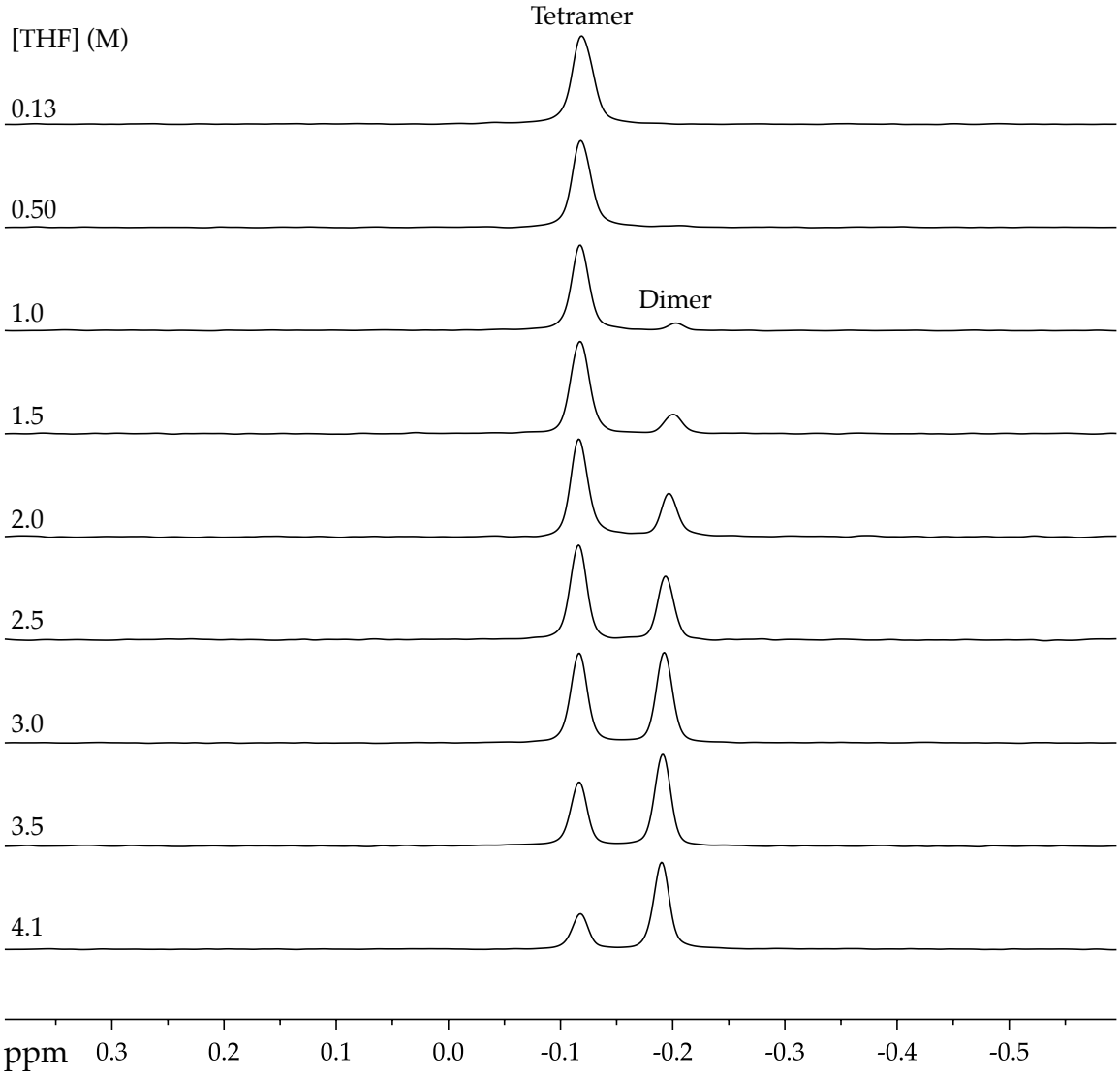


Figure 56. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** with varying concentrations of THF and toluene at –80 °C with 0.11 M [^{6}Li]LDA.

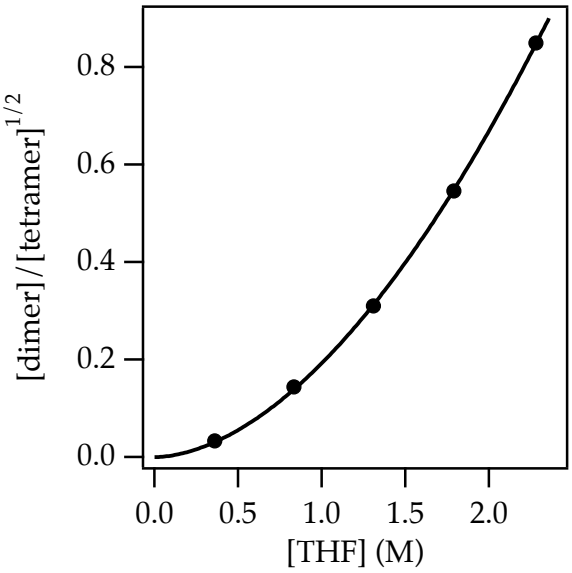


Figure 57. Plot of [dimer]/[tetramer]$^{1/2}$ of [^{6}Li]**3** versus. [THF] in toluene at –80 °C. The curve depicts an unweighted least–squares fit to y=K_{eq}[THF]^n [K_{eq} = (1.93 ± 0.02) × 10^{-1} ; n = 1.80 ± 0.02].

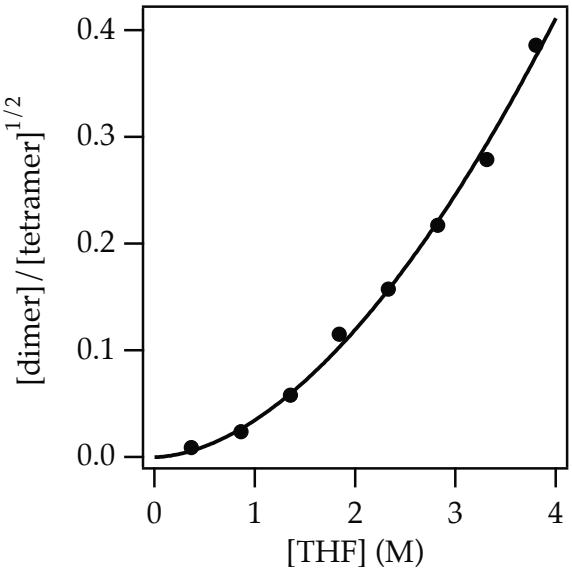


Figure 58. Plot of [dimer]/[tetramer]$^{1/2}$ of [^{6}Li]**2j** versus. [THF] in toluene at –80 °C. The curve depicts an unweighted least–squares fit to y=K_{eq}[THF]^n [K_{eq} = (3.5 ± 0.3) × 10^{-2} ; n = 1.78 ± 0.08].

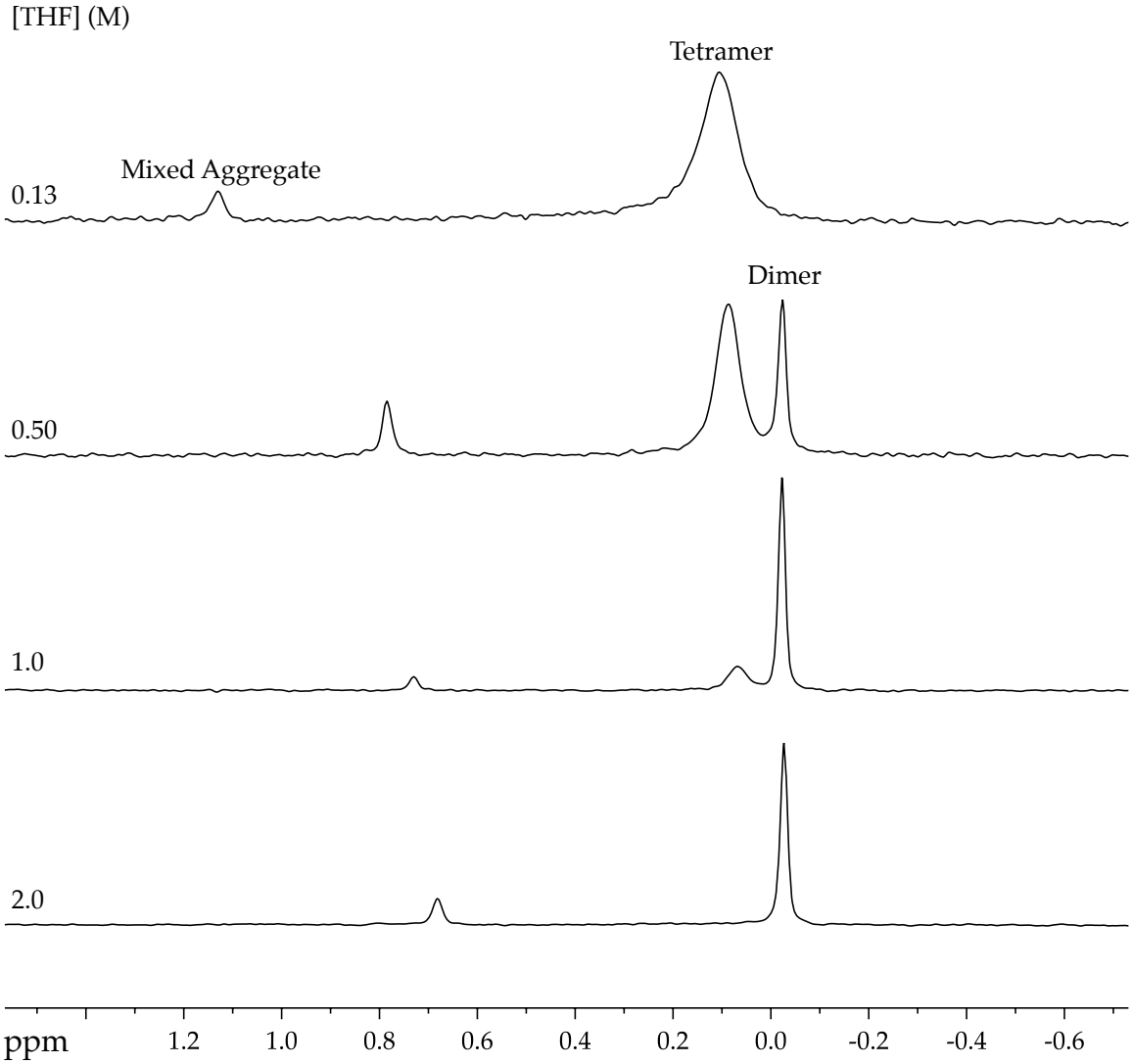


Figure 59. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**5** with varying concentrations of THF and toluene at –80 °C with 0.13 M [^{6}Li]LDA.

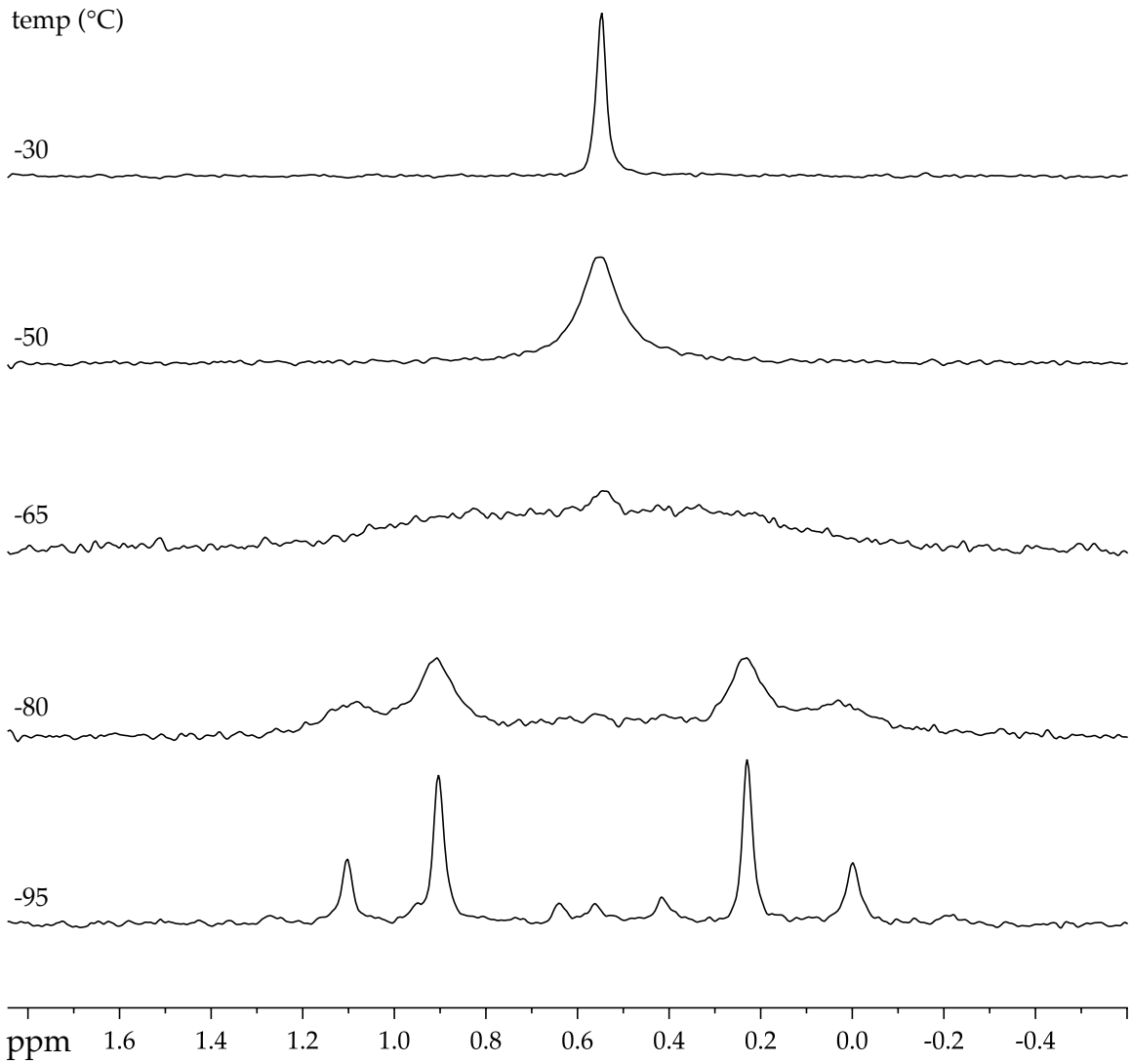


Figure 60. ^{6}Li NMR spectra for a 0.10 M solution of [^{6}Li]**2j** in 0.090 M THF and 0.060 M pyridine in toluene with 0.10 M [^{6}Li]LDA with varying temperature.

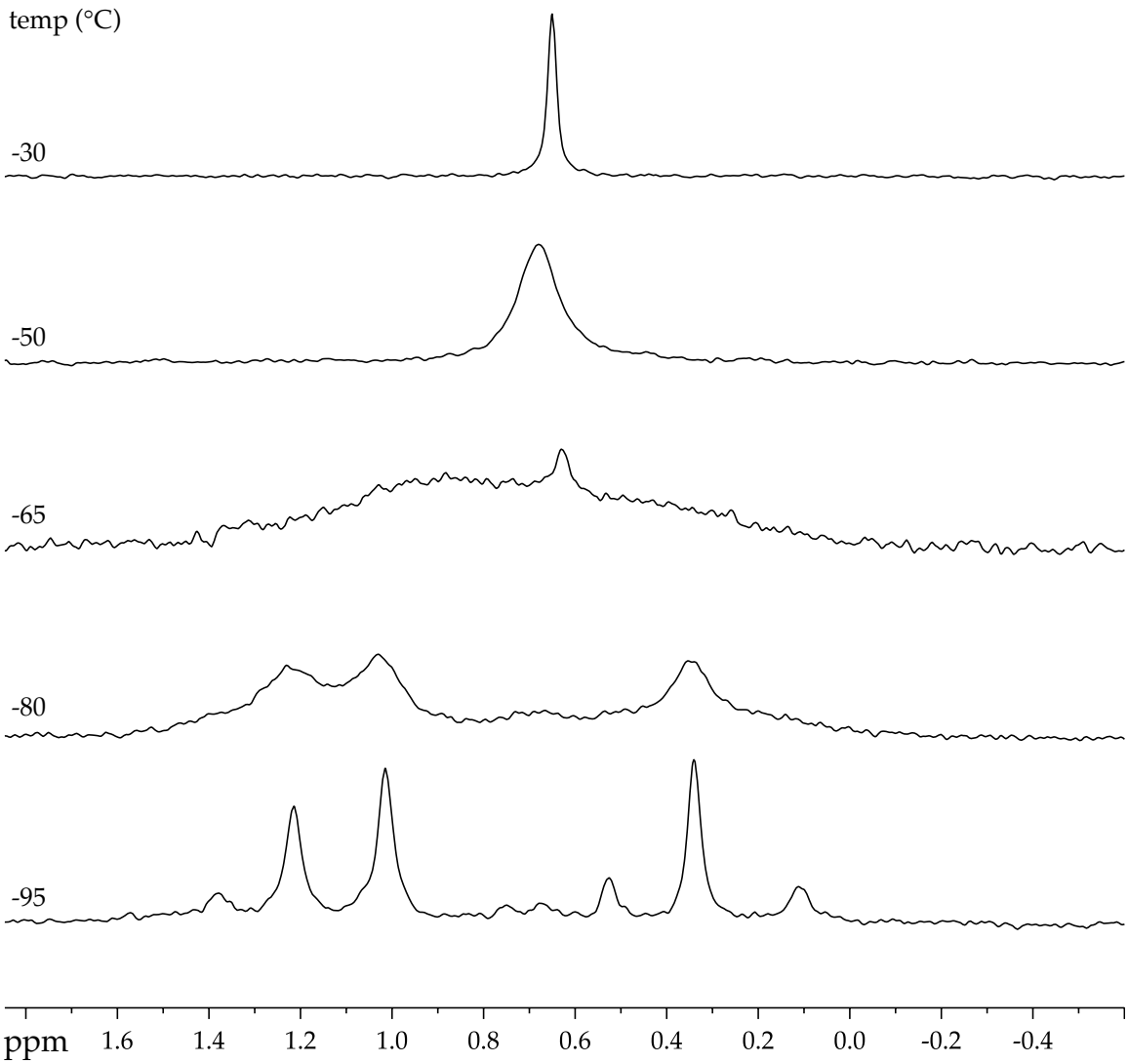


Figure 61. ^{6}Li NMR spectra for a 0.10 M solution of [^{6}Li]**2j** in 0.30 M THF and 0.20 M pyridine in toluene with 0.10 M [^{6}Li]LDA with varying temperature.

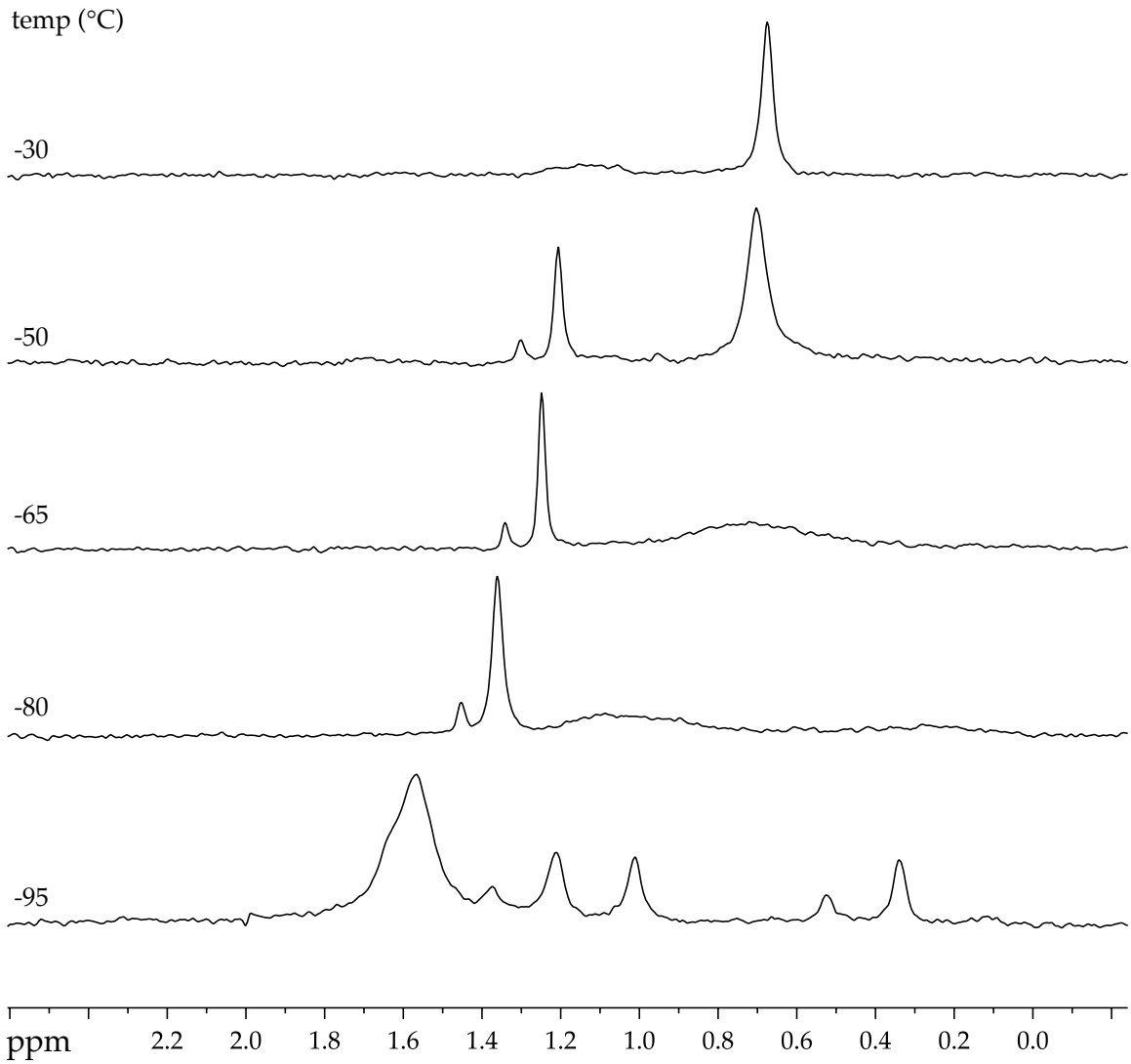


Figure 62. ^{6}Li NMR spectra for a 0.10 M solution of [^{6}Li]**2j** in 0.60 M THF and 0.40 M pyridine in toluene with 0.10 M [^{6}Li]LDA with varying temperature.

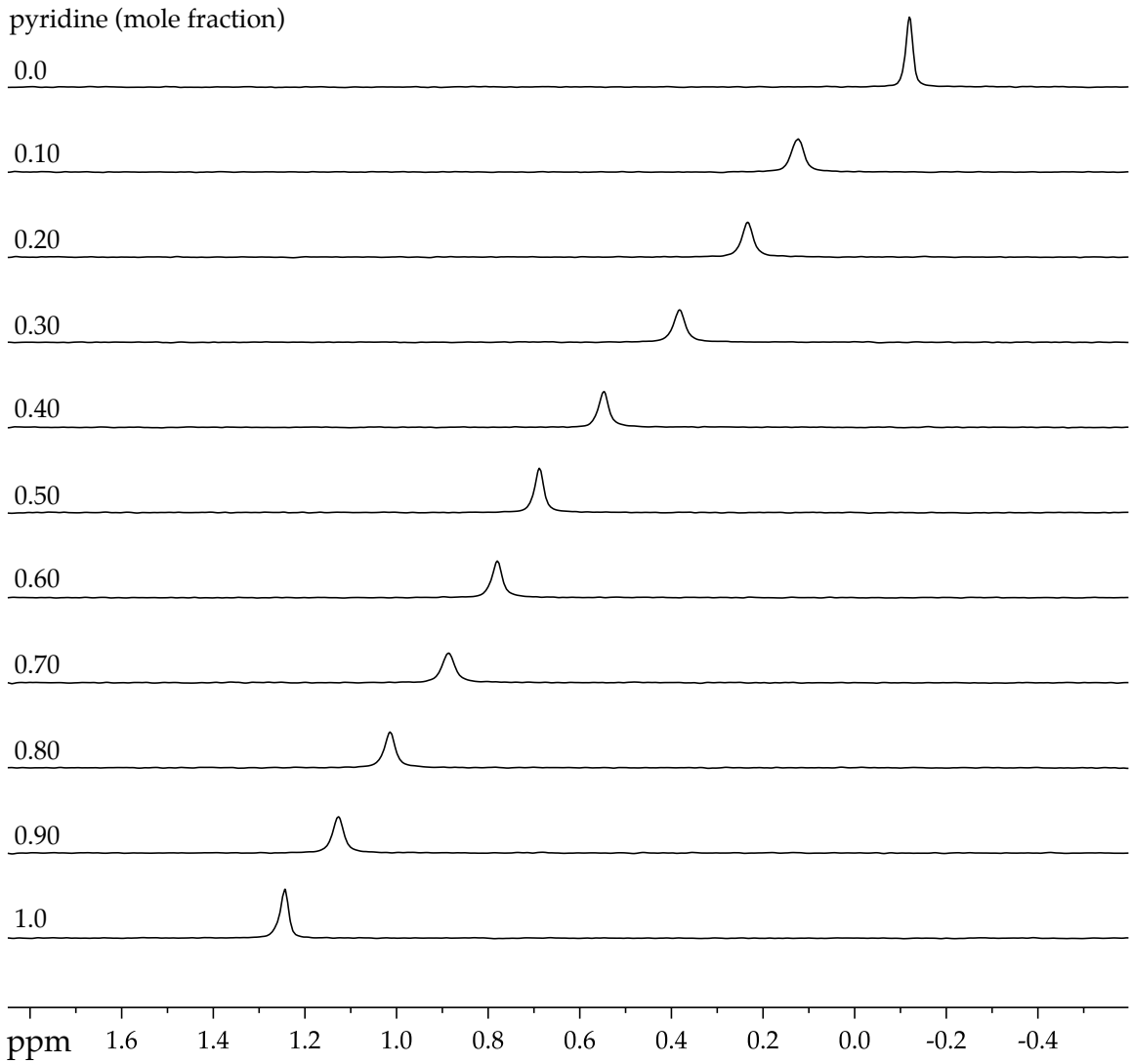


Figure 63. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** with 0.15 M total concentration of THF and pyridine in toluene at –30 °C with 0.11 M [^{6}Li]LDA.

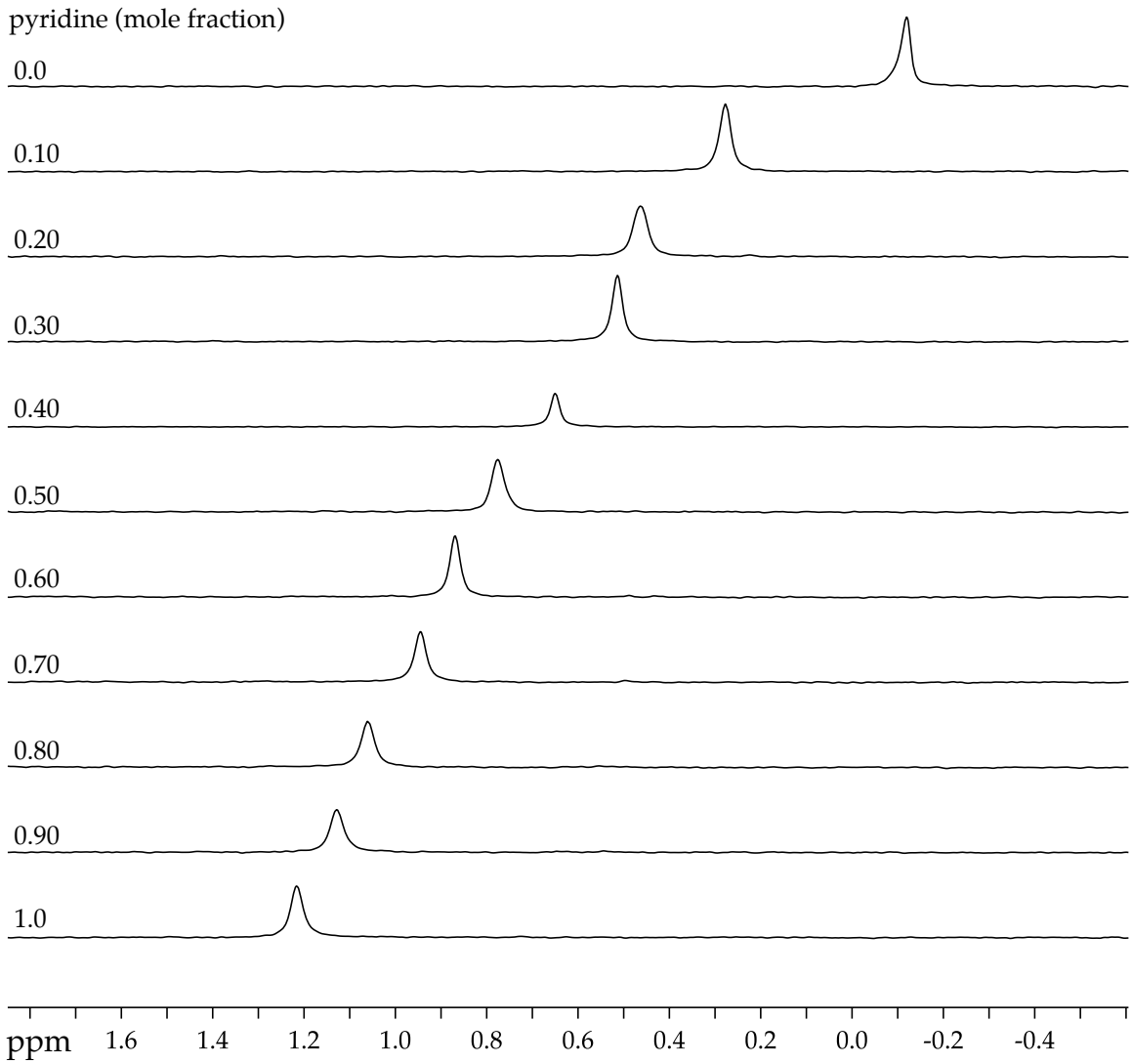


Figure 64. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** with 0.50 M total concentration of THF and pyridine in toluene at –30 °C with 0.11 M [^{6}Li]LDA.

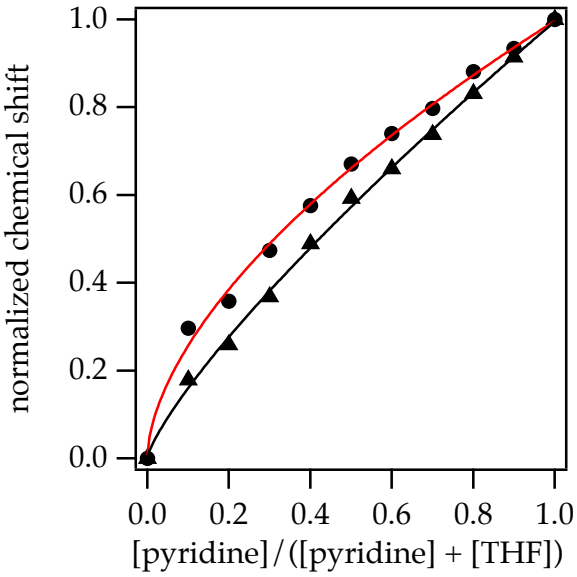


Figure 65. Plot of normalized chemical shift versus. [pyridine]/([pyridine] + [THF]) in toluene at –80 °C: the black line depicts a best–fit line for the ^{6}Li NMR chemical shifts of [^{6}Li]**2j** with 0.15 M total concentration of THF and pyridine mixtures in toluene at –30 °C; the red line depicts a best–fit line for the ^{6}Li NMR chemical shifts of [^{6}Li]**2j** with 0.50 M total concentration of THF and pyridine mixtures in toluene at –30 °C.

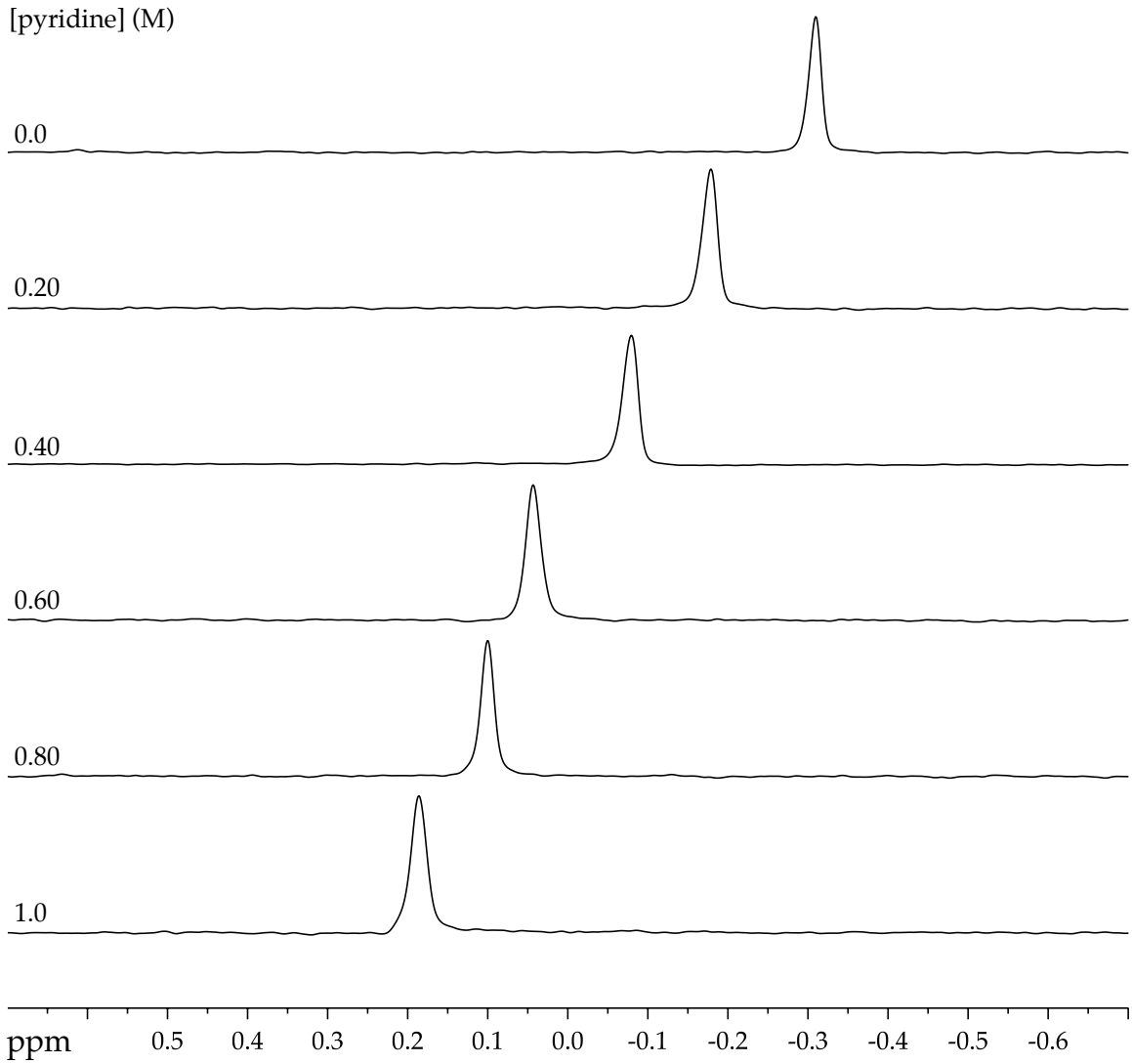


Figure 66. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**3** with varying amounts of pyridine in THF at –80 °C with 0.11 M [^{6}Li]LDA.

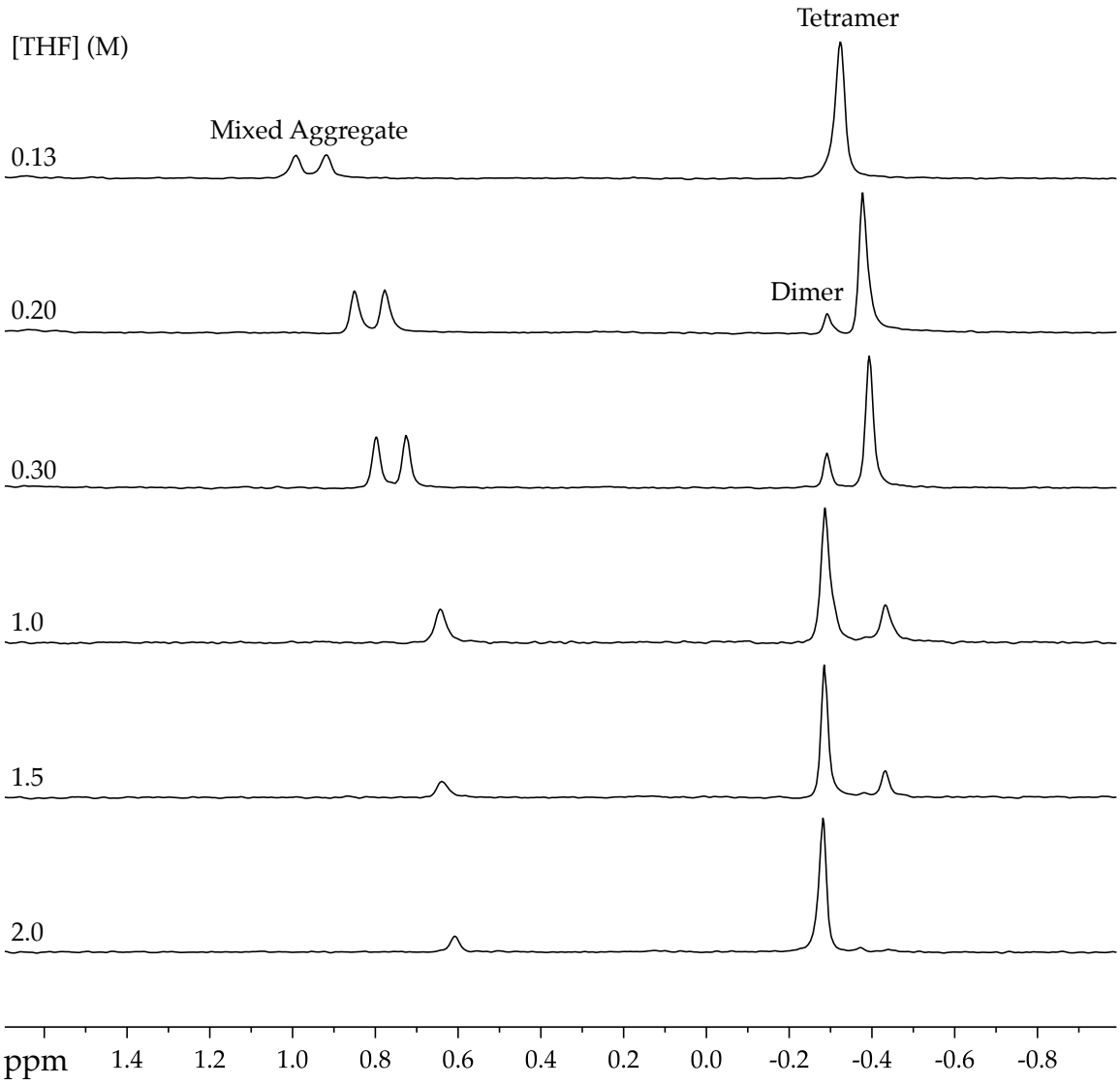


Figure 67. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2k** with varying amounts of THF in toluene at –80 °C. The top three spectra have 0.13 M [^{6}Li ,^{15}N]LDA; the bottom three spectra have 0.13 M [^{6}Li]LDA.

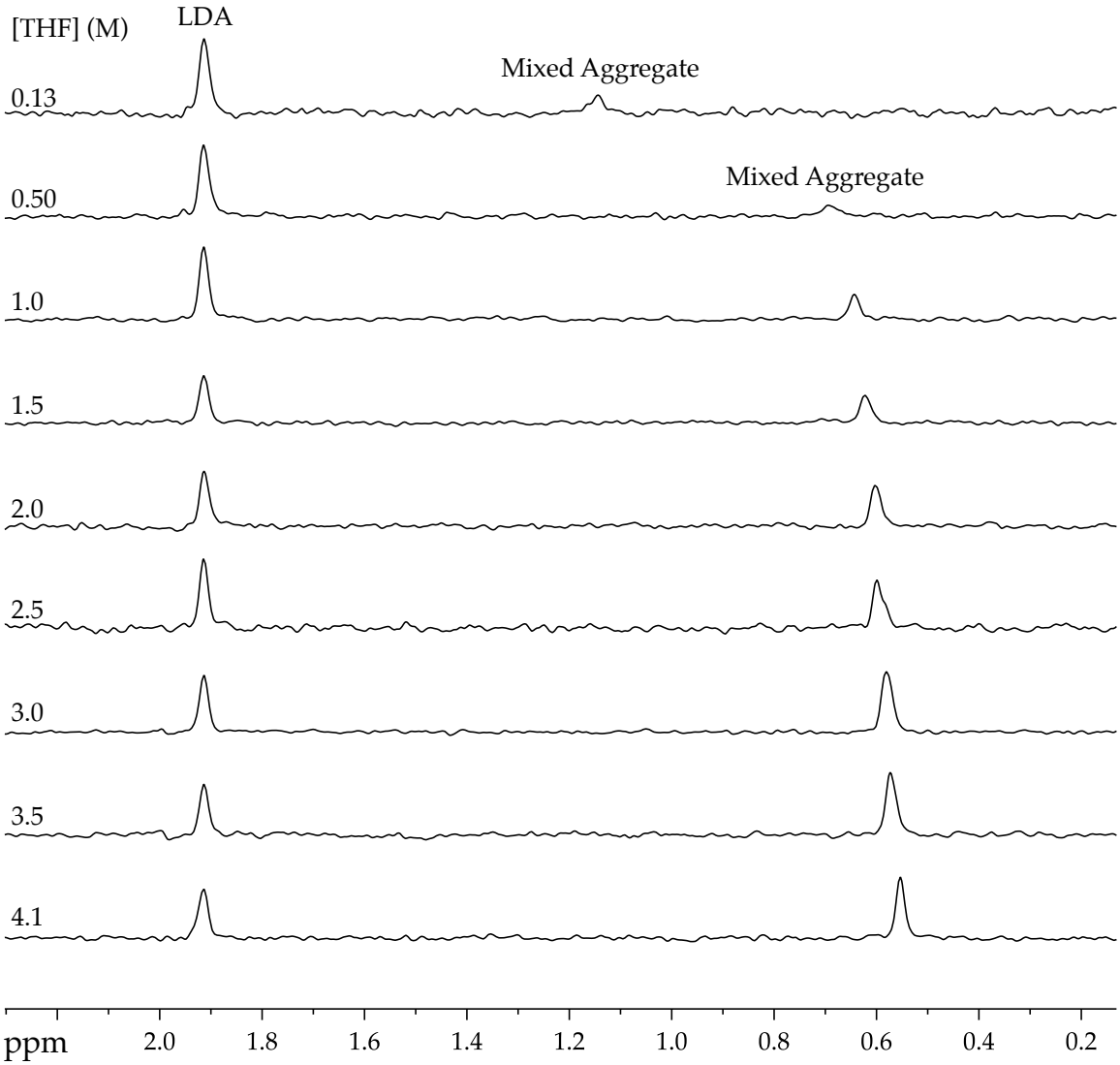


Figure 68. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**2j** with varying amounts of THF in toluene at –80 °C with 0.13 M [^{6}Li]LDA.

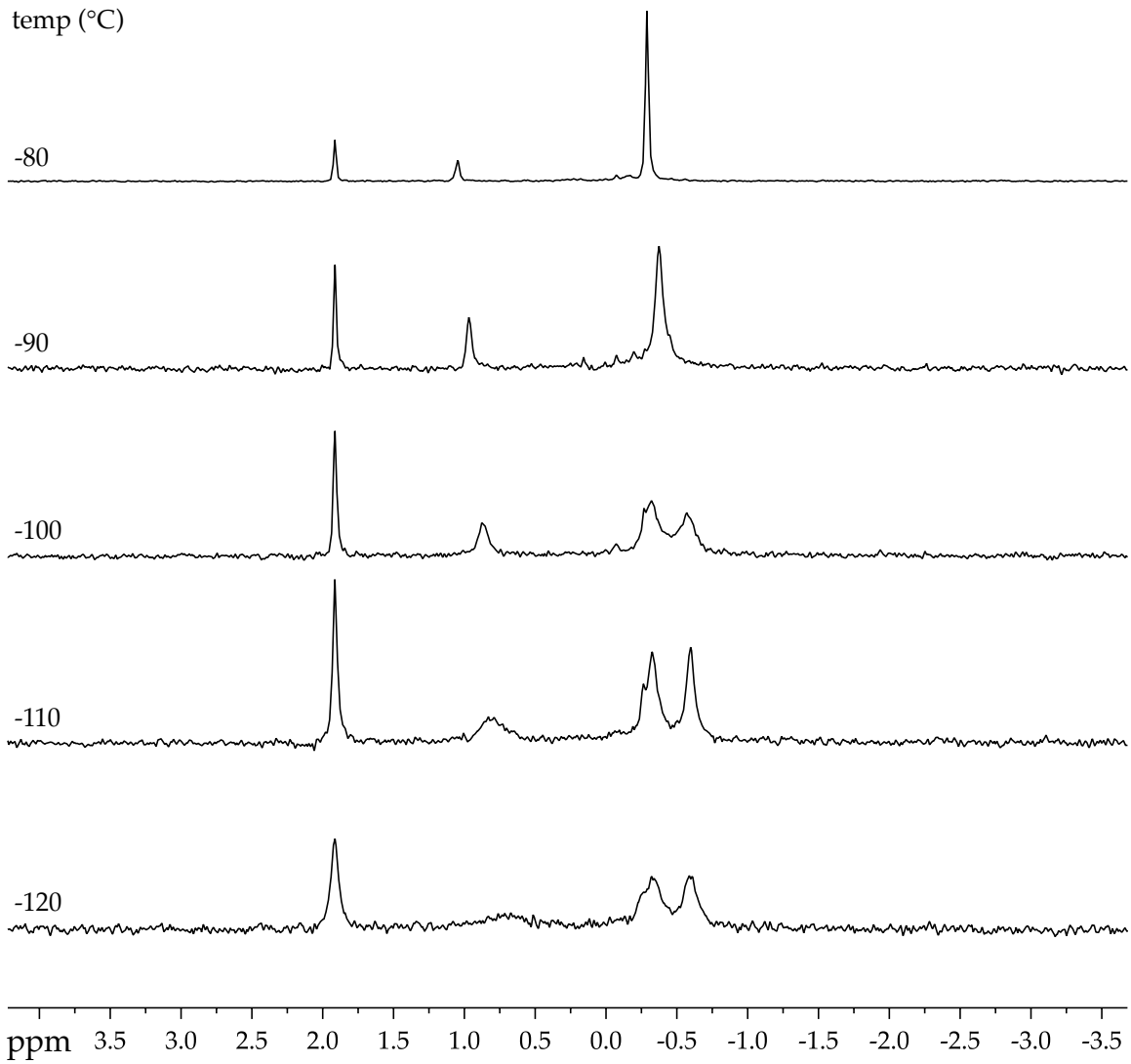


Figure 69. ^{6}Li NMR spectra of a 0.10 M solution of [^{6}Li]**2k** in 0.17 M THF and toluene with 0.13 M [^{6}Li]LDA recorded at varying temperatures.

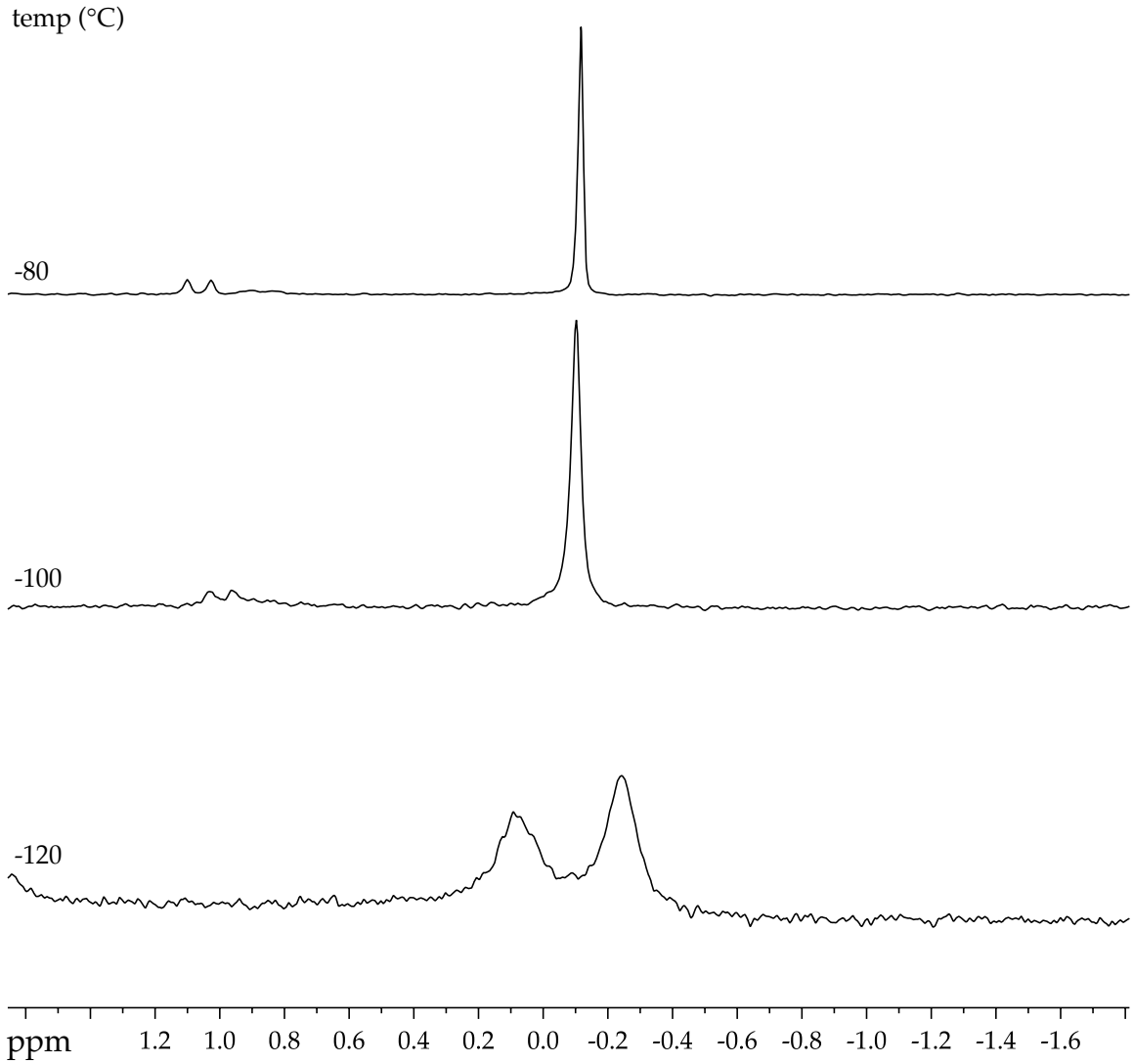


Figure 70. ^{6}Li NMR spectra of a 0.10 M solution of [^{6}Li]**2j** in 0.13 M THF and toluene with 0.11 M [^{6}Li]LDA recorded at varying temperatures.

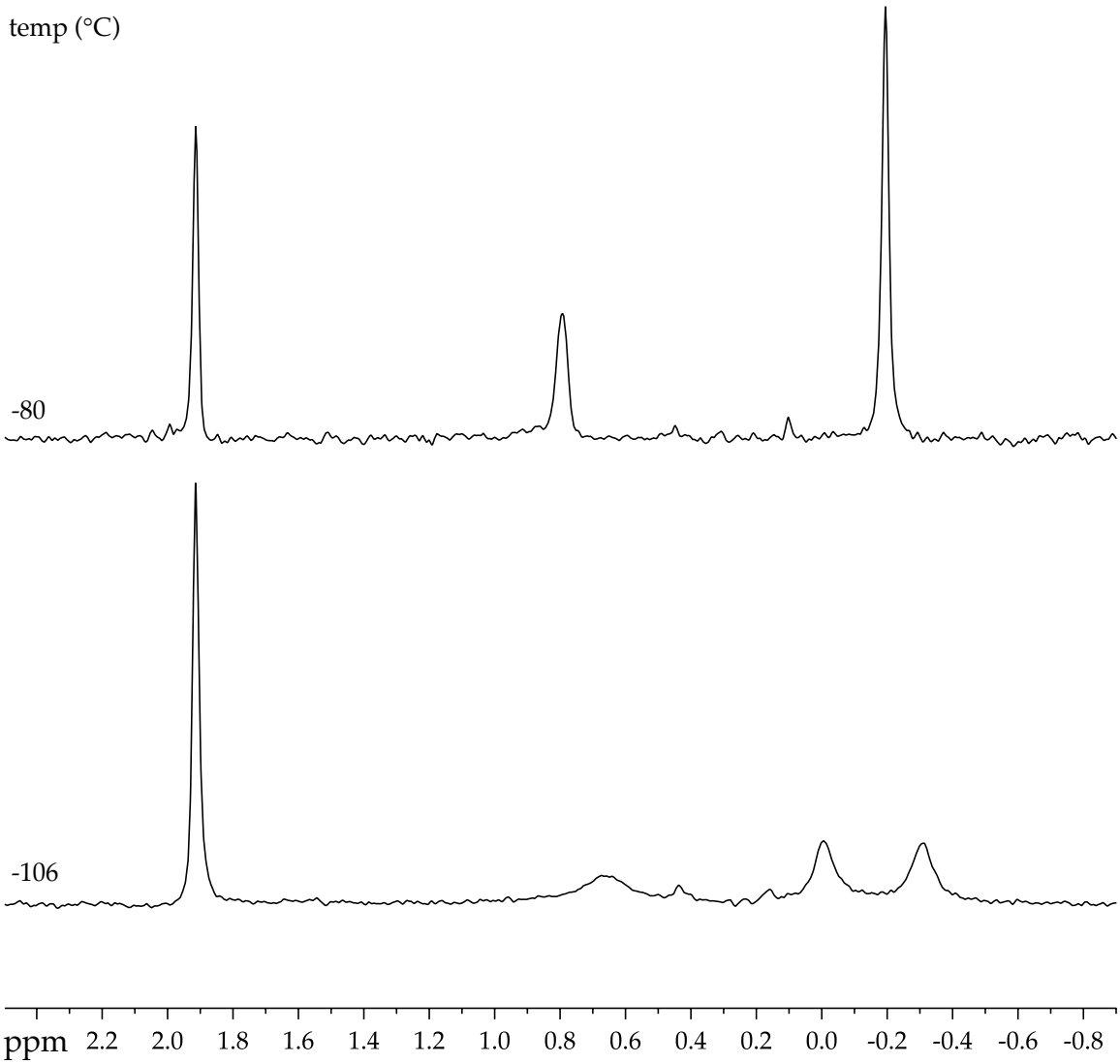


Figure 71. ^{6}Li NMR spectra of a 0.10 M solution of [^{6}Li]**2i** in 0.26 M THF and toluene with 0.2 M [^{6}Li]LDA recorded at varying temperatures.

Part 2: Derivation for Job Plot with relative integration vs intended mole fraction and Matlab code

$K_{eq}(1)=[THF_3Pyr][THF]/\{[THF_4][Pyr]\}$
$K_{eq}(2)=[THF_2Pyr_2][THF]/\{[THF_3Pyr][Pyr]\}$
$K_{eq}(3)=[THFPyr_3][THF]/\{[THF_2Pyr_2][Pyr]\}$
$K_{eq}(4)=[Pyr_4][THF]/\{[THFPyr_3][Pyr]\}$

The distributions of homo- and heterosolvated enolate tetramers are assumed to track as power functions of the pyridine and THF mole fractions. While the fit is superficially similar to that described previously for two subunits aggregating to form one or more ensembles, we substitute the measured mole fraction for the total mole fraction of solvent and consequently obviate parametric fitting. Accordingly,

$$[THF_4] = c\phi_0(1-\chi_{Pyr})^4$$
$$[THF_3Pyr] = 4c\phi_1(1-\chi_{Pyr})^3\chi_{Pyr}$$
$$[THF_2Pyr_2] = 6c\phi_2(1-\chi_{Pyr})^2\chi_{Pyr}^2$$
$$[THFPyr_3] = 4c\phi_3(1-\chi_{Pyr})\chi_{Pyr}^3$$
$$[Pyr_4] = c\phi_4\chi_{Pyr}^4$$

The c prefactor subsumes the concentration units and normalization such that $[enolate_4]_{total} = [THF_4]+[THF_3Pyr]+[THF_2Pyr_2]+[THFPyr_3]+[Pyr_4]$. Therefore,

$$c = \frac{[enolate_4]_{total}}{\left(\phi_0(1-\chi_{Pyr})^4 + 4\phi_1(1-\chi_{Pyr})^3\chi_{Pyr} + 6\phi_2(1-\chi_{Pyr})^2\chi_{Pyr}^2 + 4\phi_3(1-\chi_{Pyr})\chi_{Pyr}^3 + \phi_4\chi_{Pyr}^4\right)}$$

We wish to compute each of the equilibrium constants defined above, and do so by substituting in the fitting functions for each homo- and heterosolvate,

$$K_{eq}(1) = \frac{[THF_3Pyr][THF]}{[THF_4][Pyr]}$$
$$= \frac{4c\phi_1(1-\chi_{Pyr})^3\chi_{Pyr}[THF]}{\phi_0(1-\chi_{Pyr})^4[Pyr]}$$
$$= \frac{4\phi_1\chi_{Pyr}[THF]}{\phi_0(1-\chi_{Pyr})[Pyr]}$$

Similarly,

$$K_{eq}(2) = \frac{3\phi_2\chi_{Pyr}[THF]}{2\phi_1(1-\chi_{Pyr})[Pyr]}; K_{eq}(3) = \frac{2\phi_3\chi_{Pyr}[THF]}{3\phi_2(1-\chi_{Pyr})[Pyr]}; K_{eq}(4) = \frac{\phi_4\chi_{Pyr}[THF]}{4\phi_3(1-\chi_{Pyr})[Pyr]}$$

From the fit, $\phi_0 = 1; \phi_1 = 5.8; \phi_2 = 27; \phi_3 = 29; \phi_4 = 1$.
Assuming the absence of unsolvated enolate tetramers, one can compute the normalities of all species and thereby extract the equilibrium constants point-wise from the data employing the equations described above.

Table 1: Normalities of homo- and heterosolvated enolate tetramers corresponding to computed molarities of free solvent

[Pyr]	[THF]	[THF_4]	[THF_3Pyr]	[THF_2Pyr_2]	[$THFPyr_3$]	[Pyr_4]
0.000	0.400	0.100	0.000	0.000	0.000	0.000
0.022	0.378	0.021	0.044	0.035	0.000	0.000
0.058	0.343	0.006	0.031	0.053	0.010	0.000
0.100	0.304	0.000	0.020	0.061	0.020	0.000
0.142	0.264	0.000	0.008	0.057	0.029	0.006
0.187	0.220	0.000	0.003	0.050	0.038	0.009
0.230	0.179	0.000	0.000	0.037	0.046	0.017
0.275	0.134	0.000	0.000	0.027	0.048	0.025
0.319	0.089	0.000	0.000	0.017	0.042	0.041
0.357	0.048	0.000	0.000	0.000	0.030	0.070
0.400	0.000	0.000	0.000	0.000	0.000	0.100

Table 2: Computed equilibrium constants corresponding to Table 1

$K_{eq}(1)$	$K_{eq}(2)$	$K_{eq}(3)$	$K_{eq}(4)$
—	—	—	—
45.2	13.6	1.39	0.437
34.1	10.3	1.05	0.330
30.2	9.09	0.932	0.292
28.8	8.68	0.889	0.278
27.4	8.25	0.845	0.265
27.0	8.14	0.834	0.261
26.3	7.91	0.811	0.254
25.9	7.79	0.799	0.250
28.1	8.47	0.868	0.272
—	—	—	—

Averaging the computed equilibrium constants gives $K_{eq}(1)$=30.3; $K_{eq}(2)$=9.14; $K_{eq}(3)$=0.936; $K_{eq}(4)$=0.293.

Data1.m

```
XA = [0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1]';

Expt_Populations =[1 0         0         0         0
0.21189921     0.43967411     0.34842669     0         0
0.05960177     0.31301703     0.53031531     0.09706589     0
0         0.19656513     0.60692209     0.19651278     0
0         0.07955415     0.5669922      0.29205193     0.06140172
0         0.03264284     0.49517675     0.37904511     0.0931353
0         0         0.37184265     0.45548373     0.17267361
0         0         0.2662237      0.48330307     0.25047323
0         0         0.16830449     0.42363026     0.40806525
0         0         0         0.29621612     0.70378193
0         0         0         0         1
];

peak_assignment = [1  2  3  4  5];

phi = [ 1  5.796  27  29  26 ];


%To see the plot:  try_fit(XA, phi, peak_assignment, Expt_Populations)

%To fit the plot:  [phi_new, error] = refine_fit(XA,phi, peak_assignment,
Expt_Populations)
```

Errorofmodel.m

```
function [mean_error, pop_error] = Error_of_Model(XA,phi, peak_assignment,
Expt_Populations, Expt_weights)

   if (nargin<5) % If no info on data given assume all points equally precise.
            Expt_weights=ones(size(Expt_Populations));
   end

   Concentrations = multimers(XA,phi);
```

```
    PP = Populations(Concentrations, peak_assignment);

    % Compute the mean error.

    diff = PP - Expt_Populations;

    mean_error = sqrt(sum(sum(diff.*diff.*Expt_weights)) / sum(sum(Expt_weights)));


    % Compute the error for each population independently.

    pop_error = sum(diff.*Expt_weights,1) ./ sum(Expt_weights,1);

    pop_error(2,:) = sqrt(sum(diff.*diff.*Expt_weights,1) ./ sum(Expt_weights,1));
```

Multnotpara.m

```
function Concentration = multimer(XA, phi)

if (nargin<2)
    phi = [ 1 1 20 400 20 1 1];
end

for j=1:length(XA)
   % Use the function bisect to find Cconc
   Concentration(j,:) = bisect(XA(j),phi);
end

function Conc = bisect(XA, phi)

    tolerance = 1e-6; % Amount XA may differ by an end of bisection..
    Amax = 1; Amin = 0;
    [Xmin, Conc]=Cparametric(Amin, phi);
    [Xmax, Conc]=Cparametric(Amax, phi);

    while ((Xmax-XA)>tolerance) % While not close enough, continue to bisect difference
of rmin and rmax.
        Atest = (Amin+Amax)/2;
        [Xtest, Conc]=Cparametric(Atest,phi);
        if (Xtest>XA)
           Amax = Atest; Xmax=Xtest;
       else
           Amin = Atest; Xmin=Xtest;
       end
   end
```

```
function [XA, Concs] = Cparametric( A, phi)

N = length(phi)-1;
B = 1-A;
Concs(1)= B^N*phi(1);
Concs(N+1)=A^N*phi(N+1);
Mn=1;

for k=2:N
   idx=k-1;
   Mn = Mn * (N+1-idx)/idx;
   Concs(k) = phi(k)*A^idx*B^(N-idx)*Mn;
end

Concs = Concs / sum(Concs);

XA = A;
```

Populations.m

```
function result = Populations(Concentrations, peak_assignment)

   result = zeros(size(Concentrations,1),max(peak_assignment));
   N = size(Concentrations,2);

   for j=1:N % Go through each type of aggregate and add to correct NMR peak.
      idx = peak_assignment(j);
      result(:,idx) = result(:,idx) + Concentrations(:,j);
   end
```

Refinefit.m

```
function [phi_new, error] = refine_fit(XA,phi, peak_assignment, Expt_Populations)

if (nargin<5)
    Expt_weight = ones(size(Expt_Populations));
 end


N = length(phi)-1;

param = [ 2:(N+1)];

step_size = 0.1*phi(param),

N_no_progress = 0;

N_max_trials = 30;
```

```
[error_best, temp] = Error_of_Model(XA,phi, peak_assignment, Expt_Populations) ; % Initial Quality of Fit

fprintf(1,'\n Initial Error of Fit = %f percent.\n', error_best * 100);

while (N_no_progress < N_max_trials)

   flag = 0;
   for k=1:length(param)

         phi_testr = phi;

         phi_testr(param(k))=abs(phi(param(k)) + step_size(k));

         [error_testr, temp] = Error_of_Model(XA,phi_testr, peak_assignment, Expt_Populations, Expt_weight);

         phi_testl = phi;

         phi_testl(param(k))=abs(phi(param(k)) - step_size(k));

         [error_testl, temp] = Error_of_Model(XA,phi_testl, peak_assignment,Expt_Populations, Expt_weight);

       if (error_testr<error_best)
            error_best=error_testr; phi=phi_testr; step_size(k) = step_size(k) * 1.5;
            N_no_progress=0;
      elseif     (error_testl <error_best)
            error_best=error_testl; phi=phi_testl; step_size(k) = step_size(k) * 1.5;
            N_no_progress=0;
      else
         flag = flag + 1;
      end
   end



   if (flag>2)
      step_size = step_size * (0.75 + 0.25*rand);
      N_no_progress=N_no_progress+1;
   end

   fprintf(1,'\nError - %f , Last Good Step - %d , Mean Step Size - %f \n ',error_best, N_no_progress, 100*mean(step_size./phi(param)));
```

```
    fprintf(1,' Phi - %f',phi);

    end

    error=error_best;

    phi_new = phi;
```

Tryfit.m

```
function try_fit(XA, phi, peak_assignment, Expt_Populations)

if (nargin<5)
            Expt_weights=ones(size(Expt_Populations));
    else
            Expt_weights = 1./( Expt_Errors + mean(mean(Expt_Errors)));
    end

hold on ; cscheme='bgrmkcybgrmkcy'; axis([0 1 0 1]); xlabel('X_A'); ylabel('Mole
Fractions');

     for j=1:size(Expt_Populations,2)

          if (nargin<5)

             plot(XA, Expt_Populations(:,j),sprintf('%so',cscheme(j)));

          else

             errorbar(XA, Expt_Populations(:,j), Expt_Errors(:,j),sprintf('%so',cscheme(j)));

          end

     end

XAc = [0:0.01:1]; TP=Populations(multnonpara(XAc,phi), peak_assignment);

     for j=1:size(TP,2)
        plot(XAc,TP(:,j),sprintf('%c',cscheme(j)) );
     end

[mean_error, pop_error] = Error_of_Model(XA,phi, peak_assignment, Expt_Populations,
Expt_weights);

    N = length(phi)-1;

          fprintf(1,'\nThe Mean mismatch is %f peAcent.\n', mean_error*100);
```

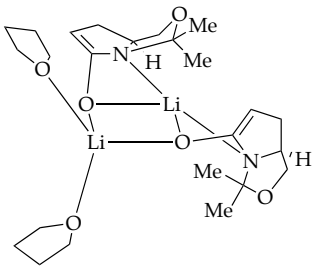
```
        for j=1:size(pop_error,2)

        fprintf(1,'Predicted value of species A%dB%d +A%dB%d exceeds measurement
by %f percent and mean square error of %f percent.\n ',j-1,N-j+1,N-j+1,j-
1,pop_error(1,j)*100,pop_error(2,j)*100);

end
```

Part 2: Computational Studies

Chart 1



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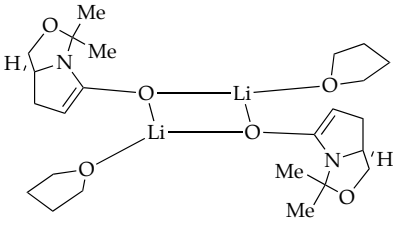
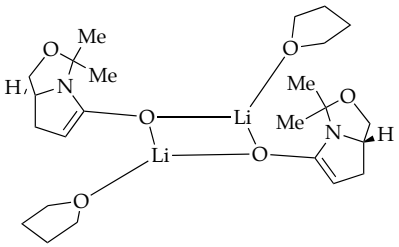


2



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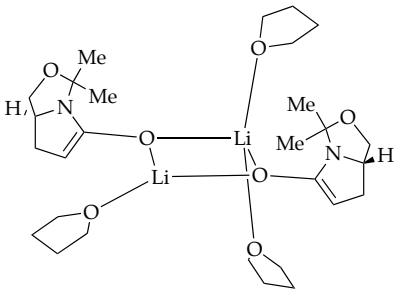

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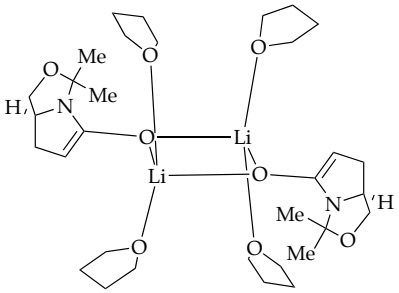
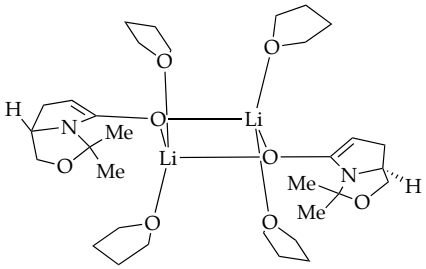
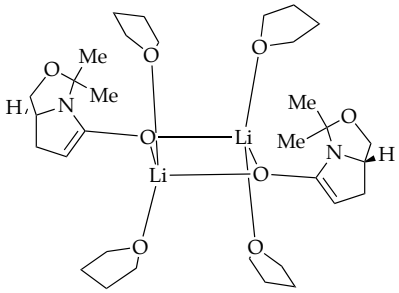


8a

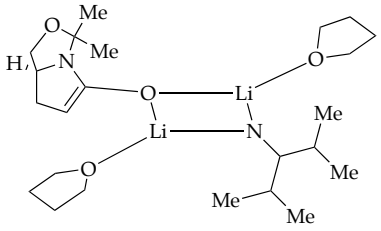


8b

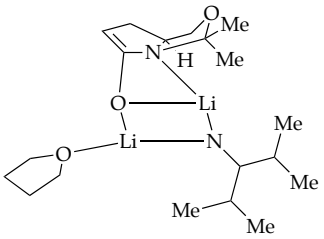


7

Chart 2



6a



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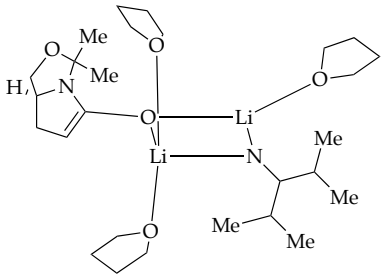
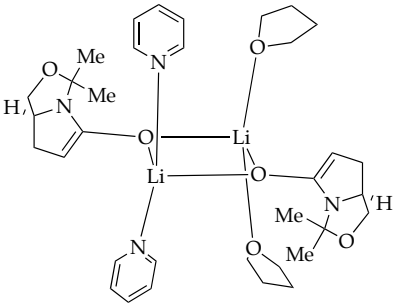


6b



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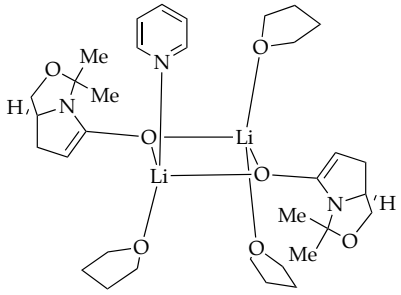

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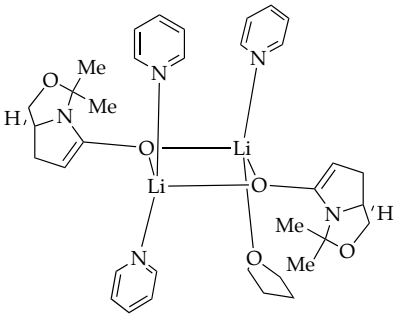

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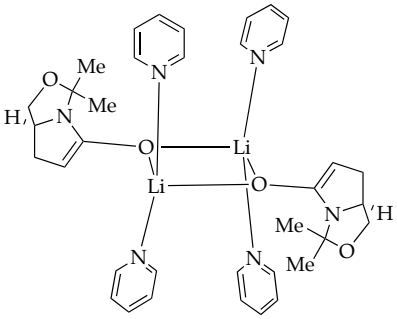
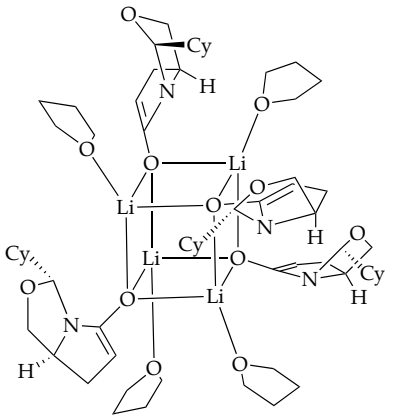
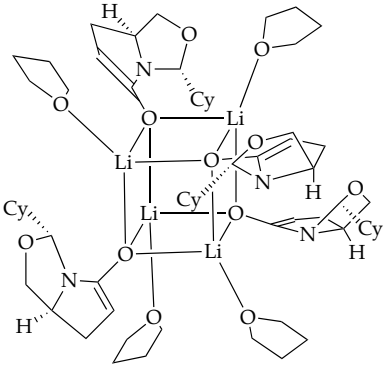


14

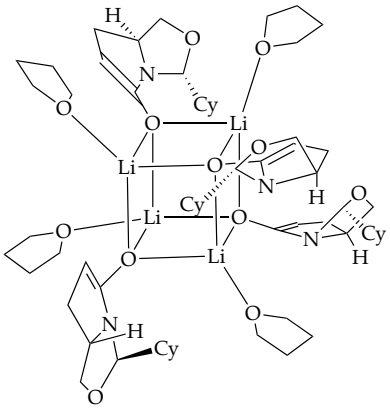
Chart 3



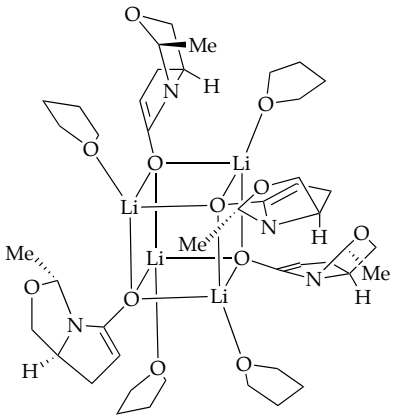
7a



7b



7c



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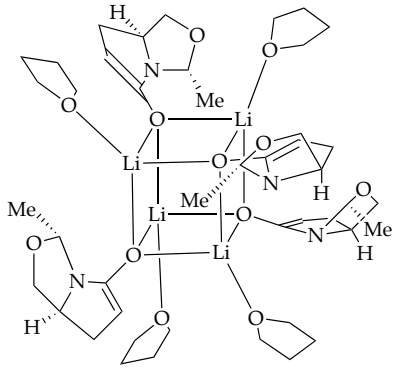

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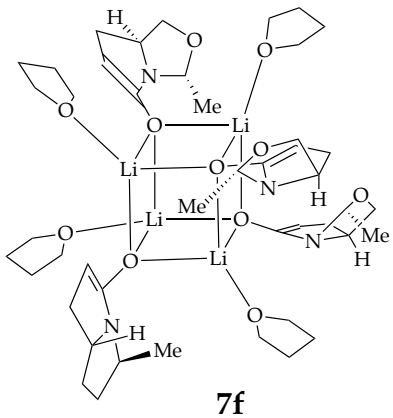

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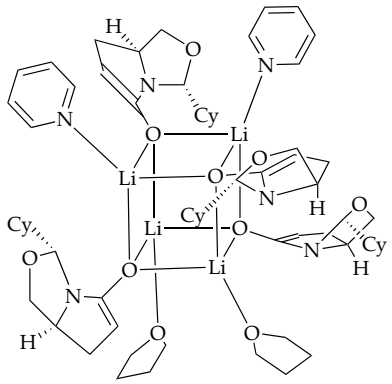
Chart 4



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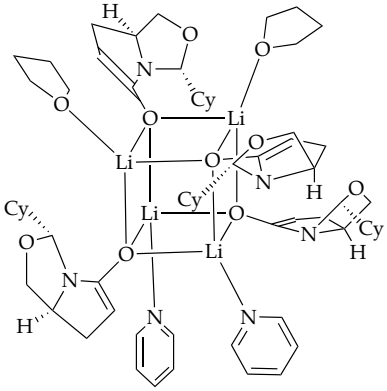

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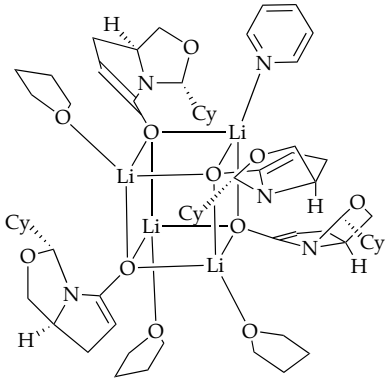

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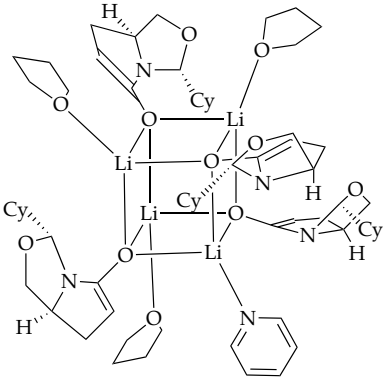

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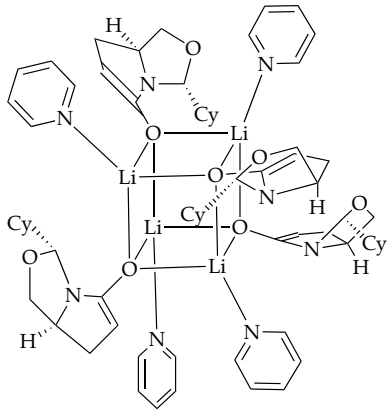

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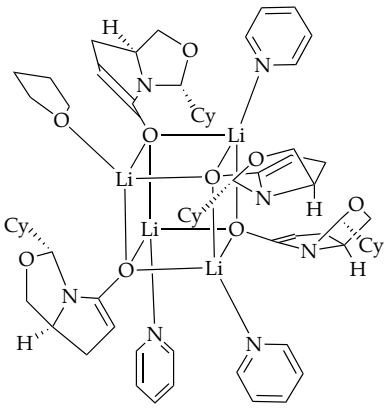
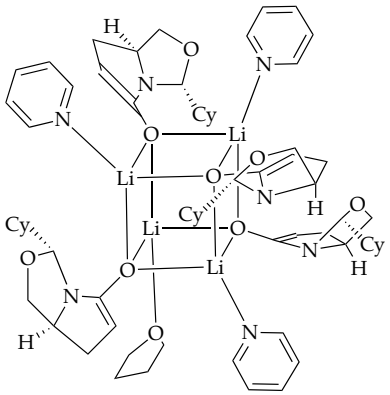
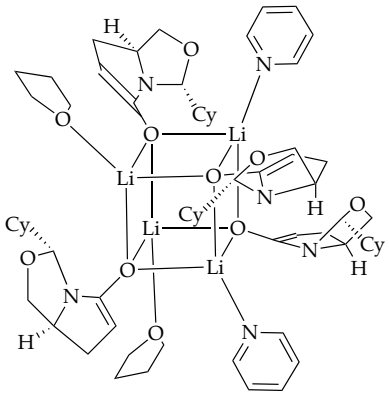


26

Chart 4 (Continued)

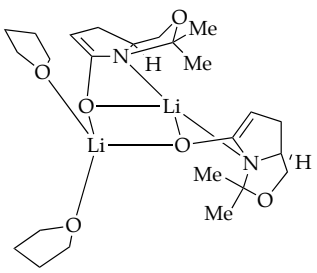


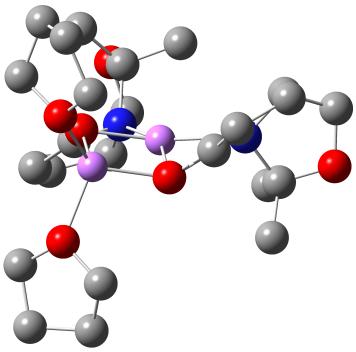
27



28

Table 2. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the L-pyroglutaminol, hemi-aminal dimers at –78 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

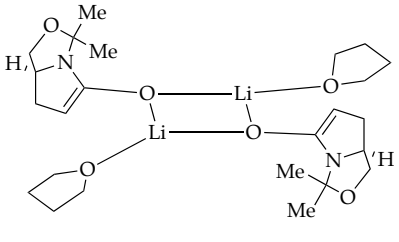


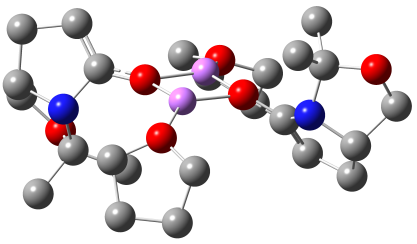


1
G = –1509.800081
G_{MP2} = –1514.095200

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-0.30519000	-6.02099000	2.39978200
C	1.16383000	1.00998400	0.20323200	H	0.10480800	-8.04194200	-1.59303800
C	2.35726300	0.21404600	-0.25857800	H	0.42721900	-7.43033700	-3.21614800
C	1.97320000	-0.89807500	-0.92992000	H	2.70473100	-7.03848500	-1.85499900
O	2.60620200	-1.90249800	-1.46551500	Li	1.15813400	-3.11322300	-0.93758600
Li	3.74032200	-3.36185700	-0.95056700	N	0.49927000	-1.01750000	-0.97685700
O	2.35142200	-4.57168500	-0.42193100	C	-0.16075800	-0.67903700	-2.30641900
C	1.55225200	-5.43782300	-0.97780800	O	-0.89579600	0.53066900	-2.06710100
C	1.73805400	-6.58309600	-1.67666900	C	-1.23979100	0.55850900	-0.68908200
C	0.42520400	-7.14813800	-2.15441700	H	-2.13115000	-0.05533600	-0.48441700
C	-0.54804100	-5.95892400	-1.91737000	H	-1.46001300	1.59460900	-0.41682900
H	-0.71145100	-5.40938600	-2.85122000	C	-1.14054500	-1.79666200	-2.68709300
N	0.12290600	-5.06347400	-0.92418700	H	-0.61077800	-2.73784600	-2.87479900
C	-0.58613900	-5.30279800	0.40079900	H	-1.86152000	-1.97512300	-1.88316600
O	-1.51035900	-6.37172100	0.14756900	H	-1.68905500	-1.52116800	-3.59432300
C	-1.86052700	-6.31688400	-1.22816500	C	0.80953700	-0.37773800	-3.44495900
H	-2.63953500	-5.56098100	-1.41532400	H	1.50694800	0.40949500	-3.14829700
H	-2.25023900	-7.29712000	-1.51680400	H	1.38136300	-1.26541900	-3.72388600
C	-1.36827300	-4.04238800	0.79211200	H	0.23531100	-0.03260500	-4.31032400
H	-1.95639300	-4.23077200	1.69678500	H	3.38881100	0.49826500	-0.08866900
H	-0.69018200	-3.20357900	0.98735100	H	0.99965000	1.92985300	-0.38294700
H	-2.04834900	-3.74178300	-0.01089900	H	1.21973400	1.31701700	1.25659600
C	0.31905100	-5.77239300	1.53591800	H	-0.24458900	-0.49446400	0.94685700
H	0.87198800	-6.66487300	1.23273400	O	4.87770100	-3.68457500	-2.56260500
H	1.03339900	-4.99656600	1.81961100	C	5.00289900	-2.60094800	-3.51169900

C	4.63289800	-3.21402200	-4.85977700	C	4.78940800	-4.25589400	1.66994000
C	5.21074600	-4.63238400	-4.72769500	O	4.91441600	-3.22723000	0.65989800
C	4.95916400	-4.95889600	-3.24839900	C	5.26497600	-1.96332700	1.27559800
H	5.76455300	-5.54798500	-2.79676800	C	5.48200600	-2.26230500	2.76459100
H	4.00936500	-5.48259400	-3.09728700	C	4.59857400	-3.50065100	2.98363700
H	4.73775900	-5.35752800	-5.39662800	H	4.89054500	-4.09268900	3.85649300
H	6.28544700	-4.62450300	-4.94448200	H	3.54864300	-3.20766700	3.10235900
H	3.54276900	-3.25036600	-4.97089900	H	6.53259700	-2.50688900	2.96119000
H	5.04614800	-2.65593200	-5.70557100	H	5.20800700	-1.41498200	3.40025100
H	6.04133500	-2.23981100	-3.50864500	H	4.43491400	-1.26709200	1.11452400
H	4.33434600	-1.80598900	-3.17669600	H	6.15937400	-1.57144000	0.77995400
H	5.71108500	-4.85472600	1.68399700	H	3.94648400	-4.88666300	1.38165200





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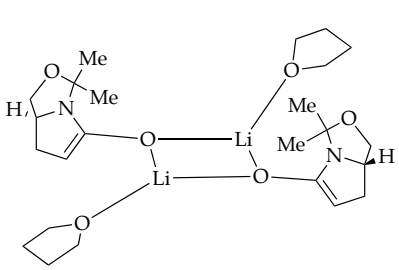
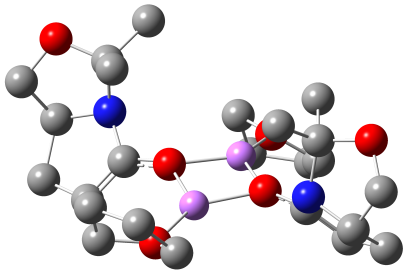
G = –1509.792741
G_{MP2} = –1514.099816

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	9.44234500	-1.13782900	0.43181400
C	0.26472100	0.23310400	1.50177400	C	8.28597400	2.06530700	1.13904900
C	1.66869800	0.76697400	1.48286400	H	8.28078200	3.01370400	0.59161600
C	2.25125000	0.53884400	0.27976600	H	7.25679800	1.82083700	1.40602800
O	3.48993100	0.74278800	-0.09358100	H	8.87723300	2.19501200	2.05088900
Li	4.50840700	2.24664500	-0.38974400	H	9.23435000	2.82283500	-3.46768900
O	6.08426800	1.34291000	-0.71295700	H	8.68154200	1.28947500	-4.12489900
C	7.15275600	1.47640600	-1.46246600	H	6.49046500	2.55620800	-3.21179300
C	7.30935300	2.12247600	-2.64845200	Li	5.05621500	-0.15550200	-0.36895500
C	8.68983100	1.89931500	-3.20893300	O	5.30079000	-2.00589000	-0.75406200
C	9.39998400	1.13450600	-2.06200900	C	4.16031900	-2.83325600	-1.09480900
H	9.89585900	0.22467500	-2.41995700	C	4.42364400	-3.35587600	-2.52903800
N	8.34747100	0.78160200	-1.06905100	C	5.82122800	-2.79422300	-2.89003900
C	8.93322900	0.95639500	0.29856800	C	6.42690300	-2.47686900	-1.52416000
O	10.3103820	1.31466000	0.05967400	H	7.17926300	-1.68392800	-1.51909400
C	10.3804070	1.94129000	-1.21263200	H	6.83962700	-3.37580800	-1.04386700
H	11.4178610	1.89246000	-1.55705400	H	6.42712300	-3.50077600	-3.46490600
H	10.0714960	2.99846000	-1.16224900	H	5.73011700	-1.87232500	-3.47419600
C	8.95837600	-0.37462400	1.04834700	H	4.42159100	-4.45021100	-2.54401600
H	9.51559500	-0.27575500	1.98642200	H	3.65777500	-3.01701100	-3.23244200
H	7.93867400	-0.70108500	1.27951700	H	3.26948000	-2.20657000	-0.99981800

H	4.09667100	-3.65421400	-0.37037900	O	0.19876600	1.50212200	-1.85114600
O	3.96443900	4.04607400	-0.71565000	C	-0.64317100	1.21208400	-0.73472000
C	4.82250800	4.97649800	-1.41368900	H	-1.66412200	0.98359000	-1.07155300
C	3.92345700	5.56606000	-2.49491100	H	-0.67986600	2.10061600	-0.09482100
C	2.58309500	5.70856500	-1.74935200	C	0.47525400	-0.69960300	-2.86218600
C	2.58936000	4.52510900	-0.76111700	H	1.17951900	-1.52170800	-3.03010200
H	2.28858200	4.81826200	0.24972400	H	-0.41776700	-1.11445400	-2.38655900
H	1.96117100	3.69152000	-1.08692000	H	0.18107900	-0.28343400	-3.83095400
H	2.54997200	6.66094900	-1.20890500	C	2.34530200	0.95275800	-2.73888100
H	1.71978700	5.67507400	-2.41953900	H	2.76022100	1.82175000	-2.23070000
H	4.29901300	6.51610000	-2.88633800	H	3.12888200	0.19754400	-2.83634600
H	3.83175200	4.86175900	-3.32952500	H	2.02743700	1.25647100	-3.74194900
H	5.16897200	5.74887100	-0.71254200	H	2.21567300	1.09637000	2.35832300
H	5.68464400	4.41378300	-1.78211000	H	-0.48763200	0.91041800	1.93266300
N	1.33914300	-0.12064800	-0.64213800	H	0.17938100	-0.71439300	2.05828100
C	1.12869000	0.39995200	-2.00242800	H	-0.58960700	-0.90470300	-0.17251700





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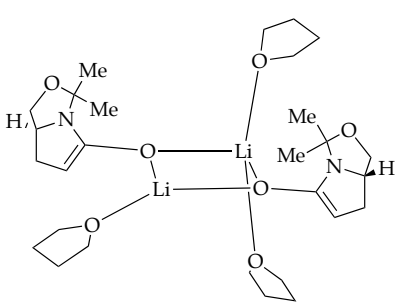
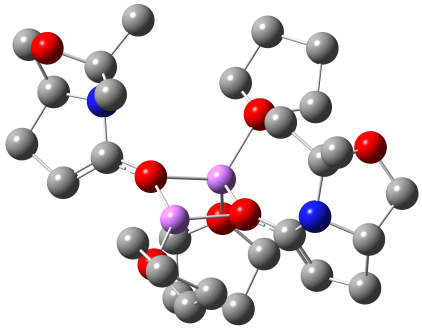
G = –1509.790487
G_{MP2} = –1514.100633

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	8.33826800	-0.61514400	2.28356400
C	0.25859900	-0.46376800	-1.45770100	H	8.49073300	-0.63060900	3.36835400
C	1.75552300	-0.34446400	-1.58027900	H	7.36650000	-1.06773600	2.05763100
C	2.29203600	0.23620700	-0.47406200	H	9.11404400	-1.22904100	1.81404700
O	3.52863400	0.60058500	-0.23397000	C	7.34812300	1.70129700	2.45139400
Li	5.18013700	-0.02978700	-0.76939900	H	7.36693400	2.71435600	2.04033300
O	6.11392300	1.48568000	-0.28954900	H	6.34209800	1.29012300	2.34430900
C	7.39944100	1.71872200	-0.40969300	H	7.59977000	1.75266400	3.51535000
C	8.05837100	2.66274000	-1.12115700	H	9.97124600	3.33839600	-0.29804300
C	9.54793800	2.54105900	-0.93289700	H	10.1163070	2.55772000	-1.87272100
C	9.67098300	1.14790300	-0.25481300	H	7.57504700	3.38834100	-1.76534600
H	9.98289700	0.40205200	-0.99592900	Li	4.45747800	2.17048900	0.07435900
N	8.31054200	0.80287700	0.25483900	O	5.66958900	-1.75080800	-1.42414600
C	8.38523500	0.82538200	1.75273000	C	4.75227800	-2.86036800	-1.47708100
O	9.66522600	1.40803000	2.06227200	H	4.80382900	-3.31903300	-2.47532400
C	10.5467110	1.08051600	0.99861500	C	5.26206900	-3.81168100	-0.39188800
H	10.9817100	0.07737800	1.13538000	C	6.79980800	-3.59849400	-0.41930100
H	11.3607710	1.81139800	0.99718500	C	6.99368300	-2.30569100	-1.24681900

H	7.59586100	-1.53546300	-0.75749900	H	3.56980700	-0.44340800	2.01390900
H	7.41488000	-2.52232700	-2.23707800	H	2.52756400	-1.29130900	3.18760500
H	7.31551000	-4.44012700	-0.89155400	H	2.30043200	-0.49609400	-2.50563500
H	7.20325100	-3.49152500	0.59146000	H	-0.13574200	-1.47931500	-1.62934400
H	4.97354200	-4.84977200	-0.58110700	H	-0.27584200	0.18875500	-2.16419300
H	4.84964600	-3.52020700	0.57955100	H	-0.77171700	0.77698900	0.05073000
H	3.74724700	-2.46226000	-1.31491100	O	3.71683400	3.92936000	0.24221600
N	1.29156900	0.53579700	0.51364200	C	4.34259100	5.07514600	-0.39679600
C	1.44678300	0.07677100	1.93158700	C	3.19338700	5.98052700	-0.87513000
O	0.20511600	-0.58958300	2.23291500	C	1.97978500	5.03363000	-0.88579600
C	-0.32041500	-1.09667500	1.01468700	C	2.28130400	4.12693800	0.30189400
H	-1.39033800	-1.27571500	1.15739800	H	1.81262500	3.13991700	0.26883200
H	0.16226500	-2.04584000	0.72908200	H	2.02834100	4.61492200	1.25339000
C	1.53574400	1.26954100	2.88183100	H	1.02611000	5.55965400	-0.78277400
H	2.46835600	1.81975800	2.71734900	H	1.95048100	4.44583200	-1.81056800
H	0.69211600	1.94351800	2.70703900	H	3.02897100	6.79791100	-0.16417800
H	1.50697000	0.93265100	3.92386400	H	3.40024000	6.42489200	-1.85280800
C	2.59665600	-0.91416300	2.16250600	H	4.95316900	4.69611300	-1.22273100
H	2.51904800	-1.76285300	1.47468200	H	5.00124300	5.56564200	0.32653800

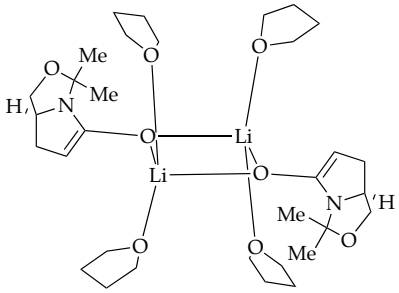


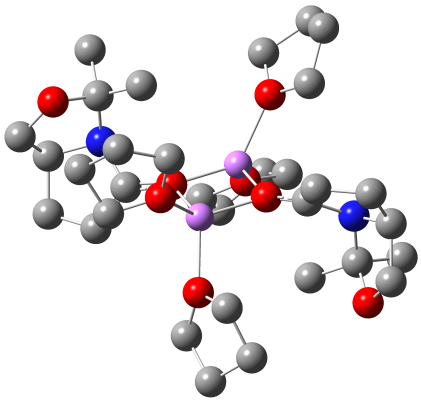


4a
$G = -1741.49226$
$G_{MP2} = -1746.449523$

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	-8.10776800	1.38187500	-1.33052000
C	0.09234400	-0.19764100	1.52523200	O	-9.34507100	2.10202900	-1.49876200
C	-1.35581200	-0.14089000	1.91977100	C	-10.3416570	1.39257700	-0.77839400
C	-2.12003700	0.34886200	0.90415800	H	-10.7506660	0.56235800	-1.37626200
O	-3.39590200	0.61110800	0.88479900	H	-11.1557280	2.08806400	-0.55316900
Li	-4.97678800	-0.45605500	1.09859700	C	-8.00061100	0.28925700	-2.40440500
O	-6.09241100	1.09349600	1.03321000	H	-8.03601700	0.73166400	-3.40628700
C	-7.38628100	1.27180600	1.09972200	H	-7.05864300	-0.25673300	-2.28980500
C	-8.14417100	1.83924500	2.07258100	H	-8.82178300	-0.42945400	-2.31273700
C	-9.60085200	1.84733500	1.69139400	C	-6.99733100	2.41653600	-1.49464800
C	-9.61758900	0.88342200	0.47170800	H	-7.06866400	3.17610900	-0.71074100
H	-10.0028000	-0.09647900	0.77899100	H	-6.01345600	1.94477100	-1.45593200
N	-8.20212400	0.74354400	0.02057000	H	-7.12260200	2.90602600	-2.46579000

H	-9.97144900	2.85056100	1.41865200	H	-4.66859800	-3.52779200	-2.60276900
H	-10.2703500	1.47426300	2.47883200	H	-4.76892900	-4.90790700	-1.50709000
H	-7.74350700	2.24747900	2.99371200	H	-4.08063600	-3.62666500	0.37436200
Li	-4.53409300	2.02644900	1.12379700	H	-3.36082900	-2.53545600	-0.84562100
N	-1.29465800	0.68945700	-0.24843000	H	-6.84905400	-1.81561700	4.16661600
C	-1.66119700	0.26931700	-1.60817000	C	-6.24034000	-0.96613700	3.81929800
O	-1.25886400	-1.12586900	-1.69303500	O	-5.27953100	-1.43615600	2.85773200
C	-0.14487000	-1.31539600	-0.81829000	C	-4.22007300	-2.06563000	3.60195400
H	0.76325200	-1.53539700	-1.39637400	C	-4.14258400	-1.32381300	4.95937400
H	-0.35963300	-2.17029400	-0.16687200	C	-5.38482100	-0.39622400	4.95240400
C	-0.84029800	1.08448000	-2.62752800	H	-5.91285300	-0.38514300	5.91078400
H	-1.14454800	2.13642400	-2.60986400	H	-5.09657900	0.63261900	4.71351300
H	0.23298900	1.03859600	-2.42437300	H	-4.17409200	-2.03506900	5.79081900
H	-1.01002400	0.68629000	-3.63288200	H	-3.21590400	-0.75035400	5.05284500
C	-3.13572800	0.34434700	-1.98848400	H	-3.31090000	-1.98437300	3.00232800
H	-3.76165600	-0.27298800	-1.34958300	H	-4.46434700	-3.12787000	3.74355000
H	-3.49469900	1.37605100	-1.93187100	H	-6.88305500	-0.23872100	3.31981600
H	-3.23635800	0.00299200	-3.02451300	H	-4.23281400	4.35364300	-0.52778800
H	-1.72628400	-0.29157500	2.92649700	C	-3.87700400	4.82342200	0.39602900
H	0.60425400	-1.14110300	1.76790300	O	-3.76577100	3.78177600	1.40198100
H	0.69723700	0.60460900	1.97989100	C	-2.42574000	3.78625200	1.95827200
H	0.83252600	0.59642300	-0.38288100	C	-1.55336200	4.35052100	0.84292000
O	-5.21975600	-1.97804400	-0.17121200	C	-2.47070400	5.42976500	0.24130300
C	-4.28536600	-3.01477000	-0.51733700	H	-2.39182100	6.36022500	0.81479000
C	-4.99467000	-3.84190800	-1.60718400	H	-2.23595400	5.65961800	-0.80197000
C	-6.50378100	-3.52968200	-1.39576400	H	-1.33417900	3.55761300	0.11970700
C	-6.51905800	-2.59727700	-0.17334100	H	-0.60697500	4.75536600	1.21418700
H	-6.64530600	-3.16452000	0.76088600	H	-2.41524300	4.42447400	2.85272000
H	-7.25861200	-1.79398700	-0.21130200	H	-2.18060200	2.75887700	2.23696400
H	-6.91920800	-3.02114000	-2.27081300	H	-4.62411900	5.55236100	0.72568900
H	-7.10043100	-4.43032000	-1.22148000				

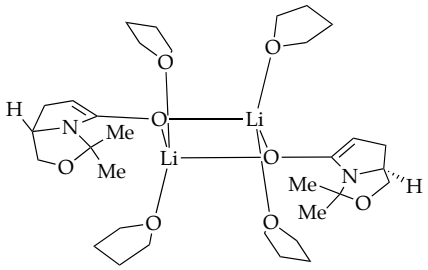


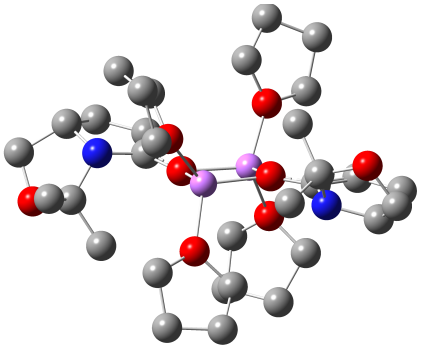


8a
G = –1973.195072
G_{MP2} = –1978.800809

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	-2.01776300	-0.94406900	0.78181500
C	-0.60775600	-0.69344400	1.23654000	C	-2.31001500	-0.20956200	-0.33099100

O	-3.44469400	-0.04891200	-0.94213600	H	0.60462700	1.74630700	-3.41891400
Li	-4.72340400	-1.36730400	-1.44444700	C	-1.77241100	0.40996400	-3.23541700
O	-6.00362600	-0.05037100	-1.94648100	H	-2.35232600	-0.50004800	-3.09482700
C	-7.13879100	-0.21193300	-2.55645500	H	-2.46182200	1.25643300	-3.22297800
C	-7.43157500	-0.94648000	-3.66908900	H	-1.27149500	0.37393500	-4.20942100
C	-8.84220600	-0.69686800	-4.12242200	H	-2.77303300	-1.43948100	1.38091300
C	-9.44932300	-0.00421700	-2.88513900	H	-0.03165300	-1.59327900	1.50258800
H	-10.1448440	0.79407500	-3.16267700	H	-0.55122700	-0.02691500	2.11413700
N	-8.30187300	0.54684000	-2.11998300	H	0.69451600	0.79885700	0.27843500
C	-8.75072000	0.54198600	-0.72227600	O	-4.74369000	2.60031100	0.08870700
O	-9.61222000	-0.62629800	-0.58820300	C	-5.50991800	3.80081100	0.29123600
C	-10.1199660	-0.97088600	-1.87487100	C	-4.71254000	4.62966200	1.29908000
H	-11.2150000	-0.88044000	-1.88853500	C	-4.09240900	3.53269900	2.17880800
H	-9.85565700	-2.01412200	-2.08857600	C	-3.77494900	2.43313200	1.16119100
C	-9.59883200	1.79973000	-0.46028900	H	-3.86974400	1.41924800	1.55503500
H	-10.0522960	1.74070800	0.53467200	H	-2.77382000	2.53698500	0.73017000
H	-8.97485700	2.69862000	-0.51397800	H	-3.20221900	3.86485500	2.72124700
H	-10.4042340	1.90222900	-1.19366100	H	-4.82468600	3.18004000	2.91484800
C	-7.67417000	0.40655000	0.34863600	H	-3.92759600	5.20137000	0.78889400
H	-7.09364000	-0.50294300	0.20722000	H	-5.34004500	5.33294900	1.85500500
H	-6.98548600	1.25360600	0.33583600	H	-6.50044600	3.53741400	0.68813900
H	-8.17415500	0.36979400	1.32309400	H	-5.64582300	4.28650200	-0.67944800
H	-9.41785800	-1.59709300	-4.38813400	O	-4.70750500	2.59977700	-2.97737300
H	-8.90009000	-0.03018700	-4.99981700	C	-3.94228100	3.80073900	-3.18076100
H	-6.67651400	-1.44116700	-4.26905100	C	-4.74404500	4.63103300	-4.18382600
Li	-4.72472600	1.25754100	-1.44415300	C	-5.36533300	3.53529500	-5.06424800
O	-3.85722300	-2.75912300	-2.66152600	C	-5.67788500	2.43254400	-4.04842400
C	-2.80789500	-3.55290000	-2.06110900	H	-5.58125500	1.41987500	-4.44497100
H	-3.21779800	-4.53208200	-1.77339700	H	-6.67833700	2.53275000	-3.61504100
C	-1.74461000	-3.68486000	-3.14877000	H	-6.25774800	3.86740800	-5.60303800
C	-2.60554400	-3.78322800	-4.42011800	H	-4.63482900	3.18566100	-5.80347300
C	-3.79983700	-2.86736700	-4.10080200	H	-5.52814900	5.20014600	-3.66945100
H	-3.66784600	-1.85897700	-4.50811800	H	-4.11947000	5.33671800	-4.74001500
H	-4.75272800	-3.26702700	-4.46444000	H	-2.95328000	3.53844400	-3.58225800
H	-2.94457200	-4.81475900	-4.57234100	H	-3.80259300	4.28442700	-2.20963300
H	-2.07556800	-3.46868200	-5.32412400	H	-5.77559300	-1.86158100	1.62053500
H	-1.10366900	-4.56008500	-3.00163600	C	-5.64384700	-2.86954200	1.21209700
H	-1.11162200	-2.79105000	-3.16409200	O	-5.58814800	-2.75974700	-0.22711900
H	-2.46708400	-3.02491100	-1.16643700	C	-6.63667800	-3.55479500	-0.82716000
N	-1.14717000	0.55021700	-0.76616900	C	-7.69922000	-3.68817300	0.26104400
C	-0.69697900	0.54601200	-2.16345700	C	-6.83748800	-3.78615700	1.53189900
O	0.16556300	-0.62152300	-2.29691400	H	-7.36717400	-3.47204800	2.43622500
C	0.67255700	-0.96578800	-1.00985300	H	-6.49777500	-4.81750100	1.68383800
H	1.76748000	-0.87415400	-0.99520500	H	-8.33302000	-2.79495000	0.27700600
H	0.40921100	-2.00935800	-0.79660400	H	-8.33940700	-4.56396000	0.11398600
C	0.15024700	1.80458800	-2.42432600	H	-6.22571100	-4.53343900	-1.11521700
H	-0.47468500	2.70281800	-2.37090300	H	-6.97855000	-3.02708600	-1.72159000
H	0.95489900	1.90762900	-1.69020900	H	-4.69045600	-3.26933700	1.57429300





8b
G = –1973.190482
G_{MP2} = –1978.797792

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	3.20465900	-3.32312500	2.54135200
C	0.09632300	1.52017500	-0.29629700	C	4.48188200	-4.16026700	2.37768500
C	1.58668000	1.70719700	-0.41092300	C	4.88964500	-3.82849500	0.94106400
C	2.23087500	0.51309500	-0.54484400	H	4.38287000	-4.48762300	0.22279000
O	3.49569700	0.24523500	-0.69210200	H	5.96764400	-3.88417400	0.76756600
Li	4.88060200	1.51099300	-0.33940900	H	5.25327100	-3.82347700	3.08033700
O	6.28553000	0.21540100	-0.47285300	H	4.32635000	-5.23267700	2.53063400
C	7.53604200	0.48482700	-0.71509800	H	2.35143800	-3.83292500	2.07797500
C	8.17642600	1.68353000	-0.82930900	H	2.95089900	-3.11979600	3.58625900
C	9.64993600	1.49861800	-1.07816700	H	2.69497000	-1.56613600	1.28878700
C	9.72103000	-0.00560200	-1.45441800	O	5.28768600	-2.20110000	-2.36954000
H	9.79715400	-0.10977900	-2.54435400	C	4.90591400	-3.52947700	-2.77559800
N	8.44778200	-0.61810700	-0.98248500	H	5.49117700	-4.26226100	-2.20259400
C	8.79456600	-1.57512900	0.10829200	C	5.22595200	-3.61322700	-4.26846300
O	10.1719050	-1.30060900	0.43607100	C	6.46581600	-2.71201800	-4.37186400
C	10.7995490	-0.83382100	-0.74869800	C	6.14441100	-1.59432600	-3.37671400
H	11.1412170	-1.67311600	-1.37612500	H	5.58197400	-0.78003200	-3.85057800
H	11.6746220	-0.24466200	-0.45791700	H	7.01890500	-1.19007200	-2.86283800
C	8.67777500	-3.01041100	-0.42788500	H	7.36216000	-3.25952300	-4.05672200
H	8.98533700	-3.73704100	0.33314400	H	6.64057900	-2.33119900	-5.38273300
H	7.64436300	-3.21220900	-0.72710900	H	4.39967000	-3.19900500	-4.85814300
H	9.31141800	-3.14579200	-1.31088700	H	5.40238800	-4.64059900	-4.60166700
C	8.01451700	-1.39788500	1.40761300	H	3.84641400	-3.66850200	-2.54522400
H	8.12223500	-0.37193600	1.76942400	N	1.29139200	-0.59685100	-0.43860000
H	6.95353700	-1.61397600	1.27262100	C	1.00592600	-1.41737100	-1.65763200
H	8.43393400	-2.07576000	2.15867600	O	-0.36604200	-1.13488600	-1.99989700
H	10.2754150	1.72203500	-0.19534100	C	-1.03903600	-0.78591400	-0.79987300
H	10.0469560	2.11351000	-1.89821300	H	-1.37409800	-1.68323500	-0.25414600
H	7.67903600	2.64379300	-0.76237200	H	-1.92095000	-0.19507800	-1.06567900
Li	4.88591600	-1.06295200	-0.72238100	C	1.14173500	-2.90553700	-1.30329800
O	4.46065400	-2.47091800	0.71442700	H	2.16839200	-3.12054400	-0.99009000
C	3.54948500	-2.04982600	1.76743900	H	0.47821300	-3.16530200	-0.47150500
H	4.07707600	-1.32505700	2.40116400	H	0.88357800	-3.53540400	-2.16268700

C	1.82598100	-1.05655300	-2.89402400	H	3.39555000	4.45935800	-3.45709900
H	1.73254200	0.01193600	-3.10608500	H	4.50055800	5.83143300	-3.24965700
H	2.88224000	-1.29715100	-2.76144300	H	5.31500700	4.97383500	-1.12972400
H	1.42942700	-1.61698200	-3.74747700	H	3.64501900	4.36007600	-1.06123600
H	2.08345600	2.67063300	-0.42942000	H	6.28726400	3.56241000	2.53417500
H	-0.45051900	1.78742200	-1.21806300	C	6.09673400	2.53084900	2.19895200
H	-0.36894500	2.09559100	0.51661100	O	4.88163500	2.50314000	1.43122500
H	-0.12809000	-0.15748400	1.07861300	C	3.80235400	2.55075800	2.38248200
O	5.06863300	2.98882700	-1.66981600	C	4.29122400	1.76374000	3.62038900
C	4.57444700	4.34216000	-1.63771500	C	5.81762700	1.60170400	3.38564200
C	4.39012700	4.75282200	-3.10150300	H	6.41389100	1.86246900	4.26545500
C	5.47481200	3.92306800	-3.80640300	H	6.05836800	0.57144300	3.10735000
C	5.43310800	2.61293100	-3.01821300	H	4.07353500	2.31196500	4.54243100
H	6.39324700	2.09325300	-2.96266300	H	3.79719800	0.79043600	3.69350300
H	4.66761400	1.92951900	-3.40798500	H	2.92152000	2.13231300	1.89068100
H	5.28216500	3.77641500	-4.87356900	H	3.60414600	3.60168900	2.63946500
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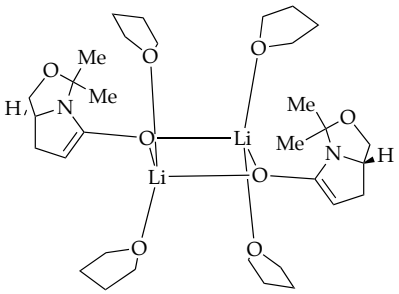
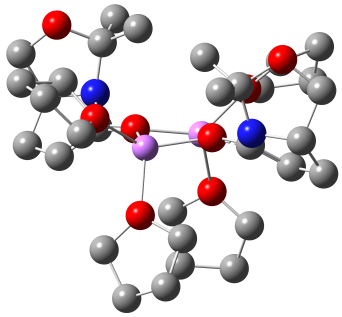


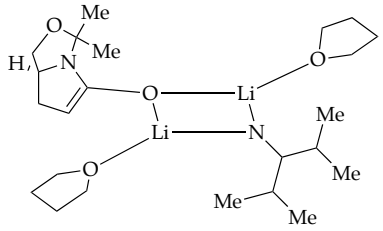


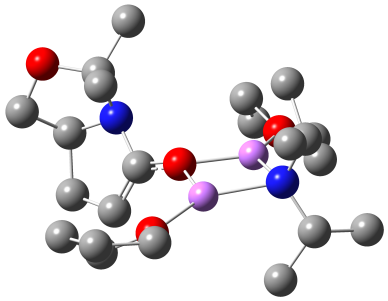
7
$G = -1978.801098$
$G_{MP2} = -1973.190260$

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	O	-9.17521900	-0.03244100	-2.67944600
C	-0.16713000	-0.78800400	1.31634200	C	-9.99618300	0.80950000	-1.88249200
C	-1.65424300	-0.99634100	1.35805300	H	-11.0364370	0.74966600	-2.22890000
C	-2.28906400	-0.18068600	0.46500500	H	-9.65885900	1.85217300	-1.97594300
O	-3.56099700	0.02877300	0.29985500	C	-9.01002100	-2.29529800	-1.85716800
Li	-4.77627500	1.48427100	0.33402100	H	-9.05702000	-2.65435000	-2.89067700
O	-6.29610200	0.34621300	0.09565300	H	-8.42096700	-3.00196200	-1.26214800
C	-7.56787800	0.60899300	0.10804800	H	-10.0281390	-2.27756500	-1.45649600
C	-8.23863400	1.65191800	0.68365900	C	-6.97399200	-0.92598000	-2.41700300
C	-9.72586700	1.44593100	0.61161600	H	-6.51756800	0.06371900	-2.41094400
C	-9.83289800	0.31592200	-0.43125900	H	-6.31869100	-1.61395900	-1.87846200
H	-10.6187000	-0.40643100	-0.18564700	H	-7.06760900	-1.26493300	-3.45461300
N	-8.50512800	-0.34811100	-0.45623400	H	-10.3073770	2.32545600	0.29347900
C	-8.37638900	-0.89419300	-1.81679100	H	-10.1634100	1.12493500	1.57248400

H	-7.76010400	2.39807500	1.30600500	C	-4.73047400	3.30770300	4.32646400
Li	-5.08384400	-1.08623400	0.51203600	C	-5.39830600	3.09242600	2.96274200
O	-4.72870100	-2.86349600	-0.38227900	H	-5.74328800	4.02293900	2.49882100
C	-5.42957500	-4.09983000	-0.13874200	H	-6.24865800	2.40388800	3.02815900
H	-5.25243700	-4.40917900	0.89958600	H	-5.44399600	3.23931000	5.15331900
C	-4.84862500	-5.10962900	-1.13130800	H	-4.25525000	4.29487300	4.37186000
C	-3.40310600	-4.61076600	-1.28031200	H	-4.11026400	1.23900600	4.60959900
C	-3.58387700	-3.09329300	-1.24589900	H	-2.84126500	2.40307300	5.03693800
H	-3.81546200	-2.69311000	-2.24081400	H	-2.45381200	2.96938100	2.69655200
H	-2.73395600	-2.55001400	-0.82823600	H	-2.81529100	1.23133000	2.53952900
H	-2.79384200	-4.94260700	-0.43087600	H	-6.87080000	2.88392900	-1.37841400
H	-2.91873200	-4.95149900	-2.20015400	C	-5.95215500	3.23678600	-1.85613000
H	-5.37390000	-5.04760800	-2.09168500	O	-4.87848800	3.06973400	-0.89027800
H	-4.92177500	-6.13987700	-0.76953500	C	-4.19114200	4.31740100	-0.70399900
H	-6.50097200	-3.92096900	-0.26927600	C	-5.23442600	5.38487300	-1.02550900
N	-1.32828800	0.59962100	-0.29542700	C	-5.98926400	4.73702700	-2.19940900
C	-1.38090900	0.66356500	-1.76481800	H	-7.01295800	5.10764300	-2.30571500
O	-0.68525500	-0.52504100	-2.22531900	H	-5.46328300	4.93404900	-3.14059700
C	0.28510600	-0.88234000	-1.24748300	H	-5.90324600	5.52705500	-0.16830900
H	1.30287100	-0.71977300	-1.63119000	H	-4.78944300	6.35214000	-1.27902900
H	0.17017300	-1.94939800	-1.02049000	H	-3.33451700	4.37697500	-1.39208500
C	-0.60659600	1.90769400	-2.23949200	H	-3.82267100	4.33362900	0.32392300
H	-1.12797300	2.82106500	-1.93358700	H	-5.73853900	2.61039100	-2.72855500
H	0.40454900	1.94017000	-1.82269000	H	-7.04333000	-0.26293900	2.92507900
H	-0.52275000	1.89541800	-3.33109700	C	-7.08266800	-1.34684100	2.76287400
C	-2.75993900	0.63835800	-2.41362400	O	-5.79115800	-1.80233500	2.29108500
H	-3.31367300	-0.25758200	-2.13960300	C	-5.03752500	-2.37741400	3.37886700
H	-3.34825500	1.51085900	-2.12122800	C	-5.89156500	-2.18568800	4.63991000
H	-2.61901600	0.65126800	-3.50004000	C	-7.31493100	-2.10925400	4.06485600
H	-2.17198900	-1.55093000	2.13219800	H	-7.70094400	-3.11494300	3.85825500
H	0.43594500	-1.70896900	1.30076600	H	-8.02270800	-1.60283000	4.72823500
H	0.20755700	-0.19469400	2.16783100	H	-5.63406700	-1.24264900	5.13711500
H	0.75989300	0.78216700	0.09001500	H	-5.75373500	-2.99482500	5.36351700
O	-4.39428000	2.49465500	2.11246600	H	-4.87107300	-3.44006000	3.15959600
C	-3.20588700	2.19036000	2.88383500	H	-4.06431000	-1.87993600	3.43659000
C	-3.66221800	2.20384900	4.34139100	H	-7.81260700	-1.54538000	1.97571800

Table 3. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the LDA mixed aggregates and pyridine solvated dimers at –78 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

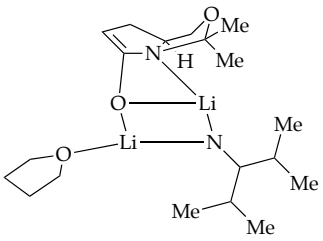


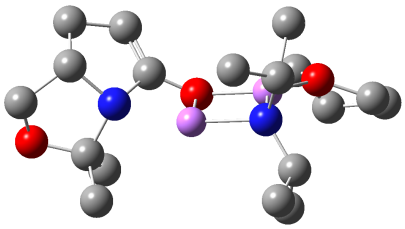


6a
G = –1288.625124
G_{MP2} = –1284.869362

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-6.20020800	1.97764000	-0.78089100
O	-1.65243600	-0.84103800	-0.00288300	C	-6.19151000	0.45089100	-0.60305400
C	-2.22101200	-1.89260600	-0.53648600	C	-5.13096500	0.26885200	0.47867000
C	-2.19091400	-2.33862400	-1.82259600	H	-4.62500800	-0.70021500	0.46456500
C	-3.11635400	-3.51161600	-2.01264800	H	-5.54781000	0.44885700	1.47925600
C	-3.55336600	-3.83229100	-0.56140200	H	-7.16402100	0.04511700	-0.30879600
H	-4.63952700	-3.95333500	-0.47331700	H	-5.87738100	-0.04491700	-1.52889600
N	-3.09622000	-2.69377200	0.28086000	H	-6.79855900	2.44876800	0.00765500
C	-2.65878800	-3.25170900	1.59700700	H	-6.60046900	2.30093300	-1.74631000
O	-2.87000600	-4.67763800	1.48400500	H	-4.19420900	2.34447300	-1.58299900
C	-2.85838800	-5.01726100	0.10589900	H	-4.55364400	3.30124900	-0.12673300
H	-3.38444200	-5.96961200	-0.01258300	N	-0.49689300	1.86162300	0.53351000
H	-1.83027000	-5.12910000	-0.27737700	C	-0.25734200	2.29630800	1.91294000
C	-3.57847300	-2.77010400	2.71888300	H	-0.45328200	3.37976700	2.02812600
H	-3.35531000	-3.30125300	3.65071600	C	1.19831600	2.06831100	2.38325300
H	-3.44543400	-1.69616900	2.88621100	H	1.91235500	2.51795000	1.68336300
H	-4.62188600	-2.95983900	2.44999000	H	1.38706700	2.50089700	3.37602700
C	-1.18358700	-3.01675100	1.94337900	H	1.41341500	0.99094800	2.44125800
H	-0.53466700	-3.36798100	1.13434300	C	-1.21958500	1.58253600	2.87624700
H	-0.97269900	-1.96117100	2.11939200	H	-1.02238500	1.84708500	3.92258200
H	-0.94994600	-3.58900500	2.84679700	H	-2.26390000	1.84681400	2.65930200
H	-2.65359700	-4.39087000	-2.49052100	H	-1.11855900	0.49091800	2.78910600
H	-3.99440900	-3.26327300	-2.62829800	C	-0.04770700	2.85937000	-0.44030500
H	-1.73383800	-1.78727400	-2.63672600	H	0.93927600	3.27824900	-0.15648000
Li	-2.23809600	0.89806700	0.32456200	C	-1.00332000	4.06701000	-0.58052700
O	-4.13890600	1.29297500	0.20014700	H	-0.58486400	4.84719700	-1.23201700
C	-4.71822900	2.33875500	-0.61975500	H	-1.96131100	3.74463900	-1.01177100

H	-1.21254700	4.52475500	0.39280400	C	3.65389700	-2.16530600	-0.16161500
C	0.14115900	2.20793300	-1.81985200	C	2.96633800	-0.77828500	-0.10888800
H	-0.79138000	1.72856500	-2.15295700	H	2.95315200	-0.32968800	0.88686300
H	0.42304100	2.94408500	-2.58282100	H	3.42896600	-0.06819600	-0.80571400
H	0.92500600	1.43897000	-1.79562200	H	4.46672200	-2.16055000	-0.89474100
O	1.59196000	-0.99244100	-0.49660000	H	4.08373900	-2.44599100	0.80388500
C	1.54095200	-2.19310100	-1.29416400	H	2.87898800	-3.93211200	-1.24695800
H	1.86627300	-1.96119900	-2.31989300	H	2.04461700	-3.58247800	0.27799800
C	2.52429200	-3.12798000	-0.59547200	H	0.50158300	-2.52991600	-1.31561100

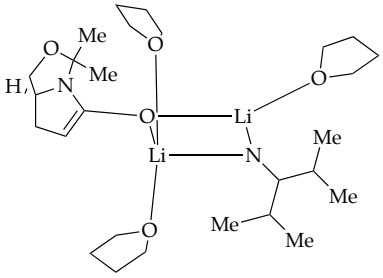


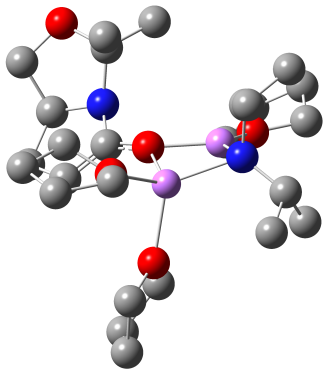


9
G = –1056.264019
G_{MP2} = –1053.168309

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	0.43431200	1.93774500	-0.32358800
O	1.61929500	-0.87798700	-0.21631000	C	0.32391200	2.75788500	0.89162500
C	2.80618000	-1.05659900	0.29884900	H	-0.46551300	3.52129200	0.76213100
C	3.28862200	-1.79185900	1.32430000	C	-0.09778400	1.89018000	2.09508700
C	4.76033400	-1.53801600	1.53001200	H	-0.15982000	2.46900400	3.02579600
C	4.99595900	-0.25886800	0.67869700	H	-1.08067400	1.43227400	1.92072600
H	4.98249400	0.62971900	1.31895800	H	0.63138600	1.08335400	2.26648600
N	3.85586700	-0.19040200	-0.28892500	C	1.62449400	3.51288000	1.25307700
C	4.41933000	-0.61504700	-1.63670800	H	1.96084300	4.14110300	0.42231100
O	5.77221200	-1.00920100	-1.37323200	H	1.50067000	4.15235200	2.13847400
C	6.21852500	-0.28678200	-0.23330500	H	2.43047700	2.79784300	1.47944200
H	6.54745800	0.72852900	-0.50529100	C	-0.20175300	2.55024900	-1.48906300
H	7.06848400	-0.82495900	0.19524600	H	-1.25316200	2.82545800	-1.25304300
C	4.41666000	0.59640500	-2.57989500	C	-0.26350800	1.53563800	-2.64160600
H	4.91554900	0.34513800	-3.52176200	H	-0.77163800	1.95254400	-3.51931300
H	3.39109900	0.90970400	-2.81492400	H	0.74670500	1.23760800	-2.95909700
H	4.93537500	1.44733700	-2.12572700	H	-0.79885600	0.62266700	-2.34762200
C	3.72742900	-1.81930300	-2.26772700	C	0.46404400	3.84810300	-2.00070100
H	3.73106300	-2.66205500	-1.57220000	H	-0.06974800	4.25910900	-2.86887100
H	2.69323400	-1.59010100	-2.53364800	H	0.47647700	4.62251200	-1.22675100
H	4.27650100	-2.10431900	-3.17044400	H	1.50477800	3.65505600	-2.29809900
Li	2.13042900	0.98794000	-0.54093800	H	5.39800500	-2.36944800	1.18600400

H	5.02859600	-1.35007400	2.57807900	H	-2.82547900	-0.24600500	-1.24586500
H	2.68680100	-2.45558600	1.93347200	H	-3.42243500	-0.44778900	0.41729800
O	-1.51832400	-1.19506600	0.04063900	H	-4.04907500	-2.71727100	0.04534800
C	-1.25022400	-2.61923800	0.00292600	H	-4.13089600	-2.22915400	-1.65337300
H	-1.45126200	-3.04737500	0.99450100	H	-2.40491700	-4.23131100	-0.93269800
C	-2.21889500	-3.15900500	-1.04385700	H	-1.82538600	-2.98084400	-2.05143100
C	-3.46902300	-2.30007700	-0.78552700	H	-0.19105500	-2.73563400	-0.23342900
C	-2.87620000	-0.93558100	-0.39632800				

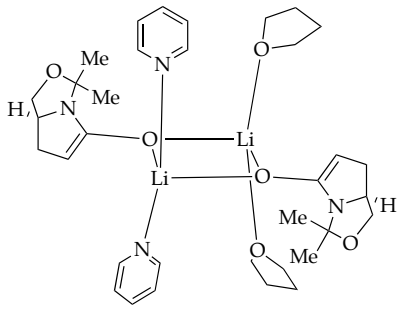


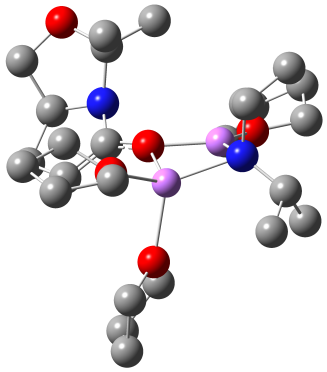


6b
$G = -1520.965486$
$G_{MP2} = -1516.559253$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.69165100	-2.68232000	1.90346700
O	1.78052300	-0.74872100	0.18810900	Li	2.24679600	1.03565900	0.05783000
C	2.25838700	-1.86864200	0.65547600	O	3.95304500	1.65308700	0.77435200
C	1.67683900	-2.79825200	1.46735400	C	4.60729500	2.92413300	0.64497000
C	2.65470000	-3.86981900	1.86893600	C	6.09686200	2.57485300	0.62417700
C	3.90223400	-3.52518600	1.01467300	C	6.18543900	1.35001500	1.57095600
H	4.80997400	-3.46148400	1.62651700	C	4.71938100	0.88171600	1.72906800
N	3.63349800	-2.20970100	0.37068200	H	4.34035600	1.09674000	2.73771300
C	4.13405700	-2.28335800	-1.04102500	H	4.55081500	-0.17082500	1.49043600
O	4.78790900	-3.56567200	-1.12664100	H	6.81354500	0.56384500	1.14346500
C	4.16724000	-4.42994000	-0.18750000	H	6.61199900	1.62162700	2.54152600
H	4.85484200	-5.25631300	0.01720300	H	6.39850900	2.29854400	-0.39115200
H	3.22320000	-4.84454500	-0.57852800	H	6.72427100	3.41088900	0.94729100
C	5.21856700	-1.23755400	-1.29366600	H	4.35189600	3.55934100	1.50651600
H	5.66263900	-1.37985500	-2.28506000	H	4.23595300	3.39637700	-0.26669500
H	4.79731800	-0.22916500	-1.23633000	N	0.61845700	1.81962800	-0.73904600
H	6.00651000	-1.33721100	-0.54079700	C	0.83513600	1.76139200	-2.19232000
C	3.03873000	-2.22595800	-2.11367000	H	1.17095800	0.73083400	-2.40446600
H	2.28980800	-3.00547500	-1.94276300	C	1.97363500	2.68587600	-2.70086100
H	2.52820300	-1.26183100	-2.12007000	H	2.91764200	2.45311100	-2.18937100
H	3.50104800	-2.40009100	-3.09053700	H	2.14373600	2.57395800	-3.78079200
H	2.31222400	-4.90040300	1.67430100	H	1.74564800	3.74234900	-2.51139300
H	2.90829600	-3.83715500	2.93975000	C	-0.41479400	1.98217100	-3.07708100

H	-0.79481100	3.00774600	-2.99087600	H	-0.39387300	-2.55226500	-2.32564900
H	-0.18777600	1.80590500	-4.13732800	H	-2.08819900	-4.21574600	-2.11250900
H	-1.22031700	1.30090400	-2.78225300	H	-2.20483700	-4.00848600	-0.36380200
C	0.01828400	3.07236200	-0.27275700	H	-3.87111500	-2.63574600	-2.36957600
H	0.16018500	3.88391000	-1.00986600	H	-3.92477100	-2.45582200	-0.61428600
C	0.69455300	3.55487200	1.02418600	H	-3.03745900	-0.26203700	-1.08675600
H	0.21743700	4.45600200	1.43339000	O	-0.84133100	-0.06479400	1.89734700
H	0.63934500	2.77235900	1.79398500	C	-2.19116500	-0.43607900	2.24063100
H	1.75339300	3.78035200	0.85039700	H	-2.38697000	-1.44059400	1.84580400
C	-1.50758300	2.97270500	-0.02548600	C	-2.26358200	-0.40276300	3.77114900
H	-1.70573600	2.23391700	0.76196000	C	-0.81477700	-0.72488200	4.16929100
H	-1.93957400	3.93323200	0.29273400	C	-0.02134100	0.00508900	3.08573200
H	-2.03245600	2.65063100	-0.93044900	H	0.13557300	1.06052700	3.34681700
O	-1.27324200	-1.29188500	-0.93020100	H	0.93942000	-0.45938400	2.85214800
C	-2.52971400	-1.08935100	-1.58731200	H	-0.62983000	-1.80414200	4.11208800
H	-2.35314100	-0.81181700	-2.63656900	H	-0.55718800	-0.38745800	5.17784500
C	-3.25972500	-2.44134500	-1.48329100	H	-2.99399800	-1.11350800	4.16960100
C	-2.10657900	-3.47058400	-1.31164000	H	-2.53982600	0.59914700	4.12013300
C	-0.83221700	-2.60588900	-1.31851500	H	-2.87789300	0.26909100	1.76040100
H	-0.06335500	-2.91584000	-0.60756200				

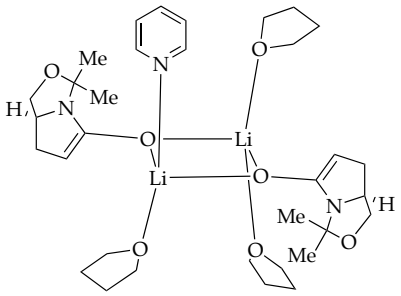


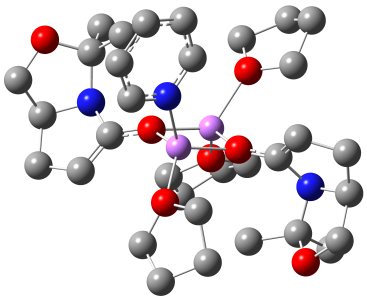


11
G = –2010.529168
G_{MP2} = –2004.814262

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	4.16724000	-4.42994000	-0.18750000
O	1.78052300	-0.74872100	0.18810900	H	4.85484200	-5.25631300	0.01720300
C	2.25838700	-1.86864200	0.65547600	H	3.22320000	-4.84454500	-0.57852800
C	1.67683900	-2.79825200	1.46735400	C	5.21856700	-1.23755400	-1.29366600
C	2.65470000	-3.86981900	1.86893600	H	5.66263900	-1.37985500	-2.28506000
C	3.90223400	-3.52518600	1.01467300	H	4.79731800	-0.22916500	-1.23633000
H	4.80997400	-3.46148400	1.62651700	H	6.00651000	-1.33721100	-0.54079700
N	3.63349800	-2.20970100	0.37068200	C	3.03873000	-2.22595800	-2.11367000
C	4.13405700	-2.28335800	-1.04102500	H	2.28980800	-3.00547500	-1.94276300
O	4.78790900	-3.56567200	-1.12664100	H	2.52820300	-1.26183100	-2.12007000

H	3.50104800	-2.40009100	-3.09053700	H	0.63934500	2.77235900	1.79398500
H	2.31222400	-4.90040300	1.67430100	H	1.75339300	3.78035200	0.85039700
H	2.90829600	-3.83715500	2.93975000	C	-1.50758300	2.97270500	-0.02548600
H	0.69165100	-2.68232000	1.90346700	H	-1.70573600	2.23391700	0.76196000
Li	2.24679600	1.03565900	0.05783000	H	-1.93957400	3.93323200	0.29273400
O	3.95304500	1.65308700	0.77435200	H	-2.03245600	2.65063100	-0.93044900
C	4.60729500	2.92413300	0.64497000	O	-1.27324200	-1.29188500	-0.93020100
C	6.09686200	2.57485300	0.62417700	C	-2.52971400	-1.08935100	-1.58731200
C	6.18543900	1.35001500	1.57095600	H	-2.35314100	-0.81181700	-2.63656900
C	4.71938100	0.88171600	1.72906800	C	-3.25972500	-2.44134500	-1.48329100
H	4.34035600	1.09674000	2.73771300	C	-2.10657900	-3.47058400	-1.31164000
H	4.55081500	-0.17082500	1.49043600	C	-0.83221700	-2.60588900	-1.31851500
H	6.81354500	0.56384500	1.14346500	H	-0.06335500	-2.91584000	-0.60756200
H	6.61199900	1.62162700	2.54152600	H	-0.39387300	-2.55226500	-2.32564900
H	6.39850900	2.29854400	-0.39115200	H	-2.08819900	-4.21574600	-2.11250900
H	6.72427100	3.41088900	0.94729100	H	-2.20483700	-4.00848600	-0.36380200
H	4.35189600	3.55934100	1.50651600	H	-3.87111500	-2.63574600	-2.36957600
H	4.23595300	3.39637700	-0.26669500	H	-3.92477100	-2.45582200	-0.61428600
N	0.61845700	1.81962800	-0.73904600	H	-3.03745900	-0.26203700	-1.08675600
C	0.83513600	1.76139200	-2.19232000	O	-0.84133100	-0.06479400	1.89734700
H	1.17095800	0.73083400	-2.40446600	C	-2.19116500	-0.43607900	2.24063100
C	1.97363500	2.68587600	-2.70086100	H	-2.38697000	-1.44059400	1.84580400
H	2.91764200	2.45311100	-2.18937100	C	-2.26358200	-0.40276300	3.77114900
H	2.14373600	2.57395800	-3.78079200	C	-0.81477700	-0.72488200	4.16929100
H	1.74564800	3.74234900	-2.51139300	C	-0.02134100	0.00508900	3.08573200
C	-0.41479400	1.98217100	-3.07708100	H	0.13557300	1.06052700	3.34681700
H	-0.79481100	3.00774600	-2.99087600	H	0.93942000	-0.45938400	2.85214800
H	-0.18777600	1.80590500	-4.13732800	H	-0.62983000	-1.80414200	4.11208800
H	-1.22031700	1.30090400	-2.78225300	H	-0.55718800	-0.38745800	5.17784500
C	0.01828400	3.07236200	-0.27275700	H	-2.99399800	-1.11350800	4.16960100
H	0.16018500	3.88391000	-1.00986600	H	-2.53982600	0.59914700	4.12013300
C	0.69455300	3.55487200	1.02418600	H	-2.87789300	0.26909100	1.76040100
H	0.21743700	4.45600200	1.43339000				

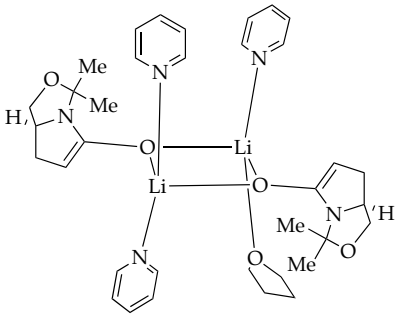


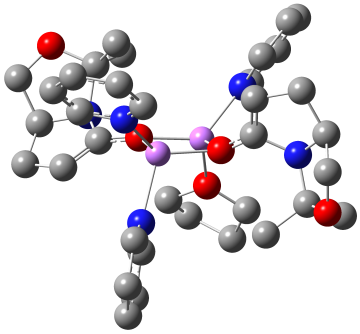


12
$G = -1994.664359$
$G_{MP2} = -1989.003963$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.34428700	-1.27303500	0.04914700
O	1.44986400	-1.19659000	-0.29953800	H	-6.39223200	-1.59152500	-0.04258000
C	2.46414800	-1.10090700	-1.11016200	H	-5.32364400	-0.18328100	0.17189500
C	2.53310500	-0.56219200	-2.36119600	C	-4.21748700	-4.00063400	-0.97364100
C	3.87046000	-0.82709700	-2.99579000	H	-4.55354300	-4.12112300	-2.00874400
C	4.69948400	-1.32828400	-1.79543300	H	-3.47558600	-4.77426700	-0.74809300
N	3.71926100	-1.74128000	-0.75979900	H	-5.07882900	-4.15793000	-0.31769100
C	4.39520500	-1.56006100	0.53992100	C	-2.45343600	-2.39785100	-1.75875300
O	5.53080200	-0.67790100	0.29027100	H	-2.04583400	-1.39179700	-1.68061600
C	5.49668500	-0.24553800	-1.06143600	H	-1.64502500	-3.10860700	-1.57466100
H	6.52713600	-0.14346100	-1.42119200	H	-2.83979800	-2.55227900	-2.77239700
H	4.98991600	0.72808300	-1.15436400	H	-5.04633700	-0.26904000	2.51903300
C	4.99012200	-2.89852800	0.99857000	H	-4.34174100	-1.64144000	3.36531100
H	4.19423000	-3.60058900	1.26966100	H	-2.33534800	0.09444700	2.66504200
H	5.58599100	-3.34430900	0.19608300	O	0.50655600	-4.20504800	-0.74454900
H	5.64095600	-2.74680300	1.86682800	C	-0.08725700	-5.50424200	-0.59518300
C	3.56241100	-0.91818600	1.64862800	C	0.83992600	-6.45573500	-1.34903100
H	3.17497100	0.05168600	1.33145900	C	1.27531000	-5.58163600	-2.53698000
H	2.71723800	-1.54306500	1.94350800	C	1.37721500	-4.18328200	-1.91231100
H	4.22005000	-0.76684300	2.51177000	H	1.04394900	-3.38124900	-2.57566700
H	5.36041500	-2.16378900	-2.05508900	H	2.38558100	-3.94140100	-1.56545500
H	4.34887000	0.05031000	-3.46039100	H	2.22044600	-5.90327700	-2.98424900
H	3.82858900	-1.59929800	-3.78244600	H	0.50840300	-5.60299900	-3.32016400
H	1.66896900	-0.19115200	-2.89850700	H	1.70381300	-6.71762700	-0.72601900
Li	0.33373100	-2.55083900	0.41293500	H	0.34121500	-7.38209300	-1.65032400
O	-1.16063400	-1.39214500	0.61252800	H	-1.09600000	-5.50189500	-1.03308500
C	-2.36724800	-1.38568500	1.09143400	H	-0.17478500	-5.71205800	0.47487400
C	-2.90934700	-0.61172800	2.07712100	O	0.51599600	-3.44334400	2.24486900
C	-4.29761700	-1.07040800	2.42196400	C	1.51693200	-4.37649400	2.69798400
C	-4.62818300	-1.98768500	1.22652700	C	0.83802400	-5.22756700	3.77391500
H	-5.19722900	-2.86992100	1.53499300	C	-0.16618500	-4.23157700	4.37515900
N	-3.32219300	-2.38925900	0.64217100	C	-0.62661500	-3.45685800	3.13974900
C	-3.60740100	-2.59947800	-0.78338400	H	-0.92077000	-2.42375400	3.33440300
O	-4.61775600	-1.60931100	-1.13023900	H	-1.46188600	-3.95303900	2.63141200

H	-0.99701700	-4.71495000	4.89790700	H	-3.96900000	2.42971600	-1.93182800
H	0.33918300	-3.56448500	5.08398700	H	-2.63389100	1.45748500	-4.11544300
H	0.30841000	-6.07375700	3.31898400	H	-2.06970800	2.96369700	-3.37365600
H	1.54977400	-5.62618900	4.50316500	H	-0.03677200	1.71344500	-3.11250100
H	2.36627200	-3.81478000	3.10795600	N	0.53100000	1.48417800	1.44579400
H	1.86699300	-4.95153000	1.83509400	C	0.52332200	1.18299700	2.75279100
O	-0.93463400	1.26701100	-1.29671500	C	1.01501600	2.04193700	3.73471300
C	-0.93843900	1.21486100	-2.74327000	C	1.54527800	3.27027400	3.34145500
H	-0.90270200	0.16240200	-3.04682400	C	1.55954600	3.59098300	1.98446200
C	-2.23807700	1.89495200	-3.19394700	C	1.04092900	2.66835500	1.07642700
C	-3.16036700	1.69344300	-1.98034800	H	1.02754900	2.87421100	0.00921300
C	-2.18192700	1.83122400	-0.81590200	H	1.96473800	4.53421000	1.63126800
H	-2.01274300	2.88498400	-0.55178300	H	1.94109500	3.96395700	4.07837000
H	-2.47844300	1.27611900	0.07798500	H	0.98335200	1.74948200	4.77975300
H	-3.60495100	0.69216900	-1.98217500	H	0.10386800	0.21381700	3.00884800

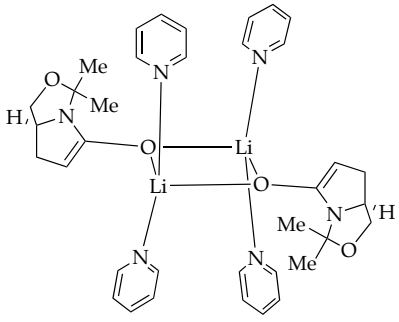


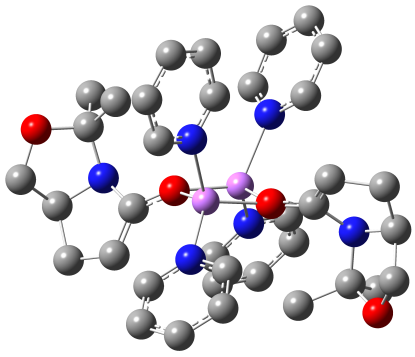


13
G = –2026.392782
G_{MP2} = –2020.627362

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.06509600	-0.81419500	-2.11245100
O	-1.49754000	-1.16184900	0.26369800	H	-2.10864500	-2.28748300	-1.90071000
C	-2.70136600	-0.84109000	0.63949800	H	-3.51279300	-2.28542000	-3.00037200
C	-3.13827400	0.25502400	1.33011900	H	-5.65357400	-1.80037300	1.44076100
C	-4.58715500	0.11792400	1.70924100	H	-5.21359100	0.99721900	1.48497900
C	-5.03105800	-1.10064500	0.87030600	H	-4.73094000	-0.08491500	2.78336300
N	-3.78629100	-1.77199500	0.40946800	H	-2.47302300	0.99731400	1.75392100
C	-4.07248800	-2.34304200	-0.93773800	Li	-0.19967200	-2.56283100	0.29618100
O	-5.40179400	-1.87201700	-1.28469400	O	1.26950100	-1.42252400	-0.11475500
C	-5.71935600	-0.76956600	-0.45248100	C	2.30884400	-1.53468600	-0.88786600
H	-6.80989100	-0.69819200	-0.38136400	C	2.46775000	-1.16164400	-2.19606200
H	-5.32676900	0.17626800	-0.86208400	C	3.79403100	-1.62943400	-2.73448200
C	-4.18037300	-3.86689300	-0.85542900	C	4.52824400	-2.06109900	-1.44735400
H	-3.20019400	-4.30756800	-0.65060800	H	5.10035800	-2.98734500	-1.57742300
H	-4.87026500	-4.14835000	-0.05387300	N	3.47797700	-2.23783500	-0.41632800
H	-4.55839800	-4.27348300	-1.80010200	C	4.12671900	-1.99372800	0.88330300
C	-3.11820300	-1.90524900	-2.05223800	O	5.36223400	-1.27243700	0.58740300

C	5.41495100	-0.99097400	-0.80333100	C	0.09723200	-6.56870500	-2.58236400
H	6.46085400	-1.03459400	-1.12823900	C	0.65628400	-5.35046300	-2.96338200
H	5.01700700	0.01330600	-1.02172000	C	0.53358700	-4.25542200	-2.10723200
C	4.54839300	-3.33048900	1.50760400	H	0.97186600	-3.29162800	-2.35749900
H	5.18858900	-3.15730300	2.37971300	H	1.18331500	-5.24177500	-3.90619000
H	3.66703600	-3.90128000	1.81987500	H	0.17467000	-7.44051400	-3.22663200
H	5.10740500	-3.92977300	0.78255800	H	-1.01277800	-7.57517800	-1.01460800
C	3.33635300	-1.14729900	1.87862900	H	-1.14029400	-5.51570500	0.39582000
H	3.07764300	-0.17814100	1.44799500	N	-0.28796900	1.53838000	-1.42981400
H	2.41194100	-1.63900900	2.18597600	C	0.64795400	2.00098700	-2.27498100
H	3.97084200	-0.98246700	2.75622200	C	0.41008200	3.03948900	-3.17494700
H	4.37374900	-0.86540500	-3.27709500	C	-0.85674500	3.62190700	-3.20350800
H	3.70274300	-2.48498900	-3.42447200	C	-1.83511400	3.14235400	-2.33312700
H	1.65403100	-0.79693300	-2.81197400	C	-1.50818200	2.10228800	-1.46304100
O	-0.46643000	-3.47378700	2.11395200	H	-2.23861600	1.69421900	-0.76513900
C	0.47250500	-4.29840300	2.83900700	H	-2.83662700	3.56150500	-2.32373400
C	-0.25664100	-4.77570900	4.10945500	H	-1.07821100	4.43206000	-3.89346000
C	-1.73930200	-4.55167800	3.76370900	H	1.20183900	3.37573900	-3.83749700
C	-1.66994200	-3.30038500	2.89310700	H	1.61188500	1.49836700	-2.23053600
H	-1.58258800	-2.39390700	3.50969500	N	0.42112700	1.17328200	1.76517500
H	-2.49881700	-3.16593600	2.19492700	C	0.12707000	0.57860700	2.93158600
H	-2.13596500	-5.39472900	3.18485700	C	0.43460400	1.14041900	4.17019000
H	-2.37180100	-4.41885600	4.64672000	C	1.07712500	2.37750600	4.20179000
H	-0.02199700	-5.81544300	4.35613600	C	1.38485000	3.00363400	2.99449500
H	0.02764200	-4.15836600	4.96925900	C	1.03720300	2.36314900	1.80565500
H	1.36988400	-3.71140000	3.06215100	H	1.25876800	2.81599100	0.84216400
H	0.75969500	-5.12824800	2.18353100	H	1.88499200	3.96685900	2.96867000
N	-0.10523000	-4.32273600	-0.92693300	H	1.33281700	2.84507900	5.14886600
C	-0.63593200	-5.50188100	-0.56693800	H	0.17271300	0.61776700	5.08509400
C	-0.56210100	-6.64813400	-1.35565300	H	-0.37870900	-0.37960200	2.85316500



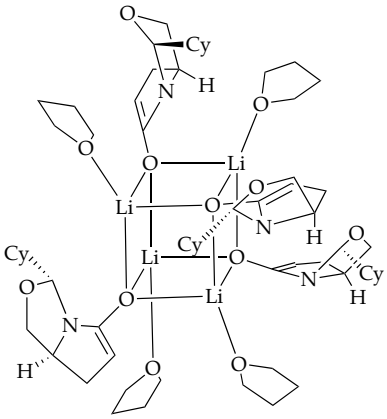


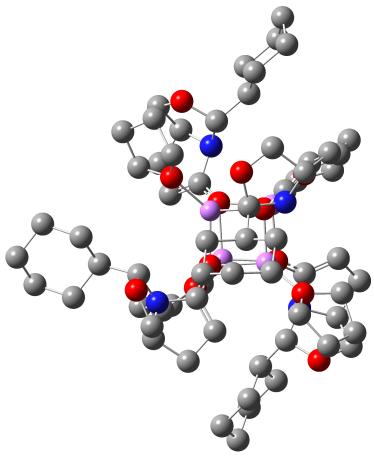
14
$G = -2042.258586$
$G_{MP2} = -2036.440946$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.32984600	-1.25383100	-1.25109800
O	1.39568500	-1.25188100	-0.34713800	C	2.26751700	-0.89814800	-2.57204600

C	3.56173900	-1.20603300	-3.27777900	N	0.35093600	-3.45415200	2.17530600
C	4.50541700	-1.51428700	-2.09604200	C	1.35989800	-4.27237400	2.51181900
N	3.63007200	-1.79830400	-0.93416200	C	1.51244300	-4.81210600	3.78829600
C	4.40885600	-1.44838300	0.26526500	C	0.57003200	-4.48806600	4.76420600
O	5.48350200	-0.57042400	-0.19336300	C	-0.48178300	-3.63831500	4.42396200
C	5.32478100	-0.32549400	-1.58280000	C	-0.55274900	-3.14379100	3.12073800
H	6.31811700	-0.24920500	-2.04022600	H	-1.35154900	-2.47176600	2.81405700
H	4.77981400	0.61574600	-1.76021300	H	-1.23964300	-3.36001500	5.14992100
C	5.09003500	-2.70663600	0.82138600	H	0.65443900	-4.89065400	5.77018100
H	4.34673600	-3.37913900	1.26375300	H	2.35042300	-5.46707700	4.00617500
H	5.61180600	-3.24410700	0.02372500	H	2.07037000	-4.49940600	1.72041300
H	5.82115800	-2.43253200	1.58981500	N	0.16060300	-4.30838200	-0.99883700
C	3.65399200	-0.70601400	1.36543400	C	-0.40855000	-5.46890200	-0.63549200
H	3.21289200	0.21629800	0.98308500	C	-0.42150700	-6.60072600	-1.44865300
H	2.85564600	-1.31584700	1.79093100	C	0.18582900	-6.52573800	-2.70229400
H	4.37395300	-0.45051000	2.15051500	C	0.77888100	-5.32513800	-3.08828300
H	5.16931100	-2.36373300	-2.29589200	C	0.74350800	-4.24298300	-2.20827300
H	3.96403900	-0.38586800	-3.89406300	H	1.19280900	-3.28643600	-2.46889100
H	3.49215400	-2.07941100	-3.94772100	H	1.26293100	-5.21983500	-4.05426700
H	1.34048300	-0.65364600	-3.07725400	H	0.19499500	-7.38714400	-3.36493300
Li	0.13790700	-2.56495400	0.22788700	H	-0.89904100	-7.51314000	-1.10493500
O	-1.30803500	-1.33313300	0.38446600	H	-0.87122500	-5.48200000	0.34818100
C	-2.51248500	-1.23678500	0.86321800	N	0.51840100	1.28289800	1.68130700
C	-2.99191500	-0.41714800	1.84897900	C	0.50728700	0.75464300	2.91451400
C	-4.41290600	-0.76659600	2.19980100	C	0.92070200	1.45408100	4.04770200
C	-4.80660100	-1.70484400	1.03923600	C	1.37058300	2.76504300	3.89635700
H	-5.40176600	-2.56343400	1.37194200	C	1.38708100	3.32296100	2.61869000
N	-3.53550400	-2.15900200	0.42359500	C	0.95188500	2.54473300	1.54658400
C	-3.83826200	-2.44064900	-0.99389800	H	0.94717000	2.94145800	0.53453000
O	-5.10121700	-1.76243500	-1.27883100	H	1.73018000	4.33904600	2.44989600
C	-5.50066900	-1.01774200	-0.14087800	H	1.70231800	3.34024000	4.75658800
H	-6.59482200	-1.03763900	-0.07481400	H	0.88970300	0.97691400	5.02239200
H	-5.17145900	0.03185600	-0.21556200	H	0.14858900	-0.26803200	2.98640400
C	-4.10908600	-3.93969500	-1.17500900	N	-0.69408400	1.49956200	-1.32240300
H	-4.52054200	-4.13107500	-2.17213400	C	-0.00631100	2.02564200	-2.34888100
H	-3.18337900	-4.51262400	-1.05834700	C	-0.53084600	3.00982800	-3.18645700
H	-4.83164000	-4.28861500	-0.43059200	C	-1.82836400	3.46452600	-2.95239100
C	-2.81863800	-1.94064300	-2.01602900	C	-2.55060300	2.91743900	-1.89212100
H	-2.65040900	-0.86688100	-1.91197000	C	-1.94489500	1.94028000	-1.10262900
H	-1.85986700	-2.45180000	-1.91963200	H	-2.47142900	1.47818700	-0.26857200
H	-3.22894300	-2.13265100	-3.01331100	H	-3.56625300	3.23505600	-1.67732800
H	-5.10267000	0.09075500	2.25986300	H	-2.27013200	4.22826500	-3.58708200
H	-4.50226600	-1.29275700	3.16497700	H	0.06660700	3.40245500	-4.00363000
H	-2.36395000	0.24480300	2.43285300	H	0.99270800	1.62237800	-2.50189600

Table 4. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the THF solvated tetramer isomers at –78 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



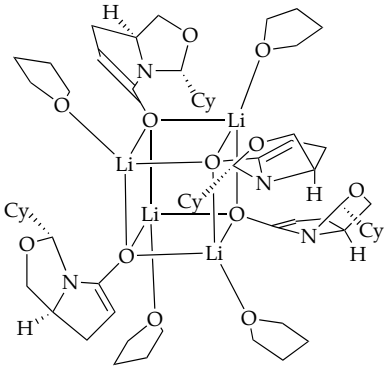


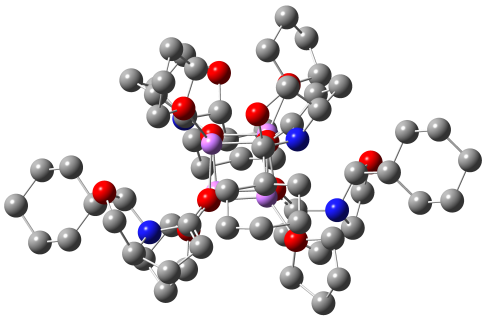
7a
G = –3652.049374
G_{MP2} = –3641.696093

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.40481300	-0.65514500	4.85855900
O	1.30886200	1.27146700	-0.81236700	H	1.90758800	-1.14088100	5.65220600
C	2.25809500	2.16153300	-0.18018400	H	2.06709400	-2.26301500	3.12665100
C	3.51623700	2.03245700	-1.02973100	Li	-1.85103700	-0.79749600	1.87725500
C	2.93444200	1.94189100	-2.45110000	O	-2.85472800	-0.60128100	3.56552200
C	1.57897800	1.24112100	-2.24257500	C	-3.44143100	0.55813900	4.18436200
H	0.76519000	1.75194800	-2.76423100	C	-4.59093700	0.02006900	5.06239700
H	1.58429600	0.19495500	-2.54488700	C	-4.27895800	-1.49573000	5.19969900
H	3.58145300	1.37832400	-3.12779500	C	-2.88743600	-1.63415800	4.56992900
H	2.78924600	2.94333500	-2.87208900	H	-2.70541200	-2.58752900	4.07009000
H	4.04647600	1.10759900	-0.78291000	H	-2.08754800	-1.44465900	5.30095100
H	4.19911800	2.87748100	-0.89776000	H	-4.29535300	-1.83996000	6.23845800
H	2.37128100	1.85610100	0.85948100	H	-5.00092100	-2.08238300	4.62599300
H	1.86248400	3.18708500	-0.19773400	H	-4.61322000	0.53058800	6.03026100
O	0.10501000	-0.70893300	1.84264500	H	-5.56196700	0.17535900	4.58356500
C	0.84489600	-0.49602300	2.91277600	H	-3.75854200	1.22490100	3.38065700
C	1.80470500	-1.27337700	3.47449600	H	-2.67534100	1.05673000	4.79189700
C	2.31016400	-0.65406500	4.74947700	O	-1.98039000	0.14853900	0.06180400
C	1.76873400	0.78433400	4.62918800	C	-3.07851000	0.86804700	-0.04362600
N	0.61091900	0.69942400	3.70151200	C	-4.23796400	0.77971400	0.66296000
C	0.54515500	1.97370300	2.99486900	C	-5.25750100	1.75648300	0.14156300
O	1.86422900	2.57092300	3.07966700	C	-4.38596500	2.67288400	-0.73730900
C	2.70848900	1.75455000	3.89006800	H	-4.89930100	3.00718200	-1.64246300
H	3.27408900	2.40075800	4.57088300	N	-3.18124300	1.87126600	-1.08328900
H	3.41638500	1.19990700	3.25748300	C	-2.08634400	2.82281900	-1.24609200
H	0.31828100	1.77679300	1.94057000	O	-2.46937900	4.03505200	-0.55283500
H	1.46276900	1.20428100	5.59056700	C	-3.76952700	3.87045400	0.00513100

H	-4.33253600	4.79952000	-0.13835800	H	2.92402200	-6.33899100	1.26251100
H	-3.69837800	3.66034300	1.08202300	H	2.07779100	-7.04869400	2.64963200
H	-1.18697300	2.41439100	-0.77128000	H	1.02406500	-4.93966800	3.20963000
H	-5.77813000	2.33558800	0.91869700	H	2.55413700	-4.33019400	2.53675200
H	-6.04389600	1.27749400	-0.46345400	O	-3.15008000	-2.16787300	-2.12125900
H	-4.44362300	0.01821200	1.40327800	C	-3.18656100	-3.49825900	-2.70436100
Li	-1.97001600	-1.70118300	-0.63637100	H	-3.60602900	-4.18554900	-1.96423200
O	-2.04592500	-2.62675100	1.10001100	C	-4.03320900	-3.37575200	-3.98036400
C	-2.59477400	-3.73443100	1.55403200	C	-3.93112900	-1.87864800	-4.32137200
C	-2.09324800	-4.66011700	2.41358400	C	-3.91067400	-1.24441200	-2.93328200
C	-3.02452900	-5.83384300	2.54001400	H	-3.42525700	-0.26796100	-2.87005500
C	-4.32417700	-5.26216600	1.94006100	H	-4.92493700	-1.15687800	-2.52126000
N	-3.90502400	-4.13318900	1.06629100	H	-4.76359400	-1.51958200	-4.93424900
C	-4.96533200	-3.13434000	1.14586200	H	-2.99666200	-1.66563200	-4.85348700
O	-5.64061400	-3.33613000	2.41388500	H	-5.07606400	-3.64706700	-3.77901600
C	-5.23890600	-4.57975500	2.98041100	H	-3.66670400	-4.02511200	-4.78095600
H	-6.12743500	-5.18212600	3.20857700	H	-2.15188000	-3.78458900	-2.91945000
H	-4.69492800	-4.39396100	3.91611900	C	3.91399500	-2.98949900	-0.26236700
H	-4.50773600	-2.14189600	1.16165000	C	4.73787200	-4.00229000	-1.07825500
H	-4.88148400	-6.00555700	1.36550100	C	4.84040800	-2.08742500	0.57982300
H	-3.18740000	-6.18661300	3.56911400	H	3.26545400	-3.54941500	0.42490700
H	-2.68944700	-6.71212300	1.96348800	C	5.70546000	-4.80966600	-0.19732300
H	-1.09386200	-4.62332000	2.82234000	H	5.31732000	-3.46033100	-1.83861400
Li	-0.00087700	-2.52097100	0.99243500	H	4.06999400	-4.69078000	-1.60977200
O	0.04322800	-1.80447300	-0.82865200	C	5.80309600	-2.90018100	1.45836600
C	0.62294500	-2.23319700	-1.93070300	H	5.41824700	-1.44531500	-0.09913700
C	0.17249600	-2.24053800	-3.21137700	H	4.23234100	-1.42360400	1.20972700
C	1.15544000	-2.92735100	-4.12070900	C	6.62319200	-3.89581900	0.62674400
C	2.41571100	-3.00191200	-3.22946800	H	6.30141000	-5.48784200	-0.82207100
H	2.95310500	-3.94501700	-3.35506000	H	5.12768800	-5.44894500	0.48834400
N	1.93105200	-2.85937800	-1.83292000	H	6.46850200	-2.22477900	2.01144000
C	2.95472500	-2.12382700	-1.09973000	H	5.22553700	-3.45344700	2.21491700
O	3.69997600	-1.35451400	-2.07745400	H	7.27463300	-4.49437700	1.27685900
C	3.38387700	-1.80688900	-3.39199800	H	7.28471700	-3.33971800	-0.05405200
H	4.30662800	-2.09183900	-3.91310100	C	-0.50542900	2.96940000	3.51900300
H	2.90878200	-0.98967300	-3.95197100	C	-0.37590600	3.28860300	5.01944700
H	2.46001300	-1.41723100	-0.42563400	C	-0.48658200	4.26351600	2.67873000
H	1.36734900	-2.39114100	-5.05777000	H	-1.47643000	2.47835200	3.35782700
H	0.83343700	-3.93982500	-4.41337300	C	-1.42617500	4.30884100	5.48757900
H	-0.81015700	-1.89953600	-3.50782800	H	0.62788000	3.69292400	5.21175600
O	0.94534100	-4.28233100	1.23881800	H	-0.47026600	2.36613300	5.60529000
C	1.66203500	-4.92289100	2.31686000	C	-1.53212100	5.28259000	3.15699300
C	1.98326400	-6.33538400	1.82524800	H	0.51535500	4.70804900	2.74279700
C	0.79894200	-6.63185800	0.89333000	H	-0.66827700	4.02969100	1.62140300
C	0.54213800	-5.27047100	0.24687900	C	-1.37935600	5.59507000	4.65187700
H	-0.51262900	-5.09812900	0.01923800	H	-1.27682800	4.53692100	6.55123500
H	1.14620700	-5.10285000	-0.64974900	H	-2.42915200	3.86279500	5.40394500
H	1.01840400	-7.40678900	0.15250400	H	-1.45448700	6.20174400	2.56251200
H	-0.07423500	-6.94876000	1.47415000	H	-2.54052500	4.88146500	2.97481100

H	-2.16132100	6.29246500	4.98022600	H	-9.34583500	-3.62784600	-0.26549100
H	-0.41682000	6.10089300	4.82040400	C	-1.75166200	3.16419000	-2.71174600
C	-5.99055400	-3.16473500	-0.00439200	C	-2.95882800	3.58801700	-3.56772500
C	-6.66827800	-4.52702000	-0.23742700	C	-0.65192000	4.24294300	-2.77534900
C	-7.04988800	-2.06512700	0.21103600	H	-1.35355300	2.23282700	-3.14555100
H	-5.41516900	-2.91242400	-0.90654500	C	-2.54717300	3.90423600	-5.01516000
C	-7.69617400	-4.46978100	-1.38060600	H	-3.42017400	4.47946500	-3.12002000
H	-7.17865600	-4.83697400	0.68574300	H	-3.71374600	2.79322900	-3.56267800
H	-5.91255800	-5.28915900	-0.46189200	C	-0.23384200	4.55942300	-4.21904100
C	-8.07523600	-2.00967200	-0.93132800	H	-1.03179100	5.15176900	-2.29228500
H	-7.56709500	-2.26196300	1.15902900	H	0.22112300	3.92664200	-2.18872500
H	-6.55375500	-1.09235300	0.31939200	C	-1.44204400	4.96853600	-5.07415300
C	-8.74505400	-3.37324900	-1.15124800	H	-3.42297100	4.23254000	-5.59011800
H	-8.18278300	-5.44721200	-1.49566000	H	-2.18621600	2.98315100	-5.49754700
H	-7.17193600	-4.27168500	-2.32856800	H	0.52340900	5.35426700	-4.22624900
H	-8.83151500	-1.24224100	-0.72103500	H	0.24067700	3.67277700	-4.66716700
H	-7.57189200	-1.70217000	-1.86124600	H	-1.13435900	5.14257500	-6.11351800
H	-9.44133500	-3.32792000	-1.99893400	H	-1.84000400	5.92358400	-4.70049300





7b

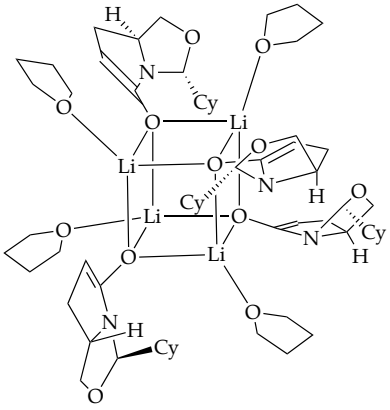
$G = -3652.059322$

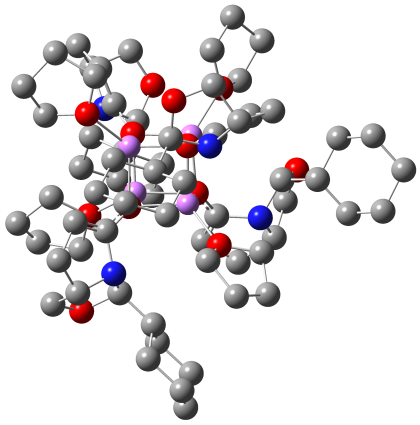
$G_{MP2} = -3641.708761$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.59963100	3.13906100	0.60210600
O	-0.17970300	1.32059100	1.48623200	H	0.80145900	3.14782900	1.69362800
C	-0.21933200	2.76642400	1.55533600	O	1.55011400	-1.27514900	0.04905200
C	-1.09940200	3.06956300	2.76298300	C	2.67557700	-0.99789100	0.67392200
C	-0.67657700	1.95780500	3.73779400	C	2.96215200	-0.02129300	1.57267700
C	-0.43023300	0.76119800	2.80733900	C	4.42066000	-0.05313600	1.94326000
H	0.44054300	0.16411100	3.09535700	C	4.85291800	-1.43015100	1.40050900
H	-1.30078800	0.10458000	2.72593400	N	3.86074900	-1.77224400	0.34891600
H	-1.43747200	1.73855200	4.49250900	C	3.73983400	-3.22594800	0.33898800
H	0.24645700	2.23648900	4.25996800	O	4.22184700	-3.69971500	1.62434200
H	-2.15562200	2.95787300	2.49928000	C	4.68393500	-2.59291600	2.39599600
H	-0.93274000	4.07607200	3.15911900	H	5.62292600	-2.87472700	2.88581600

H	3.94585300	-2.33321800	3.16882100	O	0.67270300	3.87735400	-1.69769400
H	2.68023000	-3.48605500	0.24628000	C	-0.17413200	4.03878200	-2.83506100
H	5.86586200	-1.42380700	0.98964500	H	-0.10480500	5.07735000	-3.17772400
H	4.62264400	0.02651400	3.02211200	H	-1.21771200	3.82197000	-2.56618200
H	5.00192200	0.74874500	1.46072700	H	1.11621200	1.99529300	-0.94049100
H	2.27554700	0.76865600	1.84320400	H	-1.62080900	3.01766500	-4.86280900
Li	0.11282100	-2.61341900	0.15159200	H	-0.39693200	2.06494800	-5.69769700
O	-1.43251700	-1.33201400	0.12669500	H	-1.91710000	0.46495600	-3.99670200
C	-2.55353300	-1.52500200	0.78938000	O	2.61654200	-1.35038000	-3.36313500
C	-2.87369400	-2.46632700	1.71463200	C	3.93292500	-0.76581700	-3.34752500
C	-4.31731700	-2.33676300	2.12433400	C	4.52981600	-1.17243800	-4.69060800
C	-4.68277800	-0.94794000	1.56187800	C	3.31861100	-1.01292500	-5.63001800
H	-5.70270100	-0.90324200	1.17005800	C	2.11024900	-1.33437400	-4.72499100
N	-3.69409200	-0.67964700	0.48461100	H	1.68598800	-2.32530600	-4.90893900
C	-3.48236400	0.76684800	0.45250600	H	1.31866300	-0.58168200	-4.79856300
O	-3.95226400	1.29050200	1.72212700	H	3.25782500	0.01759200	-5.99589500
C	-4.42962200	0.21933900	2.53090000	H	3.36854500	-1.67326500	-6.50082300
H	-5.33588000	0.55107800	3.04963500	H	5.38129600	-0.55003100	-4.98237200
H	-3.67588300	-0.06355200	3.28073000	H	4.86234200	-2.21635300	-4.65420900
H	-2.40830800	0.96224000	0.37143400	H	4.44768500	-1.15343600	-2.46615500
H	-4.49188500	-2.38046800	3.20998800	H	3.84762900	0.32588600	-3.26621300
H	-4.95917400	-3.11209800	1.67738900	O	-2.73438100	-1.79762000	-3.19032800
H	-2.22836000	-3.29214700	1.98351100	C	-4.12944900	-1.42774400	-3.17948400
Li	-1.33144000	-1.50000500	-1.83358100	C	-4.77753000	-2.31087100	-4.24168600
O	0.01341200	-2.93523300	-1.78383700	C	-3.67319600	-2.37597800	-5.30971800
C	0.19897800	-4.06332700	-2.43894500	C	-2.38533000	-2.39067700	-4.47347200
C	1.30068700	-4.53077700	-3.07952500	H	-1.58357300	-1.79301900	-4.91912700
C	1.01328900	-5.85503800	-3.73574500	H	-2.01879100	-3.40038900	-4.27027300
C	-0.32338700	-6.24880400	-3.07551000	H	-3.75192200	-3.25478300	-5.95664200
N	-0.92029400	-4.97690900	-2.59239500	H	-3.71182900	-1.48484300	-5.94719200
C	-1.69935900	-5.30259200	-1.40260300	H	-4.98206200	-3.30769500	-3.83541500
O	-1.19190300	-6.56356900	-0.89708700	H	-5.71681200	-1.89371400	-4.61775400
C	-0.18276000	-7.05891400	-1.77310800	H	-4.22383000	-0.36399700	-3.43933000
H	-0.34187300	-8.13320400	-1.92222500	H	-4.49954400	-1.57448100	-2.16282300
H	0.81251100	-6.91013700	-1.32898800	O	0.33364100	-3.85455400	1.65480700
H	-1.53051600	-4.52852100	-0.64552700	C	0.55523800	-3.28341500	2.97225500
H	-1.00255400	-6.75522800	-3.76634500	C	0.80767300	-4.47373000	3.89954800
H	1.77963800	-6.62534000	-3.56384000	C	1.44842600	-5.49674700	2.94842000
H	0.89304700	-5.77845800	-4.82843700	C	0.65939600	-5.27050100	1.65998400
H	2.22051000	-3.97244900	-3.18804700	H	1.23149500	-5.48583200	0.75440800
Li	1.32386900	-1.39764400	-1.88960400	H	-0.27259000	-5.84449100	1.62637300
O	-0.01955200	0.03639500	-1.96463300	H	1.36957600	-6.52778500	3.30670200
C	-0.13460700	0.96633000	-2.88905500	H	2.50424000	-5.25603500	2.78701500
C	-1.09004900	1.14263200	-3.83763300	H	-0.13882000	-4.85757600	4.29916500
C	-0.77250400	2.33666200	-4.69772700	H	1.45055500	-4.20843300	4.74430800
C	0.33573200	3.02672100	-3.87695300	H	-0.33209400	-2.70038600	3.23492900
H	1.10730100	3.48097100	-4.50402300	H	1.42097300	-2.61402800	2.91494800
N	0.91584700	1.96268900	-3.01692000	C	-3.21795900	-5.41389900	-1.63266500
C	1.38294700	2.61803700	-1.80153800	C	-3.62010300	-6.42388700	-2.72286100

C	-3.93515600	-5.73254600	-0.30540600	C	6.02224000	-3.63861500	-0.80682000
H	-3.53382500	-4.41138600	-1.96003500	C	4.25089800	-5.44907500	-0.75604500
C	-5.14566900	-6.52545500	-2.88540000	H	4.07817800	-3.53891400	-1.72519400
H	-3.22063500	-7.41211500	-2.45534000	C	6.74159800	-4.38199900	-1.94422700
H	-3.16703700	-6.14096200	-3.68069300	H	6.45268100	-3.94715300	0.15600400
C	-5.45886900	-5.82292000	-0.47539700	H	6.19521300	-2.56022800	-0.90686500
H	-3.55295700	-6.68840500	0.07709500	C	4.97270900	-6.18907300	-1.89209300
H	-3.68244500	-4.96675800	0.43926400	H	4.58630300	-5.84306100	0.21281500
C	-5.84299300	-6.84399800	-1.55569400	H	3.17040700	-5.63292900	-0.82513700
H	-5.39126600	-7.28614600	-3.63817600	C	6.47902400	-5.89337000	-1.89196400
H	-5.53497400	-5.57118000	-3.27279300	H	7.81978600	-4.17944700	-1.89979900
H	-5.92886300	-6.08571100	0.48135000	H	6.39210800	-3.98968700	-2.91184900
H	-5.85494600	-4.83464500	-0.75525200	H	4.79640100	-7.26949700	-1.80836300
H	-6.93212900	-6.86875500	-1.69234400	H	4.54371100	-5.87700900	-2.85604300
H	-5.54530600	-7.84978000	-1.22382300	H	6.96854600	-6.39557800	-2.73670000
C	-4.19609100	1.50340700	-0.69403700	H	6.92957500	-6.30666100	-0.97726100
C	-5.71387700	1.25630700	-0.75150600	C	2.90094600	2.87035200	-1.74070800
C	-3.89989900	3.01525800	-0.63931300	C	3.46429500	3.64879200	-2.94245400
H	-3.74591700	1.11157000	-1.61843100	C	3.28440200	3.56332500	-0.41799200
C	-6.37753100	2.01642500	-1.91133300	H	3.35956400	1.86997000	-1.73692200
H	-6.16133800	1.58216100	0.19783200	C	4.98069300	3.87225000	-2.82192400
H	-5.91437200	0.18267400	-0.84903400	H	2.95963600	4.62319600	-3.00383600
C	-4.55658800	3.77194500	-1.80398200	H	3.24276600	3.11038800	-3.87175700
H	-4.26988500	3.41471400	0.31420900	C	4.79966600	3.78890100	-0.30046000
H	-2.81375300	3.18150900	-0.65176800	H	2.76190200	4.52737900	-0.36162500
C	-6.07062100	3.51927700	-1.85556700	H	2.93454500	2.95676000	0.42785000
H	-7.46239200	1.84776300	-1.89763400	C	5.34989800	4.56724200	-1.50394000
H	-6.01276900	1.61103200	-2.86767900	H	5.34191200	4.45807300	-3.67743100
H	-4.35288800	4.84714900	-1.71681100	H	5.49513400	2.90036800	-2.87107700
H	-4.10273800	3.44296500	-2.75094900	H	5.02906100	4.31828500	0.63356400
H	-6.51530500	4.03223700	-2.71838700	H	5.30732300	2.81444200	-0.23873900
H	-6.53973500	3.95013800	-0.95849100	H	6.43908500	4.67887700	-1.42286500
C	4.51099400	-3.93013300	-0.79211600	H	4.92899600	5.58381800	-1.50121200





7c
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$G_{MP2} = -3641.706832$

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O	-0.66181200	-0.96867600	-1.64630400	C	3.39119700	-2.67145900	3.49987800
C	-1.11114400	-0.31161300	-2.86660700	H	4.11640800	-1.95681700	3.89907800
C	-0.88578000	-1.31819900	-4.00247600	H	2.64128500	-2.90467900	4.26370000
C	-0.88464000	-2.66809000	-3.26775300	H	4.19690800	-4.69666300	3.71495700
C	-0.19349600	-2.30564900	-1.95651900	H	4.98381600	-3.71644900	2.46003600
H	-0.45794400	-2.95034600	-1.11591200	H	2.15893400	-4.90422800	2.38062800
H	0.89739000	-2.27802400	-2.06621100	H	3.39943800	-5.02895600	1.12009200
H	-0.35696800	-3.45522400	-3.81492600	H	3.08566700	-2.72013300	0.44828400
H	-1.90969000	-3.00815000	-3.07904000	H	1.44004700	-3.03306000	1.08035700
H	0.08502900	-1.15083100	-4.48228100	O	1.99837700	0.21198500	0.05549800
H	-1.65993100	-1.24518600	-4.77190800	C	2.83021000	-0.07171900	-0.92408000
H	-0.53937900	0.61310400	-2.99416000	C	2.61642500	-0.13899100	-2.26525400
H	-2.16496000	-0.04996000	-2.74380700	C	3.86078600	-0.58962100	-2.98315100
O	-0.14018300	-0.65558900	1.89426200	C	4.93288500	-0.41460100	-1.88837800
C	-0.94871700	-1.62914500	2.25362600	H	5.69251100	-1.20048600	-1.90913100
C	-1.67559400	-2.48932900	1.49306400	N	4.19610500	-0.43294800	-0.59846200
C	-2.50277900	-3.39855200	2.36280100	C	4.92257800	0.44284000	0.31827800
C	-1.87459500	-3.16270100	3.75072600	O	5.75084400	1.31291700	-0.49627700
N	-1.21329100	-1.83648900	3.66442600	C	5.59432900	0.97477600	-1.87054800
C	-0.08172800	-1.86617100	4.58278700	H	6.58001100	0.98396000	-2.34955800
O	0.22543900	-3.26552200	4.82321600	H	4.95084300	1.71251400	-2.37230100
C	-0.69035100	-4.08270300	4.09626000	H	4.19676600	1.05959600	0.86089100
H	-0.97532400	-4.93200600	4.72710900	H	4.11337100	-0.00153200	-3.87820800
H	-0.22061400	-4.46355600	3.17726200	H	3.81365300	-1.64110900	-3.30951600
H	0.77741600	-1.39861800	4.09149000	H	1.65140000	-0.00818100	-2.73333100
H	-2.61187000	-3.17575600	4.55774000	Li	1.56552500	2.04122000	0.65619400
H	-2.45951500	-4.46266200	2.08570200	O	1.62005700	1.58366900	2.56807300
H	-3.57052500	-3.12674100	2.37517000	C	2.24897100	1.97510500	3.65646200
H	-1.78740300	-2.40385200	0.42093700	C	3.06793700	1.27988500	4.48596000
Li	1.80579100	-0.33590800	1.93222600	C	3.50354100	2.13668800	5.64516000
O	2.73676300	-2.04870300	2.36826700	C	3.10645700	3.54401100	5.15585000
C	2.50732300	-3.03617300	1.32191700	N	2.03998200	3.32785100	4.14271600
C	2.98609900	-4.37507300	1.89417800	C	2.15048700	4.41815600	3.17834200

O	3.48665700	4.96500800	3.30872200	H	4.80830700	5.61234900	-1.36468100
C	4.18985300	4.26296900	4.33256200	H	3.19445300	6.09078000	-0.80061900
H	4.76322800	4.98832900	4.92037600	H	3.80998100	4.45807100	0.90320700
H	4.88360600	3.53615300	3.88776900	C	1.12028900	5.55085600	3.33520100
H	2.03725800	4.00347700	2.17156500	C	1.04656700	6.15993800	4.74672800
H	2.74636400	4.18927800	5.96168900	C	1.37888100	6.65497200	2.29039700
H	4.57892300	2.08748400	5.87080000	H	0.14550500	5.09525300	3.10442200
H	2.97802100	1.89289700	6.58205000	C	0.00199000	7.28593100	4.82771900
H	3.27721300	0.22182200	4.39218600	H	2.03392300	6.56303800	5.01278200
Li	-0.31856600	1.23273200	2.40696500	H	0.80970400	5.38064700	5.48131900
O	-0.42284100	1.83889600	0.51458700	C	0.33412400	7.77847300	2.36654600
C	-1.25418200	2.83495100	0.28515200	H	2.38085500	7.06988700	2.45986000
C	-1.00453800	4.15639800	0.10017000	H	1.38562900	6.21809400	1.28250300
C	-2.29136900	4.91872000	-0.07541500	C	0.25754800	8.37697100	3.77863100
C	-3.29933000	3.77768000	-0.31843200	H	-0.00261100	7.72020900	5.83613400
H	-4.28039600	3.97432900	0.12233700	H	-1.00088600	6.86146400	4.66789100
N	-2.68306300	2.56924200	0.28648800	H	0.56944900	8.56141500	1.63372000
C	-3.16079700	1.42627900	-0.48083300	H	-0.65212600	7.37749500	2.08883600
O	-3.62181600	1.93619700	-1.75825600	H	-0.52627900	9.14410200	3.82778000
C	-3.44678400	3.35169600	-1.79014400	H	1.20693500	8.88336400	4.00833800
H	-4.31740700	3.79865300	-2.28269600	C	5.80728100	-0.27780500	1.35013100
H	-2.54151500	3.61387100	-2.35672800	C	6.88372300	-1.18740600	0.73079900
H	-2.31781900	0.75077300	-0.65429100	C	6.44132800	0.74980900	2.30889000
H	-2.29123000	5.62897100	-0.91571600	H	5.11728700	-0.90838600	1.92866600
H	-2.57587600	5.49807600	0.81782800	C	7.77006900	-1.84658200	1.80053300
H	-0.02628400	4.60835100	0.19602100	H	7.51509800	-0.58538600	0.06287900
O	-1.56102400	1.79030600	3.81846600	H	6.40942000	-1.96271700	0.11644200
C	-2.91536500	1.29274200	3.89412600	C	7.32502000	0.08444400	3.37407500
C	-3.48435900	1.81518400	5.23497500	H	7.04324200	1.45485900	1.72019100
C	-2.40895600	2.80839100	5.74568500	H	5.64665400	1.33163800	2.79500500
C	-1.54188700	3.05161000	4.50902400	C	8.40040400	-0.80789600	2.73860700
H	-0.49688100	3.29080500	4.71332000	H	8.55052100	-2.44999400	1.31852300
H	-1.97674700	3.82794000	3.86182200	H	7.16364800	-2.54537800	2.39723800
H	-2.83802700	3.73424800	6.14088100	H	7.79065400	0.85036300	4.00781600
H	-1.80681300	2.35091700	6.53746100	H	6.69590200	-0.52706100	4.03911300
H	-4.44752200	2.31089800	5.07796400	H	8.99416600	-1.30680600	3.51577000
H	-3.64534200	1.00291100	5.94950000	H	9.09853300	-0.17984700	2.16536800
H	-2.84886000	0.20519300	3.83011700	C	-4.28542900	0.60608900	0.17696100
H	-3.47483900	1.68339700	3.03645600	C	-5.52720200	1.42525000	0.56929300
O	2.50186600	3.46668900	-0.35243400	C	-4.68260400	-0.57233300	-0.73499100
C	3.78051400	4.11891000	-0.13422200	H	-3.84465500	0.18510200	1.09322900
H	4.58947800	3.39825400	-0.30594500	C	-6.61730000	0.54404400	1.20191500
C	3.79717300	5.24809900	-1.15877200	H	-5.93037600	1.91080300	-0.33039000
C	3.13689100	4.58241000	-2.37904900	H	-5.24461000	2.22329400	1.26689100
C	2.12630900	3.60303400	-1.75289200	C	-5.76983200	-1.45341500	-0.10197800
H	1.09855800	3.97666100	-1.76912900	H	-5.04569100	-0.16982900	-1.68996300
H	2.15974300	2.61232700	-2.21804500	H	-3.79384600	-1.17747200	-0.96033600
H	3.88729400	4.03733700	-2.96285200	C	-7.00379000	-0.62665700	0.28695600
H	2.65266300	5.30068000	-3.04763000	H	-7.50083200	1.15189600	1.43730600

H	-6.24999500	0.14484700	2.15952500	H	-2.44488200	-1.53261600	6.11042500
H	-6.05290500	-2.25817700	-0.79320800	C	0.78687700	-0.48895200	8.13459200
H	-5.36350100	-1.94180800	0.79633200	H	1.19412400	-2.27873900	6.98544300
H	-7.75210700	-1.26290400	0.77745900	H	1.80483700	-0.79625500	6.24399300
H	-7.47666400	-0.23185600	-0.62470000	C	-0.43115500	-1.00980100	8.91051400
C	-0.31296500	-1.14993200	5.92538800	H	-2.55879900	-1.34527500	8.60182500
C	-1.53573900	-1.65761100	6.71105000	H	-1.94023200	0.12951100	7.86631400
C	0.95747800	-1.22306100	6.79601900	H	1.69739100	-0.59356400	8.73892900
H	-0.48579000	-0.09578800	5.66144000	H	0.66106600	0.58784700	7.94485100
C	-1.70274900	-0.92874500	8.05471700	H	-0.56239600	-0.44625500	9.84356000
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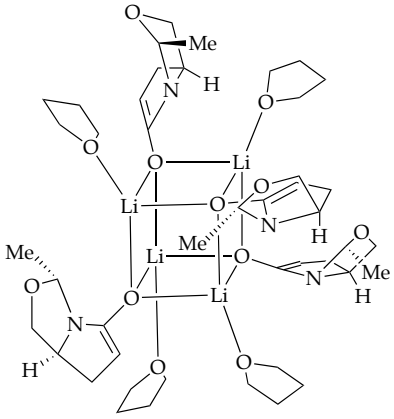

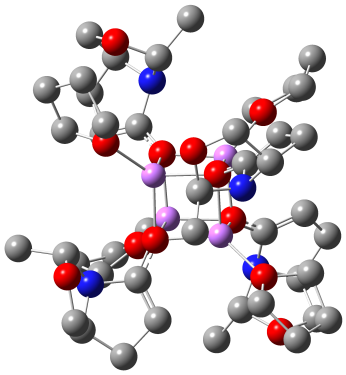

7d

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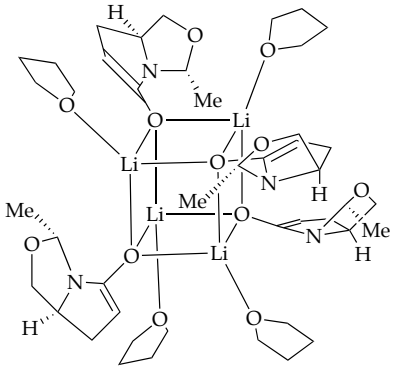
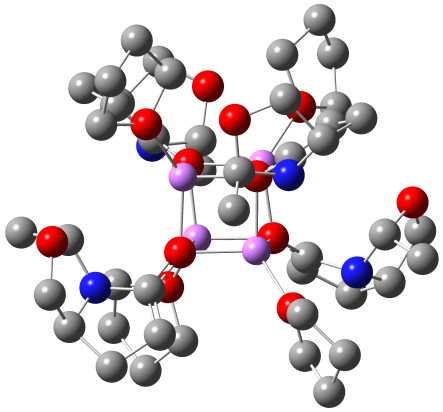
O	-1.80915900	0.73291300	0.41585700	C	-0.99949600	2.54006500	-4.35117800
C	-2.63522400	1.64549300	-0.34145600	H	-1.26601300	3.40592900	-4.97079000
C	-4.03389100	1.05014500	-0.22919000	H	-1.69230000	1.72028300	-4.57582800
C	-4.06603700	0.54845200	1.22774500	H	0.01322500	2.24591300	-1.36111900
C	-2.58007900	0.29143000	1.56556600	C	0.82689100	4.08047800	-2.14607700
H	-2.26356900	0.86753100	2.44215800	H	1.74680700	3.98644900	-1.56130500
H	-2.33879300	-0.76003200	1.72481700	H	1.06924100	4.54228500	-3.10977400
H	-4.66616600	-0.35816900	1.32833400	H	0.14027500	4.74310400	-1.61013300
H	-4.48356500	1.31090800	1.89454700	H	1.05639700	2.91631500	-5.01089300
H	-4.13621400	0.20514300	-0.91644700	H	-0.14784300	0.65183300	-6.08723600
H	-4.81884700	1.78043300	-0.44921000	H	1.59815100	0.75277700	-5.86627600
H	-2.24166700	1.70361200	-1.35637400	H	0.54477400	-1.29820000	-4.33081000
H	-2.58428700	2.64499600	0.11598500	Li	2.58041800	0.12074800	-0.88035700
O	0.84018900	-0.10357700	-1.78939600	O	4.05413600	1.02042300	-1.79746900
C	0.75049800	0.39483100	-3.00531200	C	4.31916400	2.42887100	-1.92469900
C	0.57930800	-0.22538300	-4.19911600	C	5.79860000	2.52670300	-2.35034500
C	0.63724900	0.77110500	-5.32643700	C	6.12468600	1.10937700	-2.89945900
C	0.47378600	2.10352100	-4.56705200	C	4.76864200	0.39265800	-2.87944600
N	0.93796100	1.82348200	-3.18621000	H	4.82035700	-0.67612800	-2.66575500
C	0.17384100	2.71484300	-2.33531900	H	4.20774500	0.55206700	-3.81231000

H	6.55864000	1.13374700	-3.90400100	Li	1.10033900	-2.03573600	-1.39513900
H	6.81980400	0.59391500	-2.23239500	O	0.14105000	-1.94705300	0.31959200
H	5.93839300	3.30914600	-3.10290200	C	-0.67715500	-2.79249500	0.90694300
H	6.43946700	2.76898500	-1.49767500	C	-0.81102600	-3.12345500	2.21722700
H	4.09467100	2.88624700	-0.95899700	C	-1.82029000	-4.22834300	2.38530200
H	3.64823600	2.84144100	-2.68800900	C	-2.52285800	-4.23133300	1.00768500
O	1.73052200	0.44445600	0.89777000	H	-2.75488100	-5.24512100	0.66797500
C	2.38584900	1.24155400	1.71652800	N	-1.56897600	-3.57795100	0.07582000
C	3.66474400	1.69898400	1.65658100	C	-2.38934700	-2.84087900	-0.87209400
C	3.98929800	2.51923500	2.87791100	O	-3.55671500	-2.40363400	-0.14117800
C	2.58426200	2.77720000	3.45971700	C	-3.78978100	-3.33171600	0.91819500
H	2.57744800	2.77843600	4.55401900	H	-4.69179800	-3.92624400	0.71695100
N	1.73826800	1.67537000	2.93655500	H	-3.95209700	-2.76410900	1.84207600
C	0.40537900	2.23865600	2.82821000	C	-2.80936000	-3.68574200	-2.07146800
O	0.56998200	3.63557400	2.50232500	H	-3.50234900	-3.11823800	-2.70087200
C	1.87699400	4.04524600	2.90818700	H	-1.93116500	-3.95596900	-2.66439100
H	1.80582000	4.83453400	3.66848700	H	-3.31057800	-4.60714700	-1.75384200
H	2.40589300	4.44840300	2.03604200	H	-1.85912500	-1.94438900	-1.20176700
C	-0.38342900	2.09834300	4.12951000	H	-2.54487200	-4.07126400	3.19759300
H	-1.33844400	2.62785400	4.04739200	H	-1.35377600	-5.20849400	2.57679100
H	-0.58003400	1.04299600	4.34805100	H	-0.17947300	-2.73691900	3.00648300
H	0.16922600	2.52672700	4.97286100	O	0.85918300	-3.72031600	-2.43293000
H	-0.12972100	1.77068100	2.00024200	C	0.75668400	-4.04028900	-3.83604700
H	4.51063300	3.46491900	2.67100200	C	0.56790000	-5.55639900	-3.90064000
H	4.61268000	1.97557900	3.60641800	C	1.37829700	-6.03006200	-2.68450800
H	4.38909800	1.39991900	0.90991000	C	1.10877700	-4.92879900	-1.65722800
Li	1.93107400	-1.50273000	1.10971600	H	1.96624900	-4.73336400	-1.00837400
O	2.92341200	-1.80619200	-0.56224300	H	0.21712300	-5.11645700	-1.05186000
C	3.93463100	-2.58923200	-0.86836500	H	1.07486600	-7.01695300	-2.32208700
C	4.17900200	-3.30631400	-1.99622800	H	2.44550100	-6.06934500	-2.93091100
C	5.41424200	-4.15021100	-1.83144600	H	-0.49075400	-5.81512900	-3.78152700
C	6.06697800	-3.50846500	-0.58771100	H	0.91724200	-5.97856500	-4.84782400
N	4.96064400	-2.82278400	0.13063100	H	1.67847400	-3.72734900	-4.34444300
C	5.56658500	-1.63804900	0.71975400	H	-0.08242600	-3.47728600	-4.25394000
O	6.58206200	-1.20179200	-0.21020800	O	2.54977800	-2.25394700	2.79751800
C	7.06088400	-2.35253600	-0.90543600	C	2.75497300	-3.68587400	2.93792600
H	8.08152200	-2.60171500	-0.58225500	H	3.56249700	-3.97864500	2.26108500
H	7.08580700	-2.11980400	-1.97607800	C	3.07227300	-3.91973300	4.42155100
C	6.18971100	-1.91307100	2.08576600	C	2.42796100	-2.70087000	5.10472100
H	6.71005800	-1.01754800	2.44002400	C	2.68498900	-1.59945300	4.07976400
H	5.41214500	-2.17757800	2.80797600	H	1.98463600	-0.76180500	4.10245300
H	6.91385700	-2.73427000	2.03897100	H	3.70419300	-1.20062000	4.17304600
H	4.82838200	-0.83854800	0.79510300	H	2.86380600	-2.47398200	6.08259500
H	6.54041700	-4.25105600	0.06111200	H	1.35078200	-2.85701400	5.23665500
H	6.10175000	-4.13657100	-2.68960200	H	4.15575200	-3.91791100	4.58978800
H	5.18607900	-5.21173200	-1.63820400	H	2.67847200	-4.87472000	4.78215000
H	3.49611700	-3.36981500	-2.83270400	H	1.82446500	-4.17767700	2.63362600





7e
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G_{MP2} = –2863.022253

Atom	X	Y	Z	Atom	X	Y	Z
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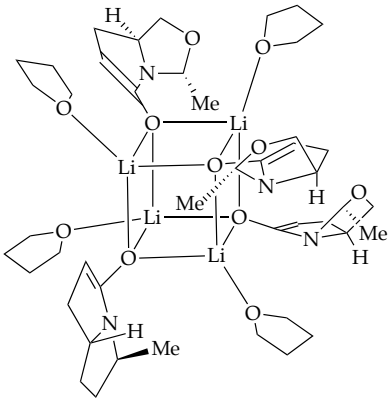
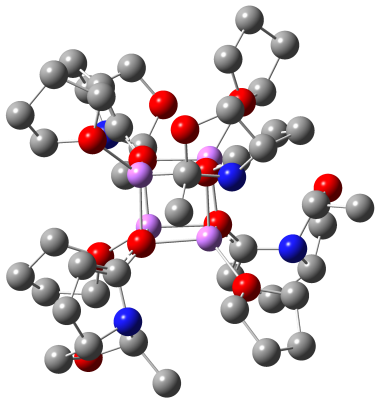
O	-1.17823600	-0.52304700	-1.49780300	Li	2.34228100	1.17554400	-0.11920500
C	-2.44312900	-1.21942600	-1.59804700	O	0.47396700	1.88823800	-0.10766000
C	-3.08416700	-0.67610300	-2.87108100	C	0.15103600	3.00151700	-0.72974200
C	-1.86004800	-0.51210500	-3.78661900	C	0.88528500	3.80171100	-1.54277500
C	-0.77032500	-0.04536500	-2.81297000	C	0.10082500	5.03080200	-1.92000900
H	0.21640300	-0.46355900	-3.03391500	C	-1.33262200	4.62511100	-1.51448200
H	-0.70723500	1.04354800	-2.75928800	H	-1.90751800	5.46519300	-1.11357300
H	-2.02212700	0.20979400	-4.59219800	N	-1.16436800	3.56974700	-0.48321800
H	-1.58930600	-1.47328500	-4.24012900	C	-2.30356500	2.68372800	-0.64586900
H	-3.54045300	0.30015900	-2.68021200	O	-2.62677700	2.68781100	-2.05736500
H	-3.84192800	-1.35256400	-3.27875000	C	-2.13560000	3.90125100	-2.63126000
H	-3.00191100	-1.03573900	-0.67873900	H	-2.97183100	4.51433400	-2.99300700
H	-2.25213800	-2.29919600	-1.67449500	H	-1.49509800	3.64822300	-3.48469300
O	1.85513500	-0.72403300	-0.03450900	C	-3.52083900	3.12028800	0.16495300
C	2.17927100	-1.87124800	-0.59010400	H	-4.38029400	2.49359100	-0.09424300
C	1.50316000	-2.65605100	-1.46624700	H	-3.32522100	3.01609200	1.23687600
C	2.26462300	-3.92852100	-1.72976600	H	-3.78436300	4.16377300	-0.04126300
C	3.66005700	-3.58047600	-1.16898000	H	-2.01721300	1.66410300	-0.38230800
N	3.42224800	-2.50050600	-0.17897100	H	0.14732400	5.29822500	-2.98569800
C	4.61648800	-1.67748400	-0.21130600	H	0.41867600	5.92676000	-1.36292500
O	5.09922000	-1.71316800	-1.57631500	H	1.93719100	3.65212700	-1.75038300
C	4.61918900	-2.91051000	-2.19283200	Li	0.60445100	1.84809600	1.86733400
H	5.46078300	-3.56716400	-2.45095100	O	2.53140600	1.41746700	1.82299000
H	4.09283300	-2.63953800	-3.11581200	C	3.59356900	1.89653700	2.43456200
H	4.35630200	-0.64218200	0.01678200	C	4.69209000	1.26396100	2.92040400
C	5.69934300	-2.17437900	0.74242900	C	5.59865700	2.24362500	3.61919800
H	5.36626400	-2.06965800	1.78018500	C	5.03304100	3.59864300	3.13771800
H	5.93770300	-3.22778700	0.55793200	N	3.63660000	3.31701500	2.72134300
H	6.61328100	-1.58735300	0.60613200	C	3.36484100	4.22561300	1.61901300
H	4.14591400	-4.43739000	-0.69285200	O	4.62073300	4.41755600	0.92811700
H	2.32672900	-4.21688800	-2.78938700	C	5.68637400	4.14981000	1.83936800
H	1.84373800	-4.79706300	-1.19770200	H	6.25979100	5.06663500	2.03316700

H	6.35844500	3.41300800	1.38263700	C	2.43154700	-1.09307400	4.70847100
C	2.82021300	5.57281400	2.08516100	H	3.12622300	-0.25462200	4.79932700
H	2.74655500	6.25445000	1.23197000	H	1.40795200	-0.73399100	4.86800800
H	1.82417400	5.44554100	2.52027700	H	1.89687700	-2.58983000	6.20801100
H	3.47513200	6.02948600	2.83589400	H	3.57404800	-2.05174200	6.33330100
H	2.66946600	3.76578000	0.91308900	H	2.90714500	-4.40928800	4.99969000
H	5.05146000	4.35880100	3.92464500	H	4.26179000	-3.39764900	4.46213300
H	6.66368800	2.14773300	3.36269000	H	2.87031000	-3.38207100	2.44055900
H	5.53956800	2.17330300	4.71755000	H	1.37329100	-3.28940300	3.42215200
H	4.82534900	0.18967900	2.92231700	O	0.03346200	3.17685900	3.19912800
Li	1.87917600	-0.45931100	1.90040100	C	-1.14097400	4.01126600	3.14020400
O	-0.05272400	-0.02762500	1.97336100	C	-0.87524500	5.11708900	4.15766900
C	-0.85307600	-0.51378100	2.89578100	C	-0.15212700	4.34792000	5.27821500
C	-1.47882400	0.09562300	3.93488600	C	0.63684100	3.26460500	4.51915200
C	-2.25219100	-0.90759800	4.74966900	H	0.56506300	2.28308800	5.00023800
C	-2.27515000	-2.12418300	3.80092100	H	1.68997900	3.51388000	4.36638000
H	-2.21140200	-3.07592100	4.33684300	H	0.50188200	4.98575800	5.88017100
N	-1.10013900	-1.94673400	2.91263400	H	-0.88440000	3.88993100	5.95288700
C	-1.47517400	-2.57169900	1.65912100	H	-0.22033000	5.88121000	3.72397500
O	-2.89897500	-2.36033000	1.50535500	H	-1.79323400	5.60627400	4.49785000
C	-3.46394200	-2.13848900	2.80060600	H	-2.02391200	3.41800100	3.42048200
H	-4.18594300	-2.93141100	3.03639900	H	-1.24787200	4.34344900	2.10538500
H	-3.98920200	-1.17636000	2.79375600	O	3.65326400	1.61182900	-1.48711100
C	-1.16088200	-4.06492100	1.62074600	C	3.40610000	1.19411100	-2.85331900
H	-1.57597400	-4.50523700	0.70850000	C	4.61988700	1.67687600	-3.64640200
H	-0.07825100	-4.22581600	1.62359400	C	5.74682400	1.54783300	-2.60926900
H	-1.59534200	-4.58614000	2.48096800	C	5.05072500	1.98092600	-1.31787000
H	-0.97301400	-2.07238200	0.82803900	H	5.42786400	1.47153800	-0.42641300
H	-3.27314600	-0.59458800	5.01248500	H	5.09521400	3.06011600	-1.14567200
H	-1.75594700	-1.17087000	5.69834900	H	6.61686300	2.17140600	-2.83779000
H	-1.36028400	1.14015200	4.18736500	H	6.06660900	0.50418800	-2.53238900
O	2.55128900	-1.57730400	3.34807800	H	4.48934100	2.72299000	-3.94908100
C	2.43520200	-3.01393900	3.37221000	H	4.79107000	1.07817100	-4.54620900
C	3.18112700	-3.41159100	4.64292600	H	2.46112800	1.64555700	-3.16964700
C	2.77485800	-2.29147100	5.62580500	H	3.31795000	0.10229100	-2.87377600





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G_{MP2} = –2863.017156

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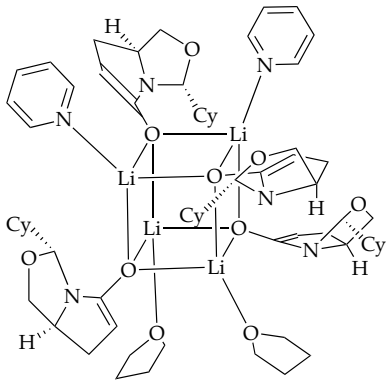
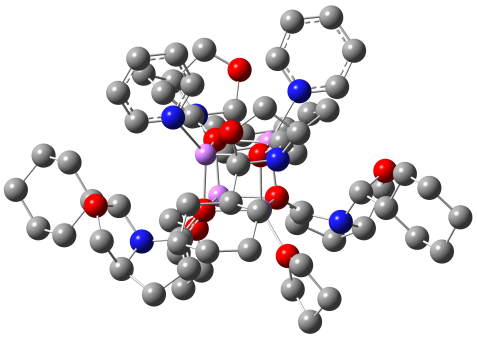
O	-0.11626900	0.07430500	1.98961200	O	0.48613300	3.56081500	-2.18528500
C	0.30329600	-1.00380900	2.87706000	C	0.34900400	4.13784600	-0.85417700
C	0.44989100	-0.37714200	4.27529600	C	-0.02238100	5.60661600	-1.07359200
C	-0.34096400	0.93716500	4.16074400	C	0.60954200	5.90821000	-2.44083500
C	-0.08143800	1.32782600	2.70968800	C	0.36859500	4.59730800	-3.18785500
H	-0.84288200	1.97667600	2.27207500	H	1.10652500	4.39364300	-3.96872400
H	0.90628700	1.78888800	2.58100300	H	-0.63975600	4.56888400	-3.61377000
H	-0.00749400	1.70160600	4.86926600	H	0.15358300	6.76341900	-2.94862700
H	-1.41140100	0.76248600	4.31997800	H	1.68394200	6.10131100	-2.33655700
H	1.50199300	-0.16412200	4.49539700	H	-1.10955400	5.71993100	-1.13322600
H	0.07079700	-1.03802900	5.06012300	H	0.35215900	6.25123000	-0.27239600
H	1.24613100	-1.41794300	2.50369700	H	1.31287900	4.01724600	-0.34899900
H	-0.45801700	-1.78526100	2.83335300	H	-0.42126800	3.57560100	-0.31819100
O	-1.21707400	0.93478800	-1.28555900	O	1.66344800	0.77861800	-0.76468200
C	-2.37725500	1.44991300	-0.94541000	C	2.69058700	1.23354300	-0.08088900
C	-2.93970100	1.63633600	0.27741800	C	3.14930000	0.89973600	1.15457000
C	-4.33204200	2.19655600	0.13953200	C	4.30722000	1.78034800	1.54639900
C	-4.34327900	2.64854700	-1.33587300	C	4.69235100	2.40815100	0.19043800
N	-3.29850100	1.83305800	-1.99649400	H	5.01260500	3.45004100	0.28563300
C	-2.79590500	2.64030600	-3.08981200	N	3.47093900	2.31423100	-0.64602200
O	-2.93885200	4.02614600	-2.68285200	C	3.94269900	2.16089600	-2.01174200
C	-3.84417300	4.09461300	-1.57850600	O	5.20501900	1.45369000	-1.93682500
H	-4.66560000	4.78166500	-1.81773500	C	5.73215400	1.58918000	-0.61760100
H	-3.31259800	4.47842500	-0.69766600	H	6.70921700	2.08848100	-0.65413700
H	-1.73189600	2.43992000	-3.23340100	H	5.86807700	0.58907100	-0.18627100
C	-3.55360400	2.40978500	-4.39312800	C	4.15224500	3.49677700	-2.71684900
H	-3.37575400	1.39143800	-4.75268200	H	4.59835000	3.32970400	-3.70238700
H	-4.63098600	2.55278800	-4.25351800	H	3.19388600	4.00827800	-2.84141000
H	-3.21038500	3.11766900	-5.15466500	H	4.82235700	4.14503800	-2.14121700
H	-5.31414400	2.49329400	-1.81687600	H	3.24619400	1.53660400	-2.57817300
H	-4.55784800	3.03770900	0.81144600	H	5.16127600	1.24840000	1.99042900
H	-5.11597700	1.44230900	0.31407800	H	4.02549300	2.56601800	2.26626300
H	-2.52558900	1.25519700	1.20108100	H	2.65971600	0.19930400	1.81657100

Li	1.64381700	-0.84939900	-1.88025000	C	-3.61960100	-2.62687400	0.74235100
O	0.65019600	0.01801400	-3.34924900	H	-3.94295900	-2.31406100	1.74063800
C	0.80505300	0.19370200	-4.64481000	H	-3.97545900	-1.89107300	0.01474300
C	0.89348500	1.33577700	-5.37151600	H	-4.07954600	-3.59618400	0.52049300
C	0.98960900	1.02343900	-6.84213900	H	-1.66405600	-1.72550500	0.83058700
C	1.32278900	-0.48255800	-6.81655900	H	0.21728700	-6.08473800	-0.66489900
N	0.81664600	-0.97137400	-5.51074300	H	-0.75511000	-5.69050800	-2.08081500
C	1.66934300	-2.08992200	-5.15149900	H	1.39693500	-3.95486300	-1.88353700
O	2.96155100	-1.84770000	-5.76313300	O	-2.48470200	-1.30486200	-3.55796800
C	2.83398200	-0.80161200	-6.72850100	C	-3.84025500	-1.43905900	-3.07833400
H	3.24506000	-1.14049300	-7.68723000	C	-4.71251100	-1.67298700	-4.33499200
H	3.39975700	0.07651300	-6.39178700	C	-3.68523700	-1.89594100	-5.47500800
C	1.13653100	-3.43477500	-5.63621000	C	-2.37602500	-2.14234400	-4.72253800
H	1.89239000	-4.20927000	-5.47065400	H	-1.47129600	-1.84268100	-5.25437000
H	0.23141200	-3.71024800	-5.08609100	H	-2.28955200	-3.19356400	-4.40738700
H	0.90544600	-3.40458900	-6.70679100	H	-3.95129300	-2.73031900	-6.13129000
H	1.80521100	-2.11623400	-4.06764100	H	-3.59333500	-0.99695600	-6.09352400
H	0.85855400	-1.03484200	-7.63961900	H	-5.35958600	-2.54535600	-4.19945700
H	1.76428600	1.58837300	-7.38077500	H	-5.35772600	-0.81462200	-4.54308500
H	0.04474800	1.19878300	-7.38097300	H	-4.07185000	-0.51705300	-2.54244400
H	0.77488900	2.33111400	-4.96326600	H	-3.88334400	-2.29305400	-2.39202900
Li	-0.99280900	-0.63954200	-2.46019700	O	3.31452600	-1.89511500	-1.86383000
O	0.00354600	-1.63922900	-1.06135600	C	4.48039300	-1.78232400	-2.72324100
C	-0.27724700	-2.92358500	-0.98958700	H	4.96682300	-0.81564900	-2.54582000
C	0.44652800	-4.00747900	-1.36857200	C	5.36187400	-2.94971100	-2.29382800
C	-0.34392700	-5.27153100	-1.14826400	C	5.17059100	-2.94752000	-0.76672500
C	-1.48337900	-4.77036600	-0.23757500	C	3.72109800	-2.45531600	-0.58389000
H	-2.43615700	-5.27342500	-0.43006500	H	3.01882300	-3.26161400	-0.35460400
N	-1.59263500	-3.31878300	-0.51780100	H	3.64074300	-1.67514300	0.18017100
C	-2.09777000	-2.71990100	0.70143200	H	5.87295600	-2.24751000	-0.30021100
O	-1.64809500	-3.55683700	1.80106700	H	5.33166500	-3.93091500	-0.31447300
C	-1.15269300	-4.78916900	1.27347100	H	6.40627200	-2.82006000	-2.59395500
H	-1.63172400	-5.62582600	1.79642900	H	4.99192800	-3.88429700	-2.73186700
H	-0.06775000	-4.84757700	1.43201500	H	4.13517200	-1.83360600	-3.75744600

Table 5. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the pyridine solvated tetramers with the lowest energy isomer at –78 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: G_{MP2} includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



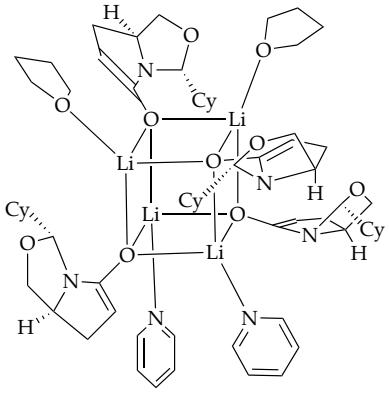


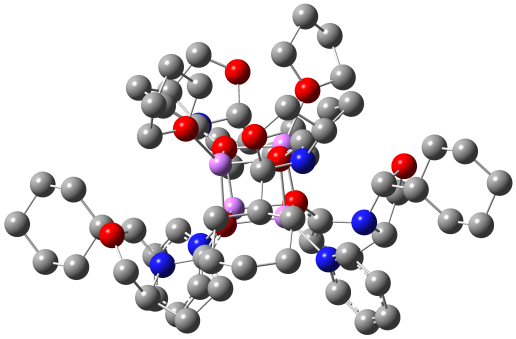
21
G = –3683.785025
G_{MP2} = –3673.334167

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-4.35193800	0.06315800	2.55919500
O	1.59445100	-1.24328000	0.04297300	H	-5.25279800	0.37303600	3.10116400
C	2.72076800	-0.96222100	0.66659600	H	-3.57188400	-0.19969300	3.28837800
C	3.00427300	0.02473500	1.55445000	H	-2.42351300	0.85966300	0.32873400
C	4.46329500	0.00098900	1.92360500	H	-4.33502700	-2.53162400	3.24711900
C	4.89524900	-1.38503600	1.40503900	H	-4.80603900	-3.28513800	1.72570900
N	3.90415200	-1.74784400	0.35787400	H	-2.05781400	-3.35144400	2.01059900
C	3.77548300	-3.20346200	0.38928600	Li	-1.27006100	-1.47904900	-1.85987200
O	4.23585200	-3.64146400	1.69103900	O	0.12615500	-2.86321000	-1.87669300
C	4.72369100	-2.52481500	2.42732600	C	0.33852000	-3.95626000	-2.57746400
H	5.66657000	-2.80447900	2.91188100	C	1.45172300	-4.38207800	-3.22663100
H	3.99979200	-2.23865200	3.20399400	C	1.19568500	-5.69438400	-3.91878900
H	2.71724600	-3.46417400	0.29040600	C	-0.13576000	-6.13224000	-3.27611700
H	5.90848000	-1.38667300	0.99477700	N	-0.76526000	-4.88329300	-2.77785300
H	4.66572700	0.09978200	3.00055800	C	-1.55584000	-5.24535600	-1.61126500
H	5.04190000	0.79550900	1.42621700	O	-1.00947900	-6.49432200	-1.10376100
H	2.31252400	0.80692900	1.83515200	C	0.01474200	-6.95991400	-1.98469500
Li	0.21438900	-2.63335300	0.08984700	H	-0.12645600	-8.03405700	-2.15039200
O	-1.37168600	-1.39428900	0.10243800	H	1.00212400	-6.79872300	-1.52971800
C	-2.47611500	-1.62263600	0.78478400	H	-1.42631200	-4.47334900	-0.84448800
C	-2.74378000	-2.56647400	1.72314400	H	-0.79665600	-6.64357300	-3.98057200
C	-4.18304100	-2.48613700	2.15825700	H	1.97707000	-6.45232800	-3.76044200
C	-4.60350300	-1.11243700	1.59928700	H	1.07916400	-5.59469100	-5.01017900
H	-5.63447500	-1.09704700	1.23506100	H	2.36450500	-3.80752700	-3.30487300
N	-3.65218000	-0.82108000	0.49373600	Li	1.40123500	-1.29358900	-1.90494600
C	-3.48635800	0.63245400	0.45494800	O	0.00176700	0.08009800	-1.96730100
O	-3.91975400	1.14285800	1.73923700	C	-0.18614200	1.06296100	-2.82158900

C	-1.24554100	1.33716700	-3.62418700	H	-3.56776900	-4.96977800	0.20409100
C	-0.98004800	2.56538700	-4.45305400	C	-5.65259100	-6.90162100	-1.82026700
C	0.25275300	3.16019600	-3.74276100	H	-5.16147700	-7.33258600	-3.89632100
H	0.95762100	3.62426900	-4.43738300	H	-5.35501000	-5.62194000	-3.53413700
N	0.88747900	2.02120700	-3.03232800	H	-5.78561700	-6.14538300	0.21521500
C	1.53358400	2.57087200	-1.85104200	H	-5.72663700	-4.89311600	-1.02062600
O	0.87940900	3.83670800	-1.56181700	H	-6.73874900	-6.95421600	-1.97160100
C	-0.07590500	4.12305200	-2.58527000	H	-5.33394600	-7.89958000	-1.48407600
H	0.01986200	5.17738600	-2.86850400	C	-4.25872200	1.35214500	-0.66344700
H	-1.09362700	3.94649400	-2.21091300	C	-5.77097400	1.07028600	-0.67599800
H	1.36111600	1.89143900	-1.00909100	C	-3.99389300	2.87001700	-0.60549000
H	-1.80876600	3.28875600	-4.47506400	H	-3.82852300	0.97758400	-1.60419200
H	-0.74164400	2.33685600	-5.50471800	C	-6.48683400	1.82515300	-1.80830100
H	-2.11665300	0.70341700	-3.71448100	H	-6.19639800	1.37797400	0.28944900
O	2.74102900	-1.14747100	-3.33176400	H	-5.95025200	-0.00697900	-0.77793500
C	4.16094300	-0.91478000	-3.30475800	C	-4.70146300	3.61972800	-1.74402300
C	4.65568700	-1.48786600	-4.62873200	H	-4.34290700	3.25267900	0.36254600
C	3.53188500	-1.05742300	-5.59057100	H	-2.91227100	3.05790400	-0.64635300
C	2.26978900	-1.07964300	-4.70375500	C	-6.21040700	3.33429200	-1.75107600
H	1.65441100	-1.96947000	-4.86680000	H	-7.56703800	1.63313800	-1.76282500
H	1.65603300	-0.18149600	-4.81848000	H	-6.14356900	1.43471300	-2.77891500
H	3.72102800	-0.04431500	-5.96235100	H	-4.51957200	4.69894000	-1.65566900
H	3.43776600	-1.71829900	-6.45720200	H	-4.26947200	3.30724200	-2.70674600
H	5.63783000	-1.10111200	-4.91749600	H	-6.69341800	3.84294700	-2.59582600
H	4.71966900	-2.58039000	-4.56643300	H	-6.66036900	3.74859100	-0.83653700
H	4.55054100	-1.39295700	-2.40447100	C	4.55272300	-3.95224000	-0.70851400
H	4.35732200	0.16492500	-3.24639000	C	6.06574800	-3.67095700	-0.72480400
O	-2.66125300	-1.76582300	-3.23241300	C	4.28431900	-5.46722100	-0.60998700
C	-4.08173100	-1.51246800	-3.23368500	H	4.12608500	-3.60200400	-1.66053900
C	-4.62498500	-2.32704100	-4.40399400	C	6.78820700	-4.46357300	-1.82662500
C	-3.48995800	-2.18895800	-5.43224400	H	6.48676800	-3.94466500	0.25258800
C	-2.23039400	-2.19729800	-4.55444400	H	6.24853100	-2.59843400	-0.86457200
H	-1.46218900	-1.50131900	-4.90620600	C	5.00513400	-6.25544700	-1.71362000
H	-1.79953100	-3.19565900	-4.44022200	H	4.61624400	-5.82115000	0.37503900
H	-3.47994100	-2.99432400	-6.17269700	H	3.20282900	-5.64877300	-0.66658300
H	-3.58163600	-1.23794500	-5.96981600	C	6.51377000	-5.96984400	-1.71732700
H	-4.75577300	-3.37488000	-4.11172500	H	7.86768500	-4.26763400	-1.78174200
H	-5.58541200	-1.94887300	-4.76765200	H	6.44948900	-4.10689800	-2.81168700
H	-4.25906400	-0.43895600	-3.38689800	H	4.82190500	-7.33087300	-1.58930900
H	-4.46790300	-1.79279800	-2.25141900	H	4.58310800	-5.97777700	-2.69119000
C	-3.06590400	-5.40433600	-1.86279100	H	7.00443200	-6.50789400	-2.53912000
C	-3.42593900	-6.42376900	-2.95850900	H	6.95629900	-6.35026400	-0.78463900
C	-3.79121700	-5.74144300	-0.54434600	C	3.05242500	2.78810900	-1.96878200
H	-3.40532100	-4.41130100	-2.19412100	C	3.48608700	3.64213200	-3.17301400
C	-4.94618000	-6.56545800	-3.14085700	C	3.61414400	3.36990900	-0.65581400
H	-3.00410800	-7.40163800	-2.68694000	H	3.47543900	1.78092000	-2.09754700
H	-2.96863700	-6.12677900	-3.90998900	C	5.01170400	3.82715500	-3.22332000
C	-5.30955600	-5.87095600	-0.73515700	H	3.00525400	4.62822800	-3.10449800
H	-3.39054100	-6.68777000	-0.15653700	H	3.14007300	3.17608600	-4.10333300

C	5.13811900	3.55522400	-0.71015700	H	-0.68875100	3.56300400	4.74775000
H	3.13350700	4.33932000	-0.46850100	H	0.17701600	3.20382700	0.54515600
H	3.34671600	2.71132400	0.18112800	H	-0.07442800	4.63696700	2.55959300
C	5.55825400	4.41169800	-1.91332500	H	-1.04628600	1.07480600	4.79449000
H	5.28329200	4.46954400	-4.07133900	H	-0.78262600	-0.20991000	2.67707800
H	5.48874700	2.85212900	-3.40742700	C	1.04005000	-3.38430200	2.77738500
H	5.49436600	4.00943300	0.22367200	C	1.23469300	-4.06281000	3.97834900
H	5.62288300	2.56971600	-0.78104000	C	0.90732600	-5.41596300	4.04188100
H	6.65179300	4.49759900	-1.96050900	C	0.40067300	-6.03536400	2.90058800
H	5.16850700	5.43240500	-1.78378100	C	0.23220100	-5.27889000	1.74161200
C	-0.08834400	2.76410700	1.50389300	N	0.54080900	-3.97056800	1.67501300
C	-0.23011500	3.56541200	2.63607800	H	1.04891100	-5.97781400	4.96132100
C	-0.57166000	2.96609100	3.84719600	H	1.30636200	-2.33427000	2.68209500
C	-0.76848700	1.58661700	3.87842400	H	1.64127400	-3.53788900	4.83710200
C	-0.61093300	0.86350500	2.69850700	H	0.13553500	-7.08803400	2.89887100
N	-0.26784100	1.43073300	1.52851400	H	-0.16770500	-5.73316500	0.83749000





22

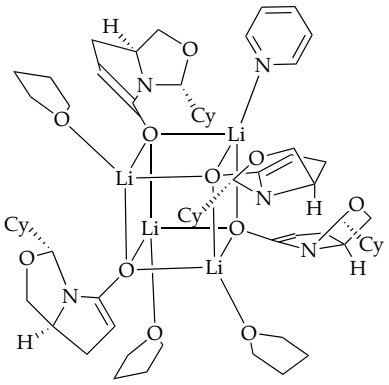
$G = -3683.789496$

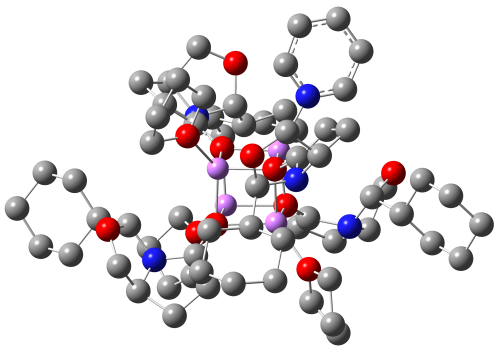
$G_{MP2} = -3673.339800$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.57654300	1.29308100	0.67766700
O	0.04303300	-1.28640200	1.50571600	C	-2.99548600	0.35887100	1.56893800
C	-0.06185700	-2.72652700	1.60004800	C	-4.42784100	0.60419700	1.96313400
C	0.79434000	-3.09120300	2.80781800	C	-4.65742800	2.03793000	1.44302800
C	0.48284800	-1.93014200	3.76722400	N	-3.63533800	2.24660600	0.38394900
C	0.33185900	-0.73026800	2.81924700	C	-3.29084300	3.66834200	0.39954900
H	-0.49142900	-0.06440000	3.09632800	O	-3.72898900	4.19471500	1.67865300
H	1.25089300	-0.14378800	2.73089300	C	-4.30921900	3.14713300	2.45035100
H	1.26851600	-1.76736200	4.51075100	H	-5.18708000	3.54390200	2.97227500
H	-0.45503700	-2.11755400	4.30330800	H	-3.59206800	2.77464700	3.19723600
H	1.85435800	-3.08209400	2.53483100	H	-2.20212000	3.76268800	0.33758900
H	0.53930500	-4.07171000	3.22156800	H	-5.66404200	2.18938400	1.04309400
H	0.27263900	-3.15103400	0.65170000	H	-4.62332400	0.54209400	3.04434400
H	-1.11465800	-3.00248900	1.74999200	H	-5.12890000	-0.09598800	1.48204500
O	-1.43334500	1.40639700	0.03578700	H	-2.42916900	-0.52614000	1.82557700

Li	0.10278600	2.62774100	0.00014100	H	0.41653400	-2.47884500	-5.51285300
O	1.53607900	1.22166200	0.03618100	H	1.97441600	-0.93980300	-3.80552800
C	2.67940300	1.33510800	0.67781400	O	0.06003700	3.91417100	1.50585800
C	3.09853300	2.26937400	1.56891900	C	-0.22843300	3.35828000	2.81956300
C	4.53094500	2.02402600	1.96288800	C	-0.38006600	4.55835300	3.76721200
C	4.76040900	0.59025700	1.44279400	C	-0.69156800	5.71913700	2.80746200
H	5.76697300	0.43880200	1.04273900	C	0.16501400	5.35429700	1.60002600
N	3.73818100	0.38158900	0.38388400	H	-0.16897900	5.77868400	0.65145500
C	3.39366600	-1.04012900	0.39955400	H	1.21778200	5.63019800	1.75041300
O	3.83157100	-1.56638700	1.67879200	H	-0.43680200	6.69977900	3.22105700
C	4.41235600	-0.51891600	2.45023900	H	-1.75151900	5.70977000	2.53422600
H	5.29037900	-0.91581500	2.97180100	H	0.55761300	4.74616000	4.30352200
H	3.69557500	-0.14633600	3.19742600	H	-1.16587900	4.39551400	4.51057200
H	2.30495500	-1.13447600	0.33749500	H	0.59522500	2.69294500	3.09685100
H	4.72660000	2.08618100	3.04406000	H	-1.14712300	2.77123300	2.73137400
H	5.23194000	2.72416600	1.48164100	C	3.35087800	5.20729400	-1.78913200
H	2.53221000	3.15431900	1.82576500	C	3.93787000	5.99531700	-2.97355400
Li	1.38584300	1.29481300	-1.92520600	C	3.91317200	5.73459600	-0.45445100
O	0.11285900	2.78524800	-1.95883400	H	3.65916900	4.15633100	-1.89487600
C	0.03482000	3.78853800	-2.81014200	C	5.47552700	5.99685000	-2.95330300
C	-0.96298100	4.13783400	-3.66213600	H	3.57415200	7.03160400	-2.92861600
C	-0.57083400	5.34817600	-4.46896300	H	3.58303900	5.56528800	-3.91742300
C	0.67753600	5.84431700	-3.70930900	C	5.44932600	5.73496000	-0.43602900
N	1.17836800	4.66655500	-2.95874700	H	3.54151600	6.75565600	-0.29511300
C	1.81274900	5.17236400	-1.74880900	H	3.53220200	5.12060000	0.37265200
O	1.29421000	6.50851800	-1.52644700	C	6.02723500	6.52268200	-1.62061800
C	0.39049300	6.84740700	-2.57760200	H	5.86038600	6.59716200	-3.78849800
H	0.57036400	7.88780900	-2.87100500	H	5.83810100	4.97047600	-3.11416000
H	-0.64890600	6.75106000	-2.23268600	H	5.81483800	6.15006300	0.51246800
H	1.51719400	4.53899600	-0.90455200	H	5.81168600	4.69670800	-0.48235600
H	1.45089100	6.23481800	-4.37661900	H	7.12423100	6.47359100	-1.61482000
H	-1.34119900	6.13250800	-4.51602100	H	5.76050300	7.58465900	-1.51294700
H	-0.31319300	5.10698500	-5.51277400	C	4.01446200	-1.87289700	-0.73458200
H	-1.87135700	3.56809800	-3.80552100	C	5.54964500	-1.80243300	-0.81222900
Li	-1.28245000	1.33306700	-1.92571200	C	3.55310800	-3.34058600	-0.63679300
O	-0.00983600	-0.15738700	-1.95868500	H	3.60060600	-1.45681000	-1.66570400
C	0.06828700	-1.16056100	-2.81014700	C	6.10096400	-2.65437000	-1.96779200
C	1.06613600	-1.50969500	-3.66214400	H	5.97063000	-2.16027700	0.13768700
C	0.67412900	-2.72004800	-4.46903500	H	5.87497100	-0.76171400	-0.93350800
C	-0.57421400	-3.21633800	-3.70945400	C	4.09734400	-4.19330600	-1.79221100
H	-1.34756400	-3.60688100	-4.37675400	H	3.89531400	-3.75482600	0.32095600
N	-1.07517700	-2.03864800	-2.95881200	H	2.45548500	-3.38292800	-0.62688800
C	-1.70955400	-2.54460400	-1.74888400	C	5.62825000	-4.11259900	-1.87531700
O	-1.19150400	-3.88100800	-1.52702200	H	7.19811000	-2.60968100	-1.97613900
C	-0.28710700	-4.21936400	-2.57774700	H	5.76364800	-2.22674300	-2.92397500
H	-0.46632700	-5.25985200	-2.87121300	H	3.77785200	-5.23695000	-1.67292600
H	0.75211800	-4.12246200	-2.23242400	H	3.66241800	-3.83822600	-2.73824800
H	-1.41367400	-1.91153300	-0.90451100	H	5.99632600	-4.68780900	-2.73494600
H	1.44457700	-3.50430300	-4.51607700	H	6.06359700	-4.57661700	-0.97767500

C	-3.91156100	4.50104900	-0.73467200	H	-5.75744200	-3.96818300	-3.78870000
C	-5.44676300	4.43081200	-0.81216700	H	-5.73484900	-2.34157200	-3.11420000
C	-3.44998800	5.96867500	-0.63703700	H	-5.71190100	-3.52161300	0.51231800
H	-3.49782300	4.08479200	-1.66576800	H	-5.70836900	-2.06812300	-0.48230600
C	-5.99802700	5.28270600	-1.96779200	H	-7.02131400	-3.84454400	-1.61503000
H	-5.86758300	4.78886600	0.13774000	H	-5.65785500	-4.95595000	-1.51327200
H	-5.77227000	3.39012900	-0.93326800	C	4.25007800	1.35435300	-2.92870700
C	-3.99418800	6.82139900	-1.79247200	C	5.30050700	1.58308400	-3.81724900
H	-3.79206300	6.38304200	0.32070300	C	5.00496100	2.04334600	-5.09999200
H	-2.35236200	6.01086400	-0.62721900	C	3.67145500	2.26592800	-5.44201900
C	-5.52510700	6.74088200	-1.87547400	C	2.68678400	2.01523800	-4.48832500
H	-7.09517900	5.23816100	-1.97609300	N	2.96246500	1.55866800	-3.25574100
H	-5.66080800	4.85493900	-2.92394700	H	5.79882900	2.22907700	-5.81861000
H	-3.67456300	7.86501000	-1.67324600	H	4.42481400	1.00030000	-1.91482100
H	-3.55936200	6.46622500	-2.73851800	H	6.32419300	1.40178000	-3.50443900
H	-5.89317000	7.31607300	-2.73512300	H	3.39353100	2.63104300	-6.42576200
H	-5.96033000	7.20503300	-0.97784100	H	1.63812900	2.19314100	-4.70881200
C	-3.24768600	-2.57910500	-1.78909400	C	-4.14727000	1.27361200	-2.92835100
C	-3.83482300	-3.36681500	-2.97364600	C	-5.19778200	1.04487500	-3.81679700
C	-3.81010400	-3.10647200	-0.45449300	C	-4.90234900	0.58478200	-5.09962500
H	-3.55572900	-1.52805200	-1.89466900	C	-3.56886400	0.36235500	-5.44183700
C	-5.37248000	-3.36803200	-2.95343600	C	-2.58411000	0.61302300	-4.48822500
H	-3.47131400	-4.40317800	-2.92884600	N	-2.85968300	1.06945400	-3.25556000
H	-3.47984700	-2.93672000	-3.91743500	H	-5.69628800	0.39906300	-5.81816800
C	-5.34626000	-3.10646700	-0.43611100	H	-4.32189400	1.62758900	-1.91441800
H	-3.43870500	-4.12764400	-0.29528500	H	-6.22144800	1.22603700	-3.50384000
H	-3.42901000	-2.49268800	0.37271300	H	-3.29102500	-0.00261400	-6.42565900
C	-5.92432900	-3.89389600	-1.62082000	H	-1.53546800	0.43519800	-4.70885000





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$G_{MP2} = -3657.521432$

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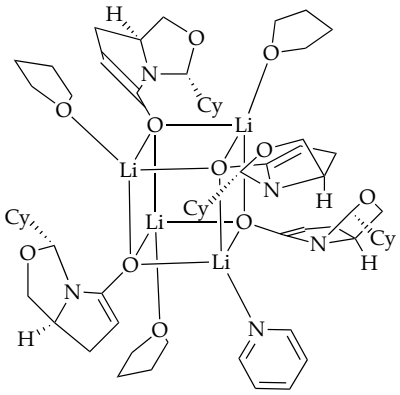
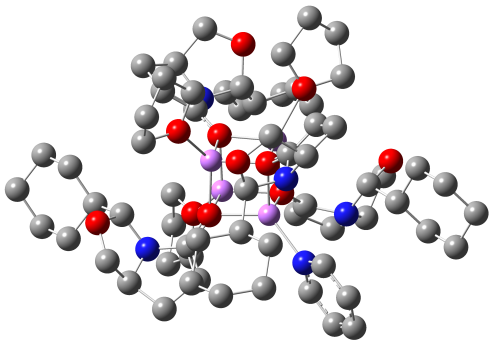
C	-4.39975700	-0.64999600	2.07092700	C	0.32308600	-1.06486300	-2.77063100
C	-5.00804500	0.69406700	1.62360600	C	1.46634500	-1.19227600	-3.49005900
N	-4.10664400	1.20889700	0.55995800	C	1.46324700	-2.48034000	-4.27024600
C	-4.14614200	2.66641900	0.64401400	C	0.28649700	-3.23810300	-3.62104100
O	-4.63485000	3.00272300	1.96927400	H	-0.28431400	-3.83115600	-4.34094900
C	-4.93319300	1.80720700	2.68458700	N	-0.56707800	-2.18961600	-3.00808800
H	-5.87704200	1.94647500	3.22404800	C	-1.21517400	-2.79109500	-1.85188800
H	-4.13884600	1.58961100	3.41384900	O	-0.42959700	-3.95912600	-1.48832300
H	-3.12708900	3.05244100	0.54504500	C	0.66310500	-4.09551400	-2.39931400
H	-6.03002400	0.59366100	1.24809300	H	0.78366500	-5.15751200	-2.63938500
H	-4.54034600	-0.80621800	3.15101000	H	1.59039100	-3.72553700	-1.93924700
H	-4.90841200	-1.48849200	1.56902100	H	-1.18620900	-2.07614900	-1.02145500
H	-2.17881900	-1.20336200	1.86764700	H	2.39524400	-3.06037500	-4.19327300
Li	-0.63333200	2.55258600	0.08816500	H	1.27674500	-2.33615600	-5.34663100
O	1.13294500	1.59106700	0.03677200	H	2.22171000	-0.42262800	-3.56708800
C	2.20384100	2.04596700	0.65489200	O	-3.06516000	0.47690400	-3.17259900
C	2.33824200	3.08546800	1.51863600	C	-4.50110100	0.35286500	-3.07890500
C	3.78477200	3.28365600	1.88614300	C	-5.00909400	0.55043300	-4.50492100
C	4.41360400	1.96225800	1.40203500	C	-3.89476100	-0.11790200	-5.32669800
H	5.41839000	2.09428300	0.99153200	C	-2.62976600	0.25197200	-4.54309000
N	3.48887500	1.43614800	0.36399800	H	-2.18445300	1.18707400	-4.90203300
C	3.57370000	-0.02243700	0.42473100	H	-1.87595300	-0.53828100	-4.53026500
O	4.11605700	-0.35962000	1.72518600	H	-4.03423900	-1.20528400	-5.33959100
C	4.40390600	0.83247400	2.44771900	H	-3.85472500	0.22934100	-6.36351100
H	5.36874900	0.71299100	2.95409500	H	-5.99421600	0.10140400	-4.66456500
H	3.62846100	1.01591500	3.20616100	H	-5.07624200	1.61874800	-4.74273700
H	2.56271900	-0.43353200	0.35107200	H	-4.85187900	1.09154400	-2.35749400
H	3.96979200	3.43773400	2.95986500	H	-4.75198100	-0.64784300	-2.70229100
H	4.24322900	4.14066000	1.36726900	O	2.23968200	2.18016900	-3.26691900
H	1.53873500	3.76986400	1.76690300	C	3.68040900	2.14363200	-3.20361400
Li	0.90171200	1.66970100	-1.92520600	C	4.13718400	3.16445200	-4.24024200
O	-0.71490800	2.77324000	-1.86866100	C	3.10145200	2.95654600	-5.35885900
C	-1.13912000	3.75064200	-2.64168900	C	1.81432200	2.62488100	-4.58504500
C	-2.27762800	3.85842900	-3.37291400	H	1.23599000	1.82027900	-5.05132300
C	-2.29677900	5.15332000	-4.14084200	H	1.17349200	3.49743400	-4.43374700
C	-1.15062700	5.93568700	-3.46629000	H	2.98008200	3.83528900	-5.99911200
N	-0.28188600	4.90684300	-2.83986600	H	3.39873200	2.11567400	-5.99617100
C	0.31104100	5.51765900	-1.65529100	H	4.06706800	4.17829300	-3.83058500
O	-0.52145500	6.65014500	-1.30145000	H	5.16692400	2.99659500	-4.57065000
C	-1.57668000	6.78128300	-2.25286500	H	4.03223300	1.13477300	-3.46451400
H	-1.70057600	7.84309000	-2.49398100	H	3.96726800	2.35705300	-2.17221000
H	-2.51778500	6.40169100	-1.83034000	O	-0.98187300	3.75005700	1.62809100
H	0.28298300	4.79235700	-0.83394600	C	-1.06304800	3.11411000	2.93479400
H	-0.58085600	6.54387900	-4.17415600	C	-1.48052500	4.21594500	3.92222000
H	-3.24412000	5.70922100	-4.07448800	C	-2.09873500	5.28631600	3.00681300
H	-2.09022800	5.02242300	-5.21537500	C	-1.22106900	5.16980000	1.76560600
H	-3.01221500	3.07041700	-3.46689600	H	-1.67769000	5.52394800	0.83982900
Li	-1.70025500	0.98349600	-1.84069900	H	-0.26079700	5.68792500	1.89676900
O	-0.07936600	-0.09867600	-1.97294900	H	-2.07809300	6.28982400	3.44295700

H	-3.13233600	5.02149400	2.76332000	H	-4.54294800	3.14944400	-1.37839800
H	-0.60360300	4.61808500	4.44294400	C	-7.29513100	3.56667700	-1.55366200
H	-2.17981700	3.84429000	4.67664600	H	-6.95213500	2.98940500	0.50400100
H	-0.08283400	2.68458300	3.16637600	H	-6.48032000	1.76015700	-0.67048100
H	-1.79955700	2.30950300	2.86120700	C	-5.82983000	5.61524800	-1.29011400
C	1.77101700	5.97576800	-1.82382500	H	-5.42625100	5.11429900	0.77967200
C	1.99137100	6.97308400	-2.97532100	H	-3.97821800	5.24957300	-0.21697200
C	2.30901100	6.54889600	-0.49779500	C	-7.27095700	5.08897200	-1.35627800
H	2.33431200	5.05730400	-2.05082500	H	-8.32941700	3.19825000	-1.55129600
C	3.45894200	7.42031800	-3.08085900	H	-6.88208200	3.32725200	-2.54562100
H	1.35718900	7.85453000	-2.80668800	H	-5.82854200	6.69589000	-1.09606600
H	1.67423800	6.52344500	-3.92399100	H	-5.34607800	5.47207600	-2.26800700
C	3.77687700	6.98791500	-0.60870700	H	-7.82410900	5.58733300	-2.16315400
H	1.68986800	7.40951800	-0.21065500	H	-7.79030600	5.33903300	-0.41912600
H	2.20346900	5.79665400	0.29486800	C	-2.68271600	-3.19840800	-2.06343900
C	3.97936200	7.99003600	-1.75400200	C	-2.91264300	-4.16799800	-3.23576300
H	3.56727000	8.16100600	-3.88411900	C	-3.27457100	-3.76749900	-0.75877700
H	4.08184200	6.55921700	-3.36832300	H	-3.20465700	-2.25740900	-2.29185300
H	4.11196300	7.42285500	0.34197400	C	-4.39592000	-4.54529100	-3.38495000
H	4.40867100	6.10426600	-0.78617200	H	-2.32264400	-5.07935900	-3.06558700
H	5.03947700	8.26093800	-1.84465700	H	-2.55063300	-3.71768500	-4.16804700
H	3.43677300	8.91852200	-1.52176200	C	-4.75593600	-4.14378200	-0.91223400
C	4.42920300	-0.68009000	-0.67177100	H	-2.69884400	-4.65775000	-0.47142100
C	5.86910300	-0.14737900	-0.76682500	H	-3.15526100	-3.03317000	0.04899200
C	4.42983500	-2.21186900	-0.49384600	C	-4.97261200	-5.11530500	-2.08133000
H	3.91395900	-0.45742500	-1.61794900	H	-4.51894500	-5.26525800	-4.20469100
C	6.67082100	-0.85826900	-1.86985300	H	-4.97058500	-3.65012300	-3.66936000
H	6.37025700	-0.29930000	0.19951100	H	-5.13131700	-4.58162700	0.02189100
H	5.85791800	0.93298800	-0.95592200	H	-5.34705900	-3.23178200	-1.08678800
C	5.22740000	-2.92097100	-1.59811600	H	-6.04072600	-5.33895000	-2.20196500
H	4.86176400	-2.45158700	0.48654600	H	-4.47558700	-6.07024000	-1.85436600
H	3.39505900	-2.58087200	-0.48076800	C	0.44216700	-2.72377200	1.50569700
C	6.66280300	-2.38263200	-1.68681400	C	0.68280100	-3.49874900	2.63957600
H	7.70203600	-0.48145700	-1.88651400	C	1.00324500	-2.86053200	3.83668000
H	6.23474100	-0.61315700	-2.85061600	C	1.08052800	-1.46904800	3.85239900
H	5.23842600	-4.00414600	-1.41865100	C	0.82938800	-0.77419900	2.67182800
H	4.72324100	-2.76916300	-2.56451500	N	0.50675900	-1.37946600	1.51566600
H	7.20473600	-2.86846400	-2.50889300	H	1.19467700	-3.43624800	4.73828400
H	7.20166300	-2.63728500	-0.76195800	H	0.18829700	-3.19448600	0.55850000
C	-5.02777000	3.35708900	-0.41223600	H	0.61725900	-4.58039400	2.57547200
C	-6.47544400	2.83929100	-0.47498500	H	1.33635300	-0.92646600	4.75701300
C	-5.01473000	4.88543700	-0.21212100	H	0.89900600	0.31003500	2.63805500





24
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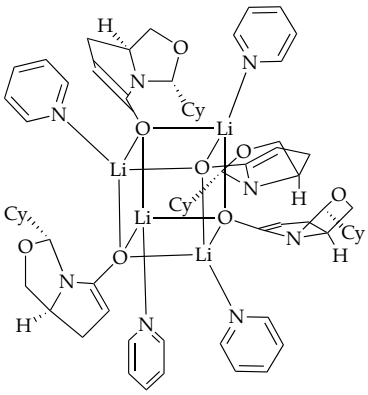
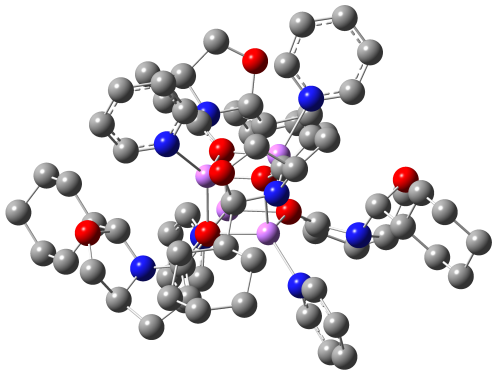
G_{MP2} = –3657.523954

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.26217200	-1.89480400	0.79619400
O	-0.26616300	1.27271100	1.47963800	C	-2.39588300	-2.86688500	1.73436400
C	-0.58012100	2.68561900	1.52896800	C	-3.81779800	-2.94431500	2.22359600
C	-1.36108300	2.86312400	2.82707000	C	-4.40913800	-1.62624300	1.68463500
C	-0.63916800	1.87621600	3.75928900	H	-5.44553200	-1.73032900	1.35200300
C	-0.30310800	0.70966800	2.82124900	N	-3.53270500	-1.22846500	0.55206500
H	0.67161600	0.25613400	3.02496200	C	-3.53830000	0.23319000	0.50476200
H	-1.07144700	-0.06982400	2.83208000	O	-4.00019600	0.69622000	1.79992700
H	-1.25371300	1.55650500	4.60607500	C	-4.27242100	-0.42516100	2.63614300
H	0.27791800	2.32609900	4.15805200	H	-5.18691500	-0.22248800	3.20465800
H	-2.40210100	2.55685800	2.68201800	H	-3.44518900	-0.58768000	3.34306800
H	-1.33839900	3.89509000	3.19059700	H	-2.51113100	0.58141900	0.35573000
H	-1.13937700	2.93669800	0.62575000	H	-3.92334600	-3.00439500	3.31740100
H	0.35456900	3.26119500	1.53011900	H	-4.36528000	-3.80756200	1.81345100
O	1.71657700	-1.04763800	-0.02293900	H	-1.62237200	-3.58236600	1.97635400
C	2.83682500	-0.66789700	0.55557200	Li	-1.12252500	-1.57243900	-1.88364800
C	3.08863200	0.39406200	1.36270200	O	0.45312400	-2.71963300	-1.98469000
C	4.55431200	0.46951700	1.69842900	C	0.79287500	-3.68545500	-2.81266000
C	5.05016900	-0.92401800	1.26033200	C	1.88428500	-3.80790900	-3.61180200
N	4.05301700	-1.41133000	0.27290600	C	1.81702200	-5.08396700	-4.40892000
C	4.01016500	-2.86456600	0.39807700	C	0.68241400	-5.84407000	-3.68967900
O	4.53663500	-3.19128400	1.71177300	N	-0.11206100	-4.80339500	-2.99067600
C	4.97835200	-2.00105700	2.35984100	C	-0.66476300	-5.42338100	-1.79376700
H	5.94977200	-2.19373600	2.82968900	O	0.14498700	-6.59375500	-1.51146900
H	4.26223300	-1.70589100	3.14106800	C	1.14470400	-6.73328800	-2.52092200
H	2.96719200	-3.19123200	0.35918200	H	1.22187300	-7.79213600	-2.79234700
H	6.04976900	-0.89673800	0.81835700	H	2.11800500	-6.39198300	-2.14043000
H	4.77386400	0.64883200	2.76167700	H	-0.56711500	-4.72131200	-0.95745500
H	5.08030600	1.25824200	1.13757000	H	0.05276600	-6.41473700	-4.37759000
H	2.36320100	1.16379300	1.58953700	H	2.74703600	-5.67245300	-4.40604600
Li	0.49967900	-2.57639400	-0.01583900	H	1.55873200	-4.92255500	-5.46806800
O	-1.21814000	-1.53993100	0.07791800	H	2.64289300	-3.04498300	-3.72107900

Li	1.49735200	-0.98016300	-1.97483800	H	-2.17432400	-6.32371600	-4.00737300
O	-0.09035800	0.17324700	-1.95023800	C	-4.13387700	-6.76963800	-0.60236600
C	-0.46706300	1.14073200	-2.76185000	H	-2.05105700	-7.29391800	-0.31402300
C	-1.59977600	1.27686800	-3.49649300	H	-2.46504100	-5.67075200	0.24591500
C	-1.54927400	2.53498000	-4.32264300	C	-4.43997100	-7.73099600	-1.75982900
C	-0.36036100	3.28422900	-3.68548000	H	-4.14135900	-7.87064100	-3.91008800
H	0.24439900	3.82281400	-4.42068300	H	-4.54396700	-6.25506700	-3.33668400
N	0.44836100	2.24101100	-3.00470000	H	-4.44212700	-7.21329500	0.35346600
C	1.06842100	2.87414700	-1.84445600	H	-4.73074800	-5.85342200	-0.72750800
O	0.31992900	4.08279200	-1.56935700	H	-5.51553800	-7.94792800	-1.80352300
C	-0.73643500	4.21348500	-2.51819100	H	-3.93421800	-8.69064600	-1.57547000
H	-0.81073300	5.26593300	-2.81420900	C	-4.42114200	0.83858700	-0.60021300
H	-1.69236700	3.90316100	-2.07169800	C	-5.89636400	0.40332600	-0.54387100
H	0.97720100	2.19982700	-0.98484500	C	-4.31392600	2.37580600	-0.59873500
H	-2.46507400	3.14386600	-4.28294400	H	-3.99128300	0.47992100	-1.54721700
H	-1.35314400	2.34181700	-5.38946800	C	-6.72344400	1.03814900	-1.67404300
H	-2.37552600	0.52624700	-3.56555400	H	-6.31753500	0.70079600	0.42648700
O	2.86231900	-0.47870700	-3.29687100	H	-5.97002000	-0.68962400	-0.60324800
C	4.29477900	-0.35436500	-3.16504300	C	-5.13727100	3.01049600	-1.72948000
C	4.83275800	-0.56563400	-4.57690600	H	-4.66194100	2.75648000	0.37093000
C	3.75644900	0.13405500	-5.42436400	H	-3.25973600	2.66779400	-0.69909800
C	2.46048400	-0.18137400	-4.66295600	C	-6.60684400	2.56888300	-1.67185400
H	1.96096400	-1.07485500	-5.05393300	H	-7.77530400	0.73619200	-1.58303100
H	1.75657700	0.65383000	-4.63446000	H	-6.37051600	0.65074800	-2.64182300
H	3.93658100	1.21517700	-5.44459100	H	-5.06649000	4.10495800	-1.67842200
H	3.72382200	-0.22049500	-6.45892100	H	-4.70731000	2.71274300	-2.69713900
H	5.83245700	-0.14188600	-4.71377000	H	-7.16811500	2.99553200	-2.51345700
H	4.87770200	-1.63566800	-4.81231500	H	-7.06789300	2.96459200	-0.75455300
H	4.62062800	-1.08316000	-2.42195600	C	4.79348200	-3.63617200	-0.67981600
H	4.53882100	0.65121300	-2.79543100	C	6.26779500	-3.21817400	-0.82374700
O	0.86647900	-3.82882000	1.47875100	C	4.69204600	-5.15499900	-0.43542500
C	1.15243400	-3.22807600	2.77361400	H	4.27724600	-3.41897700	-1.62784200
C	1.52700700	-4.38699200	3.71204100	C	6.98857200	-4.02793700	-1.91420200
C	1.89994300	-5.51769400	2.73836300	H	6.77845800	-3.37151500	0.13760300
C	0.92521600	-5.26971100	1.59269800	H	6.33510900	-2.14819900	-1.05468500
H	1.22950700	-5.67266200	0.62500800	C	5.40967200	-5.96673500	-1.52444000
H	-0.07738800	-5.65520700	1.82671000	H	5.13391400	-5.38303200	0.54361400
H	1.79006900	-6.51537900	3.17449000	H	3.63555700	-5.45259700	-0.38350800
H	2.93081300	-5.39166300	2.39277700	C	6.87734100	-5.53879500	-1.66756300
H	0.66758400	-4.67898100	4.32688500	H	8.04295500	-3.72669200	-1.96942600
H	2.34685300	-4.11759400	4.38372100	H	6.54504600	-3.79073300	-2.89325400
H	0.26234300	-2.68202700	3.10183800	H	5.34628900	-7.03898100	-1.29709800
H	1.97471700	-2.52368700	2.62981300	H	4.89433900	-5.81974700	-2.48546200
C	-2.14674500	-5.82386600	-1.89608300	H	7.36145600	-6.09534300	-2.48070400
C	-2.46531500	-6.78372700	-3.05570600	H	7.41989200	-5.79503100	-0.74533000
C	-2.64328700	-6.40079000	-0.55562600	C	2.55846800	3.21649800	-2.01663200
H	-2.68577700	-4.88280900	-2.07904900	C	2.86381200	4.10252800	-3.23698100
C	-3.95670300	-7.15464300	-3.09815200	C	3.12081200	3.85018100	-0.72937900
H	-1.86677300	-7.69790000	-2.93755700	H	3.05704400	2.24672900	-2.16339200

C	4.36236700	4.42600200	-3.35365000	H	4.43990500	6.04056900	-1.91806200
H	2.29754800	5.03997100	-3.14602600	C	-3.93888100	-2.31708600	-2.74912800
H	2.51991100	3.60543000	-4.15221600	C	-4.94690400	-2.76457600	-3.60314300
C	4.61867400	4.16972800	-0.84843400	C	-4.62009800	-3.06870100	-4.92435900
H	2.56332400	4.77259600	-0.51836500	C	-3.29695400	-2.92081000	-5.33954100
H	2.95154500	3.17155600	0.11698300	C	-2.35477100	-2.47074400	-4.41687100
C	4.91103900	5.05747700	-2.06652700	N	-2.66368400	-2.16482100	-3.14633400
H	4.53640300	5.09148700	-4.20951500	H	-5.38138100	-3.41745200	-5.61711200
H	4.91875900	3.49928700	-3.56399200	H	-4.13904300	-2.06740600	-1.70902200
H	4.97401700	4.65463300	0.07019800	H	-5.96249800	-2.86992400	-3.23432900
H	5.18419700	3.22990900	-0.94205500	H	-2.99426400	-3.15157400	-6.35607900
H	5.98998000	5.23842300	-2.15962900	H	-1.31135500	-2.35463200	-4.69592700





25
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$G_{MP2} = -3704.964308$

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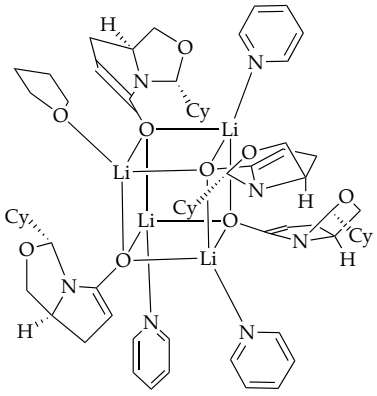
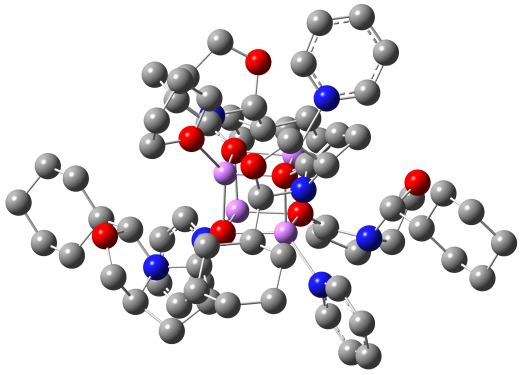
O	-1.49399800	1.36720500	0.03930500	C	2.60905900	1.43830000	0.70313200
C	-2.62014700	1.20750400	0.70337500	C	2.95719500	2.37485800	1.62202500
C	-2.96848000	0.27090100	1.62213900	C	4.39355300	2.20223100	2.03882800
C	-4.40492100	0.44352000	2.03866800	C	4.70843500	0.79306300	1.50105000
C	-4.71969100	1.85271000	1.50089400	H	5.73113600	0.69898500	1.12604800
N	-3.73666500	2.09531900	0.41077000	N	3.72559400	0.55048000	0.41073600
C	-3.47407900	3.53571900	0.39890500	C	3.46298600	-0.88992100	0.39879800
O	-3.86774100	4.04822800	1.69493200	O	3.85647900	-1.40247500	1.69485300
C	-4.39962500	2.99142200	2.48551700	C	4.38820400	-0.34568500	2.48557200
H	-5.28678800	3.35891900	3.01413300	H	5.27527200	-0.71319700	3.01433400
H	-3.65860300	2.65913200	3.22704400	H	3.64704200	-0.01343200	3.22697400
H	-2.39886900	3.69534800	0.27270400	H	2.38778900	-1.04952700	0.27245000
H	-5.74233300	1.94681200	1.12573100	H	4.56488800	2.25674000	3.12431700
H	-4.57645100	0.38895400	3.12412200	H	5.06304600	2.94804600	1.58176000
H	-5.07433500	-0.30226500	1.58143700	H	2.33332500	3.21172000	1.90395300
H	-2.34467700	-0.56595700	1.90421500	Li	1.32809200	1.33050500	-1.92518600
Li	-0.01092800	2.64604100	0.00002100	O	0.03772200	2.78792800	-1.96699900

C	-0.10209800	3.84868800	-2.73546400	C	4.19124600	-1.67708700	-0.70489300
C	-1.18413400	4.29496900	-3.42223800	C	5.71961900	-1.49777300	-0.71786000
C	-0.84677800	5.54810000	-4.18603800	C	3.82667400	-3.17259400	-0.62465200
C	0.49898500	5.94890700	-3.54933100	H	3.79169900	-1.29091100	-1.65460300
N	1.05238700	4.69823000	-2.97264800	C	6.37936700	-2.30902900	-1.84505300
C	1.85747000	5.08395300	-1.82444500	H	6.12563900	-1.82364800	0.25008600
O	1.38535000	6.39445100	-1.40063900	H	5.97515400	-0.43671000	-0.82923100
C	0.37877400	6.85062900	-2.30609800	C	4.48476700	-3.98641600	-1.74905400
H	0.55996600	7.90864200	-2.52655100	H	4.14606400	-3.56111700	0.35122100
H	-0.61480700	6.74719600	-1.84795100	H	2.73528500	-3.28600200	-0.66939400
H	1.67837000	4.37110600	-1.01118900	C	6.00882300	-3.79643200	-1.76471400
H	1.19581000	6.38456400	-4.26991300	H	7.46994400	-2.18547000	-1.80774900
H	-1.58662600	6.35606500	-4.08464200	H	6.05280500	-1.90851400	-2.81693000
H	-0.72308900	5.37681200	-5.26754400	H	4.23599500	-5.05020100	-1.63893800
H	-2.12511700	3.76577700	-3.48808000	H	4.06996100	-3.66691100	-2.71679900
Li	-1.33968400	1.31586100	-1.92468400	H	6.45517300	-4.34681000	-2.60342000
O	-0.04920300	-0.14170000	-1.96725900	H	6.43590100	-4.22473200	-0.84559600
C	0.09069900	-1.20264400	-2.73543500	C	-4.20220600	4.32290700	-0.70485600
C	1.17282700	-1.64906700	-3.42198400	C	-5.73058200	4.14361500	-0.71800200
C	0.83557200	-2.90229800	-4.18564500	C	-3.83762800	5.81840800	-0.62456700
C	-0.51028400	-3.30300100	-3.54905600	H	-3.80255200	3.93674500	-1.65453000
H	-1.20701000	-3.73874300	-4.26968300	C	-6.39018600	4.95485000	-1.84529300
N	-1.06374700	-2.05225400	-2.97260500	H	-6.13670900	4.46953000	0.24988600
C	-1.86894100	-2.43781600	-1.82444700	H	-5.98611600	3.08255200	-0.82936300
O	-1.39675300	-3.74819500	-1.40032100	C	-4.49557500	6.63222100	-1.74906200
C	-0.39022700	-4.20459900	-2.30571000	H	-4.15712900	6.20694100	0.35126400
H	-0.57153600	-5.26261500	-2.52607500	H	-2.74623200	5.93180800	-0.66917700
H	0.60335100	-4.10126100	-1.84753400	C	-6.01963300	6.44224700	-1.76492500
H	-1.68999600	-1.72480600	-1.01129600	H	-7.48076900	4.83130500	-1.80811600
H	1.57538800	-3.71026800	-4.08403400	H	-6.06351600	4.55431300	-2.81712400
H	0.71203100	-2.73117000	-5.26719300	H	-4.24682000	7.69600800	-1.63892400
H	2.11379900	-1.11985500	-3.48783300	H	-4.08064400	6.31270100	-2.71674800
C	3.37507900	5.13636900	-2.07303400	H	-6.46585300	6.99263100	-2.60369700
C	3.80228400	6.04532300	-3.23897600	H	-6.44683300	6.87056200	-0.84587100
C	4.11664700	5.52363600	-0.77755800	C	-3.38652400	-2.49042600	-2.07317600
H	3.66020200	4.10612800	-2.32966300	C	-3.81354200	-3.39968300	-3.23895800
C	5.32864800	6.05694100	-3.42361000	C	-4.12816500	-2.87748100	-0.77768100
H	3.45273400	7.06896100	-3.04331100	H	-3.67173100	-1.46027300	-2.33005700
H	3.32433100	5.70866600	-4.16636700	C	-5.33989100	-3.41150100	-3.42372100
C	5.64103300	5.53290800	-0.96695000	H	-3.46391000	-4.42324400	-3.04303800
H	3.78062900	6.52105700	-0.46341700	H	-3.33554500	-3.06317600	-4.16638000
H	3.84143900	4.82642400	0.02542700	C	-5.65253500	-2.88694400	-0.96720400
C	6.05742000	6.44555400	-2.12947800	H	-3.79207700	-3.87479800	-0.46329400
H	5.60206900	6.74342600	-4.23597300	H	-3.85308800	-2.18007100	0.02517700
H	5.65992100	5.05550700	-3.73731000	C	-6.06873100	-3.79989300	-2.12956300
H	6.13374600	5.84966000	-0.03828600	H	-5.61316700	-4.09820400	-4.23594800
H	5.98864700	4.50865900	-1.17023100	H	-5.67124000	-2.41017500	-3.73768100
H	7.14490200	6.40736700	-2.27702400	H	-6.14529500	-3.20354300	-0.03851300
H	5.81180100	7.48766400	-1.87574000	H	-6.00023700	-1.86277700	-1.17074200

H	-7.15620500	-3.76185300	-2.27720800	H	0.58013400	5.75811500	0.60577500
H	-5.82302800	-4.84192100	-1.87556800	C	2.56370400	1.89187100	-4.55359600
C	-0.21912200	-2.70985100	1.54560000	C	3.51830900	2.06584900	-5.55373800
C	-0.15882300	-3.51164300	2.68478600	C	4.86172700	1.86665100	-5.23623400
C	0.32070300	-2.96101100	3.87209500	C	5.19650300	1.50793100	-3.93091000
C	0.73064300	-1.62890100	3.87327500	C	4.17386900	1.35517700	-2.99472200
C	0.63948800	-0.90149600	2.68894300	N	2.87691400	1.53509000	-3.29781800
N	0.16726100	-1.42061800	1.54200900	H	5.63302000	1.99239500	-5.99148000
H	0.37910600	-3.55952900	4.77733100	H	1.50812100	2.04975700	-4.75571100
H	-0.59167500	-3.11159900	0.60560600	H	3.21060100	2.35340800	-6.55418900
H	-0.48433100	-4.54587100	2.63191400	H	6.22902100	1.34824800	-3.63605500
H	1.12051600	-1.15730000	4.76988800	H	4.38041100	1.08461700	-1.96140400
H	0.96973100	0.13357000	2.64463400	C	-4.18537000	1.29058600	-2.99489300
C	-0.65055000	3.54737300	2.68871300	C	-5.20769100	1.13739200	-3.93135000
C	-0.74192100	4.27455500	3.87316300	C	-4.87243100	0.77853600	-5.23651300
C	-0.33232600	5.60677300	3.87221600	C	-3.52886500	0.57964800	-5.55358800
C	0.14710000	6.15773300	2.68502100	C	-2.57460100	0.75405100	-4.55319600
C	0.20764500	5.35614700	1.54570200	N	-2.88828100	1.11095700	-3.29757000
N	-0.17841600	4.06682300	1.54188200	H	-5.64346700	0.65245400	-5.99196500
H	-0.39091900	6.20512100	4.77755100	H	-4.39227900	1.56127100	-1.96168400
H	-0.98053800	2.51223800	2.64421000	H	-6.24034100	1.29684600	-3.63683200
H	-1.13169700	3.80271200	4.76969100	H	-3.22078800	0.29200100	-6.55390000
H	0.47234100	7.19205500	2.63234000	H	-1.51891500	0.59643200	-4.75497200



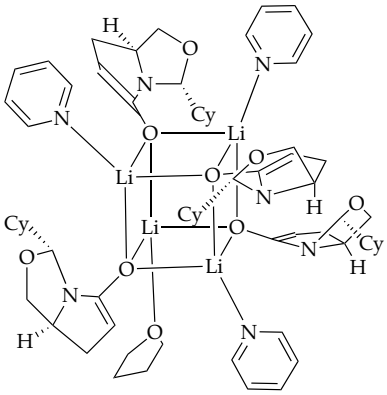


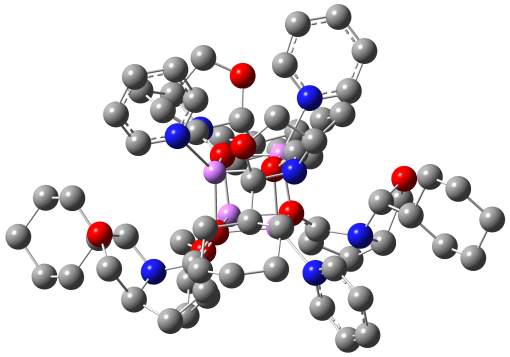
26
$G = -3699.651839$
$G_{MP2} = -3689.151808$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.38895000	3.58648700	0.53847300
O	-1.48086800	1.37120600	0.11241400	O	-3.78925600	4.08721800	1.84017600
C	-2.60414700	1.22848700	0.78372600	C	-4.34693100	3.02574900	2.60916000
C	-2.97682800	0.28221100	1.68176600	H	-5.22772900	3.40334400	3.14077000
C	-4.40580000	0.48663700	2.10963200	H	-3.61756000	2.66240200	3.34824600
C	-4.68668800	1.91454600	1.60010900	H	-2.30670900	3.71284400	0.43648900
N	-3.69624500	2.15631700	0.51761000	H	-5.70626400	2.03913900	1.22487600

H	-4.57322400	0.41605600	3.19483000	H	0.59228000	-4.04450200	-1.92049600
H	-5.09794900	-0.23174900	1.64261000	H	-1.70793900	-1.70819300	-1.01021500
H	-2.37323500	-0.57504800	1.94727500	H	1.52453800	-3.60700400	-4.16755400
Li	0.00973800	2.63796900	0.05562600	H	0.62953900	-2.62278700	-5.32257500
O	1.48975600	1.27761300	0.01892200	H	2.04076400	-1.01655100	-3.54607400
C	2.63273200	1.44631600	0.65057600	O	-0.05003300	3.91140300	1.57343700
C	3.00028300	2.38867500	1.55684100	C	-0.31366300	3.35154800	2.89049300
C	4.44795500	2.22291000	1.93627900	C	-0.47465100	4.54928500	3.84031100
C	4.75280900	0.81199500	1.39652700	C	-0.80033600	5.70918100	2.88404700
H	5.76631200	0.71873900	0.99718500	C	0.04881000	5.35160400	1.66927200
N	3.74395800	0.56499300	0.33178300	H	-0.29433800	5.77569900	0.72389400
C	3.49004800	-0.87644200	0.32132800	H	1.10140100	5.63297600	1.81164400
O	3.92565800	-1.39017100	1.60375300	H	-0.54891800	6.69098600	3.29696500
C	4.45742100	-0.32755100	2.38728600	H	-1.86214300	5.69206300	2.61941200
H	5.35414100	-0.68730500	2.90460100	H	0.46227400	4.74532700	4.37498400
H	3.72293100	0.00002100	3.13761300	H	-1.25732000	4.37751000	4.58487500
H	2.41252300	-1.04214500	0.22530700	H	0.52611200	2.70271700	3.16016900
H	4.64935800	2.28297000	3.01645700	H	-1.22097800	2.74666400	2.81301200
H	5.10253800	2.96836400	1.45737600	C	3.19054500	5.29574700	-1.80802500
H	2.38514100	3.23572100	1.82744600	C	3.71675500	6.11666500	-2.99854700
Li	1.26848700	1.38370200	-1.93418100	C	3.80057500	5.80275900	-0.48634400
O	-0.03829300	2.84441500	-1.89957000	H	3.50943800	4.25213000	-1.94901800
C	-0.15495400	3.86557600	-2.72461500	C	5.25349100	6.13918900	-3.04144600
C	-1.18777300	4.22868600	-3.52778800	H	3.34200600	7.14678000	-2.91615900
C	-0.83163000	5.45561600	-4.32588800	H	3.32887800	5.70176400	-3.93601300
C	0.44151100	5.94339100	-3.60374300	C	5.33600800	5.82644500	-0.53112000
N	0.97833000	4.75253800	-2.89998400	H	3.42159700	6.81454100	-0.28952700
C	1.65598100	5.23676400	-1.70475600	H	3.46246800	5.16514100	0.34146300
O	1.12844400	6.55936400	-1.42653000	C	5.85254100	6.64661500	-1.72216400
C	0.19031900	6.91916400	-2.43970400	H	5.59590000	6.76077200	-3.87957700
H	0.35749000	7.96649900	-2.71580500	H	5.62242600	5.12115900	-3.23733400
H	-0.83678600	6.81207600	-2.06255200	H	5.73435500	6.22830700	0.40985000
H	1.40480900	4.57865400	-0.86498600	H	5.71179500	4.79522700	-0.61360000
H	1.18599200	6.35437600	-4.29112900	H	6.94943900	6.61455700	-1.76282500
H	-1.60635900	6.23697900	-4.33025000	H	5.57472700	7.70197500	-1.58174300
H	-0.61127200	5.23464200	-5.38274200	C	4.19132700	-1.65153000	-0.80777800
H	-2.09846300	3.65772800	-3.64762700	C	5.71814100	-1.46571400	-0.85793400
Li	-1.39930400	1.35845900	-1.85630100	C	3.83339900	-3.14875900	-0.73150000
O	-0.10425700	-0.09215300	-1.96882600	H	3.76597800	-1.25726700	-1.74304000
C	0.03380500	-1.13834100	-2.75726400	C	6.35364200	-2.26700500	-2.00591200
C	1.10842900	-1.56003900	-3.47058700	H	6.14875300	-1.79548600	0.09793700
C	0.77333200	-2.80697600	-4.24577200	H	5.96559400	-0.40278800	-0.96969100
C	-0.55687200	-3.23325400	-3.59239200	C	4.46712400	-3.95122400	-1.87786100
H	-1.26088200	-3.66581600	-4.30795900	H	4.17675800	-3.54472600	0.23325300
N	-1.11454200	-1.99808300	-2.98720400	H	2.74147600	-3.26526400	-0.75119700
C	-1.89586000	-2.40978400	-1.83128900	C	5.98977900	-3.75615300	-1.92758700
O	-1.40536000	-3.72283100	-1.43826400	H	7.44437800	-2.14017600	-1.99289800
C	-0.40682200	-4.15258600	-2.36544700	H	6.00390000	-1.86050500	-2.96709500
H	-0.57895800	-5.20915600	-2.59941900	H	4.22397900	-5.01661900	-1.77102500

H	4.02914800	-3.62464700	-2.83298600	H	-7.18075300	-3.76834500	-2.19924700
H	6.41806300	-4.29903100	-2.78045700	H	-5.83401900	-4.84186100	-1.82653300
H	6.43948600	-4.18971600	-1.02182500	C	4.09066500	1.50835100	-3.04619900
C	-4.07476800	4.41734900	-0.55986600	C	5.09536400	1.73950200	-3.98568600
C	-5.60820500	4.29208900	-0.59319000	C	4.73240900	2.15304000	-5.26692700
C	-3.66508300	5.89932800	-0.44918100	C	3.37966800	2.32838600	-5.55716800
H	-3.67516900	4.03489300	-1.51135700	C	2.44444500	2.07865900	-4.55482200
C	-6.22385200	5.13988400	-1.71875200	N	2.78511300	1.66687200	-3.32309600
H	-6.01419000	4.62074300	0.37380500	H	5.48930300	2.33934200	-6.02423800
H	-5.89992200	3.24226200	-0.72001000	H	4.31985900	1.18951000	-2.03147400
C	-4.27393500	6.74954600	-1.57407900	H	6.13617300	1.59597700	-3.71234000
H	-3.99477200	6.28443100	0.52488900	H	3.04986900	2.65669900	-6.53785600
H	-2.56991900	5.98258200	-0.46948800	H	1.38241600	2.22076200	-4.73445100
C	-5.80282100	6.61283600	-1.61564000	C	-4.27630500	1.35596100	-2.85880000
H	-7.31843900	5.05440300	-1.69701700	C	-5.32336600	1.20481000	-3.76764200
H	-5.89826800	4.73956400	-2.69082900	C	-5.02688000	0.80666400	-5.07090800
H	-3.99008100	7.80242900	-1.44615100	C	-3.69625100	0.56601000	-5.41242900
H	-3.85358500	6.42619800	-2.53787500	C	-2.71499100	0.73998500	-4.43824100
H	-6.21628200	7.18726200	-2.45495100	N	-2.99105500	1.13673100	-3.18530200
H	-6.22929900	7.04625500	-0.69863600	H	-5.81781700	0.68198100	-5.80575100
C	-3.41716200	-2.47196100	-2.05312400	H	-4.45230600	1.65619300	-1.82827700
C	-3.85776900	-3.37811300	-3.21631400	H	-6.34488100	1.39646900	-3.45406700
C	-4.13323100	-2.87212400	-0.74713300	H	-3.41819100	0.24609400	-6.41173500
H	-3.71459200	-1.44243300	-2.29785300	H	-1.66913200	0.54773300	-4.65862900
C	-5.38688400	-3.39983600	-3.37489600	C	-0.20062200	-2.73896700	1.50131800
H	-3.49719600	-4.39992700	-3.03175900	C	-0.11824300	-3.56031600	2.62515100
H	-3.39849500	-3.03404900	-4.15035800	C	0.39073000	-3.03242800	3.81048100
C	-5.66054000	-2.89074900	-0.91043700	C	0.80710800	-1.70240600	3.82494700
H	-3.78530800	-3.86905900	-0.44430900	C	0.69251600	-0.95493400	2.65534200
H	-3.84958700	-2.17737300	0.05518800	N	0.19212800	-1.45161900	1.51062700
C	-6.09068200	-3.80007700	-2.07054100	H	0.46679300	-3.64658800	4.70382700
H	-5.66928700	-4.08427000	-4.18590100	H	-0.59454000	-3.12368100	0.56298100
H	-5.73054300	-2.39924000	-3.67774600	H	-0.44965500	-4.59209100	2.56200300
H	-6.13520000	-3.21549100	0.02483000	H	1.21955300	-1.24802500	4.72032300
H	-6.01803800	-1.86770100	-1.10247000	H	1.02539200	0.07939800	2.62092100





27
G = –3699.650604
G_{MP2} = –3689.149397

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.01481900	-3.38264100	1.96915300
O	1.59147600	-1.23964100	0.02147000	Li	-1.25041300	-1.43416000	-1.89320700
C	2.72034000	-0.98195100	0.65163700	O	0.15963200	-2.78831300	-1.95510100
C	3.02463400	0.01134400	1.52544500	C	0.37639500	-3.82843900	-2.73188300
C	4.47866200	-0.05002800	1.91057600	C	1.47918900	-4.17491600	-3.44411700
C	4.87398800	-1.45595500	1.41772000	C	1.23896100	-5.45126600	-4.20603800
N	3.88359300	-1.80509700	0.36519700	C	-0.05504500	-5.97037200	-3.54598100
C	3.71768100	-3.25641700	0.41204000	N	-0.70233200	-4.77523500	-2.95028000
O	4.16382000	-3.69164300	1.72025800	C	-1.44325100	-5.23272700	-1.78548100
C	4.65417200	-2.57404700	2.45337600	O	-0.84387000	-6.49322500	-1.37411900
H	5.57768100	-2.86635300	2.96660800	C	0.16548800	-6.86893300	-2.31297700
H	3.91619700	-2.25897900	3.20542300	H	0.05458900	-7.93555200	-2.53926600
H	2.65406100	-3.49189500	0.31152100	H	1.16183800	-6.69984300	-1.88137900
H	5.89126800	-1.49586000	1.01939200	H	-1.30939400	-4.50587800	-0.97633700
H	4.67241300	0.05886000	2.98818000	H	-0.72530100	-6.45876100	-4.25779200
H	5.08620200	0.71918600	1.40770900	H	2.04826100	-6.19183000	-4.12138300
H	2.35283000	0.81638700	1.78944900	H	1.07949800	-5.29083800	-5.28475700
Li	0.21920000	-2.63588000	0.01566700	H	2.36892300	-3.56450800	-3.51983400
O	-1.37802200	-1.39609700	0.07402700	Li	1.42340600	-1.21410900	-1.93318300
C	-2.46722900	-1.64309100	0.77262300	O	-0.00451800	0.13807900	-1.97056400
C	-2.71131300	-2.59938600	1.70448700	C	-0.26628400	1.17629200	-2.73713600
C	-4.14211700	-2.53796700	2.16818000	C	-1.40651200	1.52859800	-3.38235600
C	-4.58690300	-1.16256100	1.63348400	C	-1.20270900	2.79749400	-4.16684400
H	-5.62461800	-1.15472700	1.28887300	C	0.13116200	3.31259700	-3.58864100
N	-3.66010700	-0.84922500	0.51284800	H	0.76166200	3.79336200	-4.34116900
C	-3.51438100	0.60748400	0.48501900	N	0.80563300	2.11615300	-3.02460700
O	-3.91857000	1.09799600	1.78592500	C	1.61043400	2.57414800	-1.90196200
C	-4.33127200	0.00653400	2.60061200	O	1.05501000	3.84798900	-1.47516200
H	-5.22732600	0.30290600	3.15794100	C	-0.01241500	4.21789700	-2.35044800
H	-3.53968500	-0.25655900	3.31719700	H	0.08364000	5.28339200	-2.58779600
H	-2.45833300	0.85052000	0.33265300	H	-0.97969400	4.04974600	-1.85651500
H	-4.27192200	-2.59693600	3.25926500	H	1.50718700	1.85646100	-1.08020500
H	-4.76513300	-3.33875900	1.73931500	H	-2.00081700	3.54408700	-4.03994900

H	-1.11004600	2.62626600	-5.25139300	C	4.47833300	-4.03988000	-0.67281600
H	-2.30222200	0.92321100	-3.41396400	C	5.99326800	-3.77258100	-0.70986900
O	2.80456600	-0.92471000	-3.31189000	C	4.19896800	-5.54990800	-0.53715500
C	4.24555100	-1.00562900	-3.28917300	H	4.04408500	-3.71289200	-1.62970200
C	4.64011100	-1.35727700	-4.72080400	C	6.69594400	-4.59184700	-1.80489700
C	3.60387000	-0.56020800	-5.53064600	H	6.42194500	-4.03249100	0.26800100
C	2.33989900	-0.66955700	-4.66684600	H	6.18293200	-2.70408000	-0.86974400
H	1.71483000	-1.52092900	-4.95966300	C	4.89753300	-6.36531800	-1.63556600
H	1.74102500	0.24410700	-4.65151700	H	4.54326200	-5.88574100	0.44979000
H	3.91809100	0.48620300	-5.62008400	H	3.11526100	-5.72570700	-0.57140100
H	3.44935400	-0.95303300	-6.54005200	C	6.40867400	-6.09319100	-1.66415100
H	5.67388700	-1.08170100	-4.95090500	H	7.77771100	-4.40573300	-1.77585300
H	4.52328800	-2.43332800	-4.89608800	H	6.34908800	-4.25033900	-2.79241400
H	4.52375800	-1.74197600	-2.53470500	H	4.70691400	-7.43659700	-1.48870800
H	4.65794800	-0.03165900	-2.99271600	H	4.46494800	-6.10145700	-2.61230400
C	-2.95518700	-5.42221900	-1.99772800	H	6.88356700	-6.65107000	-2.48197000
C	-3.32692300	-6.37479000	-3.14782900	H	6.85980500	-6.46045700	-0.73029400
C	-3.62857800	-5.86488100	-0.68272700	C	3.11167900	2.73278200	-2.19477600
H	-3.33707400	-4.42342600	-2.25196800	C	3.44015300	3.68303500	-3.35956800
C	-4.84997700	-6.52410500	-3.29641400	C	3.86491100	3.15365300	-0.91734600
H	-2.88337300	-7.36169700	-2.95401500	H	3.44993700	1.72422700	-2.47289700
H	-2.90277800	-6.00490400	-4.08855300	C	4.95556700	3.80736700	-3.58987400
C	-5.15012500	-6.01004900	-0.83603600	H	3.02589800	4.67631900	-3.13703600
H	-3.19810000	-6.82634100	-0.37167700	H	2.95680100	3.32877100	-4.27806800
H	-3.39831900	-5.14044200	0.11038600	C	5.37815600	3.27473000	-1.15191800
C	-5.51171700	-6.96472600	-1.98307900	H	3.46865600	4.12033200	-0.57777400
H	-5.07915500	-7.23947600	-4.09747000	H	3.66512800	2.42762100	-0.11797700
H	-5.27639700	-5.55915000	-3.60913400	C	5.69472500	4.22911900	-2.31228000
H	-5.59178400	-6.36095300	0.10590900	H	5.15329000	4.52231100	-4.39941100
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H	-6.60150800	-7.02216200	-2.10517600	H	5.87510100	3.61333700	-0.23342700
H	-5.17124900	-7.97975000	-1.72923600	H	5.79180900	2.28044100	-1.37987700
C	-4.32986000	1.32303400	-0.60595300	H	6.77698700	4.26843000	-2.49293800
C	-5.84199400	1.04139000	-0.56227200	H	5.38576800	5.24840600	-2.03635200
C	-4.06346000	2.84087600	-0.56201100	C	0.01804600	2.73186500	1.52552400
H	-3.93706100	0.94660200	-1.56211100	C	-0.09319200	3.53276100	2.66144500
C	-6.59502600	1.78985100	-1.67441400	C	-0.49027500	2.94730700	3.86250700
H	-6.23377600	1.35306500	0.41600700	C	-0.76849100	1.58179900	3.88071300
H	-6.02870600	-0.03598900	-0.65283300	C	-0.63566600	0.85799800	2.69815100
C	-4.81442000	3.58970800	-1.67296500	N	-0.24351100	1.41185500	1.53736600
H	-4.37233400	3.22557200	0.41892500	H	-0.58563600	3.54429800	4.76558800
H	-2.98439500	3.02481600	-0.65023000	H	0.33135100	3.15991300	0.57569600
C	-6.32169900	3.29995300	-1.62869000	H	0.13010000	4.59303700	2.59584200
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H	-4.41538600	3.28064700	-2.65057900	C	1.12480600	-4.16148700	3.89216800
H	-6.83398400	3.80546800	-2.45789300	C	0.84440300	-5.52655900	3.90509000
H	-6.74254400	3.71437900	-0.70039500	C	0.40715100	-6.13056600	2.72733300

C	0.25802400	-5.34773000	1.58326400	C	-4.87991800	-2.35604600	-5.01399800
N	0.52007000	-4.02774600	1.56566800	C	-5.17629000	-2.04617800	-3.68713500
H	0.96962900	-6.10934900	4.81378700	C	-4.12594500	-1.76797200	-2.81234600
H	1.18358000	-2.39524900	2.64756500	N	-2.83729500	-1.78325400	-3.19511200
H	1.47784100	-3.64749700	4.78067300	H	-5.67414300	-2.57620400	-5.72240300
H	0.18167500	-7.19161600	2.68594800	H	-1.50739300	-2.11132000	-4.74038300
H	-0.08478200	-5.79054800	0.65051000	H	-3.26474100	-2.62399600	-6.43519500
C	-2.55976000	-2.09186500	-4.47193100	H	-6.20078000	-2.01908500	-3.32904500
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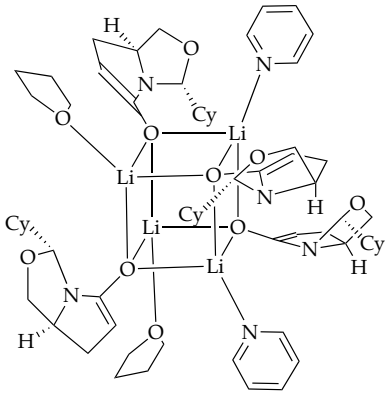

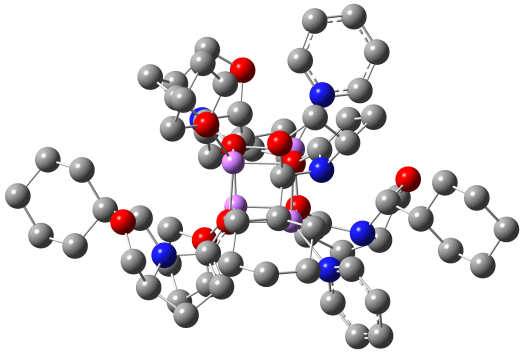

28
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G_{MP2} = –3673.336078

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O	-0.07678700	1.29647200	1.50085100	C	4.65426100	-2.74532800	2.22619200
C	-0.05476300	2.74102300	1.57953300	H	5.59226000	-3.06174900	2.69689100
C	-0.89102800	3.06619700	2.81209600	H	3.95238600	-2.43220700	3.01300700
C	-0.47775900	1.93747100	3.77236900	H	2.54679300	-3.58876100	0.15966100
C	-0.26651100	0.73945600	2.83207100	H	5.84929300	-1.66596800	0.75947700
H	0.62093300	0.15032900	3.08559900	H	4.74996100	-0.11597800	2.79935400
H	-1.13345900	0.07468900	2.78720500	H	5.10584100	0.55791700	1.21074200
H	-1.23306800	1.72938300	4.53575300	H	2.39845100	0.71526500	1.68692200
H	0.45703400	2.19376500	4.28472600	Li	0.07043600	-2.63746600	0.02495700
H	-1.95643100	2.98882000	2.57442600	O	-1.44950300	-1.30836100	0.12947600
H	-0.68276700	4.06499400	3.20805500	C	-2.54396100	-1.46440600	0.84383100
H	-0.44478000	3.13504700	0.63917000	C	-2.84941600	-2.38554100	1.79231300
H	0.98414600	3.08099600	1.69233700	C	-4.27111700	-2.21875500	2.25908400
O	1.51830400	-1.31488300	-0.04774900	C	-4.62571000	-0.82615000	1.70035600
C	2.67746300	-1.08658500	0.53520000	H	-5.66042000	-0.75752600	1.35305700
C	3.03790600	-0.11131200	1.40927300	N	-3.67916500	-0.59057500	0.57776700
C	4.50580100	-0.20622900	1.73012100	C	-3.43035400	0.85137100	0.53019800
C	4.85110400	-1.61266400	1.20183100	O	-3.82640800	1.39208600	1.81662700
N	3.80969600	-1.92557000	0.18863800	C	-4.30139100	0.33957800	2.65026300
C	3.61867400	-3.37435900	0.21556500	H	-5.17750100	0.69896700	3.20155900

H	-3.52715100	0.04057500	3.37223000	H	4.56871800	-2.46045700	-4.76418900
H	-2.35654300	1.01749400	0.39821500	H	4.36897100	-1.43599800	-2.52417500
H	-4.40096900	-2.24962400	3.35129600	H	4.13924700	0.17437400	-3.25198800
H	-4.94824500	-2.98286700	1.84569600	C	-3.36537200	-5.26064500	-1.87208700
H	-2.20334400	-3.20658600	2.07231100	C	-3.79941900	-6.23045200	-2.98558500
Li	-1.41973000	-1.37593500	-1.83830100	C	-4.05286800	-5.61737500	-0.53850000
O	-0.09762200	-2.80736100	-1.94019000	H	-3.69180500	-4.25140100	-2.15966600
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C	1.12213000	-4.32081600	-3.38980500	H	-3.40921000	-7.23322900	-2.76091900
C	0.80096700	-5.60589800	-4.10553500	H	-3.36377100	-5.91789100	-3.94174900
C	-0.51455800	-6.02529500	-3.41901500	C	-5.58134100	-5.68078400	-0.67735500
N	-1.08622000	-4.77542200	-2.85852000	H	-3.67604000	-6.59068400	-0.19598800
C	-1.84328500	-5.15169900	-1.67479900	H	-3.77474900	-4.88046400	0.22732000
O	-1.31644700	-6.43338200	-1.22864200	C	-6.00449700	-6.65449800	-1.78661900
C	-0.33409200	-6.89315000	-2.15835100	H	-5.60548200	-7.02789400	-3.89241900
H	-0.50284000	-7.95925900	-2.34800700	H	-5.70367600	-5.32290900	-3.46277200
H	0.67251500	-6.76280100	-1.73649400	H	-6.03442100	-5.97226600	0.27930500
H	-1.66114600	-4.40932900	-0.88914200	H	-5.96723400	-4.67708400	-0.91206300
H	-1.21908700	-6.49767500	-4.10829300	H	-7.09670000	-6.65571100	-1.90025400
H	1.56673200	-6.38878300	-4.00074400	H	-5.71845700	-7.67694100	-1.49774500
H	0.64205100	-5.47335800	-5.18805100	C	-4.17581400	1.60277800	-0.58626400
H	2.04744700	-3.76966500	-3.48700400	C	-5.70182200	1.40173000	-0.57576700
Li	1.24220400	-1.29297000	-1.98643600	C	-3.83688400	3.10588700	-0.55065200
O	-0.09900200	0.14514500	-1.95407400	H	-3.77969800	1.19819600	-1.53017100
C	-0.25898700	1.12527600	-2.81953200	C	-6.38530300	2.16556200	-1.72147300
C	-1.29734200	1.39956200	-3.64912100	H	-6.10109100	1.75381200	0.38570100
C	-0.99327900	2.60390900	-4.49959200	H	-5.94336600	0.33419400	-0.64782900
C	0.23450700	3.19583100	-3.77823000	C	-4.51538900	3.87368700	-1.69532900
H	0.96571000	3.62177000	-4.47038700	H	-4.16047200	3.51868300	0.41404700
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H	-1.13708300	4.06832000	-2.31805500	H	-4.10231500	3.52878300	-2.65486100
H	1.22350700	1.99775200	-0.96824200	H	-6.49665500	4.17583800	-2.54592300
H	-1.80908100	3.33994300	-4.55695400	H	-6.46372200	4.11237100	-0.78539300
H	-0.73875000	2.34420500	-5.53997900	C	4.31653500	-4.14295300	-0.92073900
H	-2.17338500	0.77477300	-3.75737600	C	5.83543200	-3.91077600	-1.00735000
O	2.55420200	-1.16522100	-3.43455800	C	4.00323300	-5.64869700	-0.81797600
C	3.96913000	-0.90249900	-3.38840700	H	3.85771600	-3.77204200	-1.84964100
C	4.47698300	-1.36814600	-4.74906800	C	6.47639100	-4.71615300	-2.14937500
C	3.34263800	-0.89860000	-5.67950600	H	6.29374800	-4.20665100	-0.05344400
C	2.08171100	-1.02033700	-4.80005800	H	6.04528100	-2.84328900	-1.14731400
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H	3.50399200	0.14424900	-5.97384900	H	2.91477800	-5.79509200	-0.82169600
H	3.26699300	-1.49523600	-6.59335000	C	6.15831300	-6.21346900	-2.03722800
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H	6.10097700	-4.33986800	-3.11357700	C	-4.32181300	-1.52629700	-2.75227100
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C	3.50560400	3.43788200	-0.59118700	H	-4.47676500	-1.19108400	-1.72938700
H	3.37228600	1.79957900	-1.97623700	H	-6.40934200	-1.61513700	-3.27136800
C	4.99098300	3.76951000	-3.12803800	H	-3.53272700	-2.74696700	-6.28468700
H	3.00142600	4.61848800	-3.09893800	H	-1.74121300	-2.28088300	-4.61214200
H	3.13112700	3.12871100	-4.04090900	C	0.92626000	-3.50183800	2.66815600
C	5.03431900	3.58870200	-0.60454300	C	1.12004900	-4.21984400	3.84585900
H	3.03947500	4.42221700	-0.45132900	C	0.72885100	-5.55696200	3.88465700
H	3.20159600	2.81420400	0.26000800	C	0.16372700	-6.12127000	2.74233100
C	5.51088200	4.39053300	-1.82414900	C	0.00177000	-5.32766900	1.60735800
H	5.30255700	4.37387500	-3.99018600	N	0.37042600	-4.03379800	1.56547000
H	5.45117600	2.77820300	-3.26142000	H	0.86703400	-6.14879700	4.78560300
H	5.37225200	4.06914200	0.32297300	H	1.23917400	-2.46351000	2.59149800
H	5.49847100	2.59099400	-0.62481700	H	1.57431900	-3.73781900	4.70582200
H	6.60709400	4.44984100	-1.83970500	H	-0.15099100	-7.15997100	2.72105000
H	5.14179900	5.42398000	-1.74429500	H	-0.43820900	-5.74069200	0.70206700

Part 4: Full References

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.