

Lithium Enolates Derived from Weinreb Amides:  
Insights into Five-Membered Chelate Rings

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**Part 1: NMR Spectroscopic Studies**

- Figure 1.**  $^6\text{Li}$  NMR spectra for 0.10 M solutions of  $[\text{}^6\text{Li}]\mathbf{3d}$  and  $[\text{}^6\text{Li}]\mathbf{3c}$  in 12.3 M THF with varying  $X_B$  at  $-80\text{ }^\circ\text{C}$ . **S4**
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- Figure 9.** Job plot of  $[\text{}^6\text{Li}]\mathbf{3e}/[\text{}^6\text{Li}]\mathbf{3g}$ . Relative integrals measured at  $-80\text{ }^\circ\text{C}$  are plotted vs measured mole fraction of  $[\text{}^6\text{Li}]\mathbf{3g}$ . **S12**
- Figure 10.**  $^6\text{Li}$  NMR spectra for 0.10 M solutions of  $[\text{}^6\text{Li}]\mathbf{3a}$  and  $[\text{}^6\text{Li}]\mathbf{3b}$  in 12.3 M THF with varying  $X_B$  at  $-80\text{ }^\circ\text{C}$ . **S13**
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## Part 2: Computational Studies

**Table 1.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for tetrameric Weinreb amide enolates at  $-78\text{ }^{\circ}\text{C}$ . **S33**

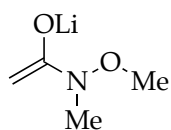
**Table 2.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for dimeric Weinreb amide enolates at  $-78\text{ }^{\circ}\text{C}$ . **S51**

**Table 3.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for dimeric Weinreb amide enolates at  $-78\text{ }^{\circ}\text{C}$ . **S56**

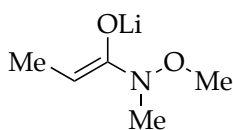
## Part 3: Full References **S68**

### Part 1: NMR Spectroscopic Studies

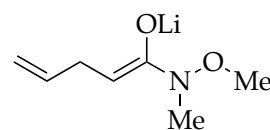
#### Chart 1



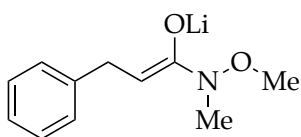
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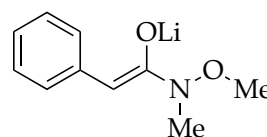
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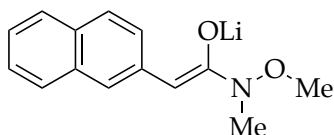
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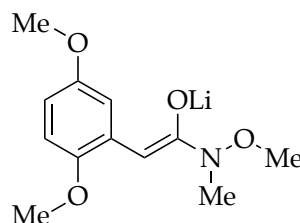
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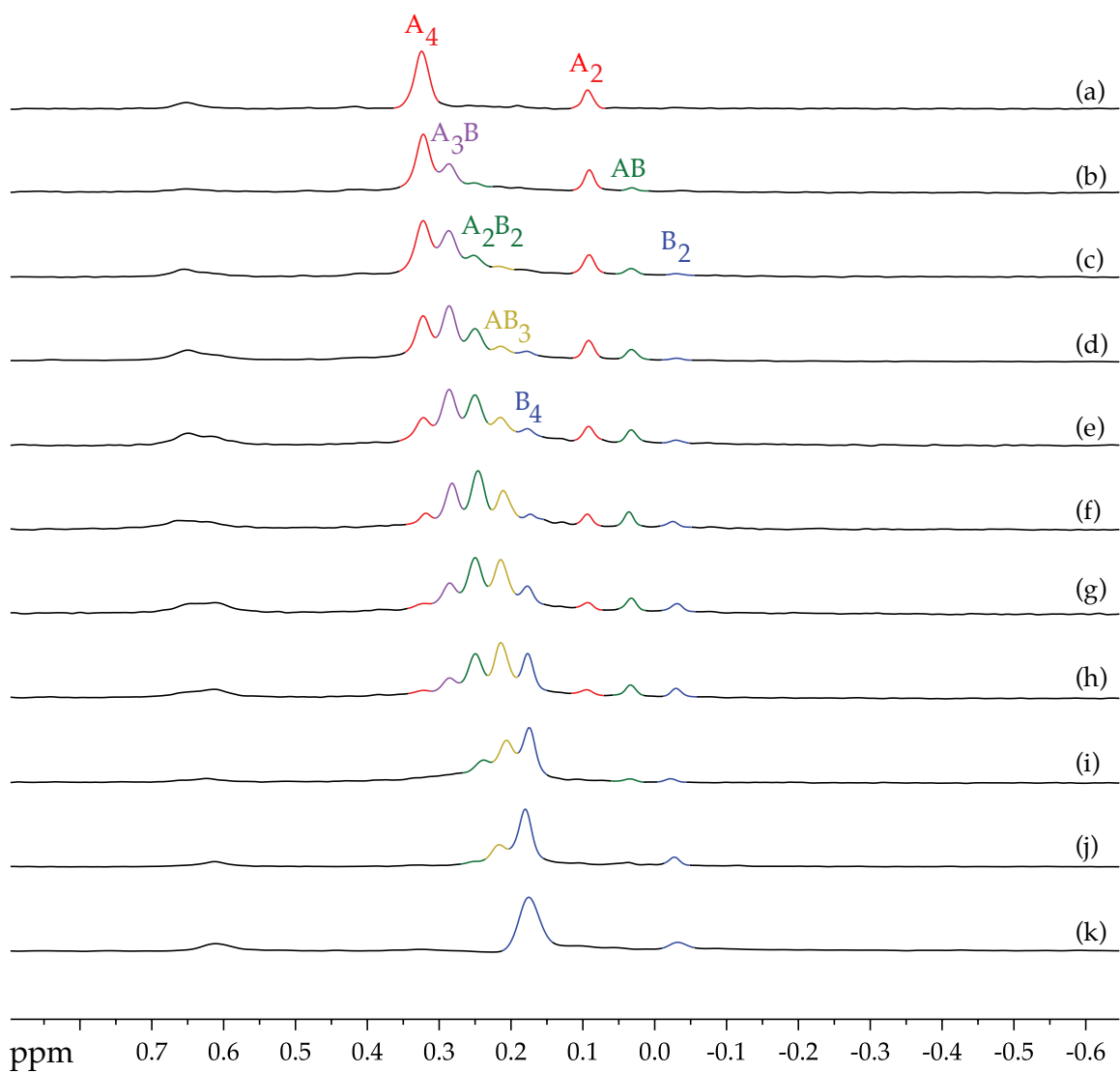
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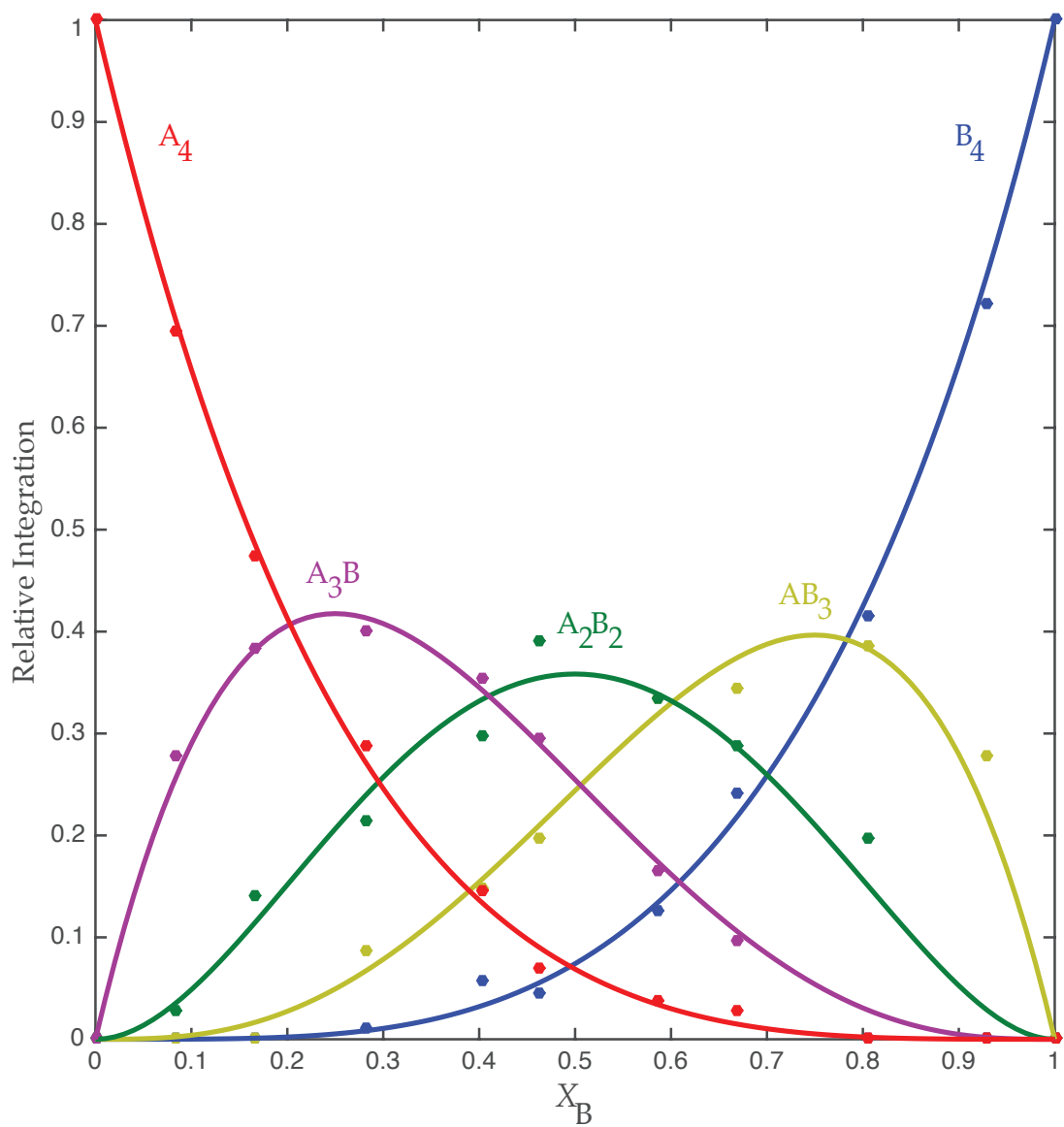
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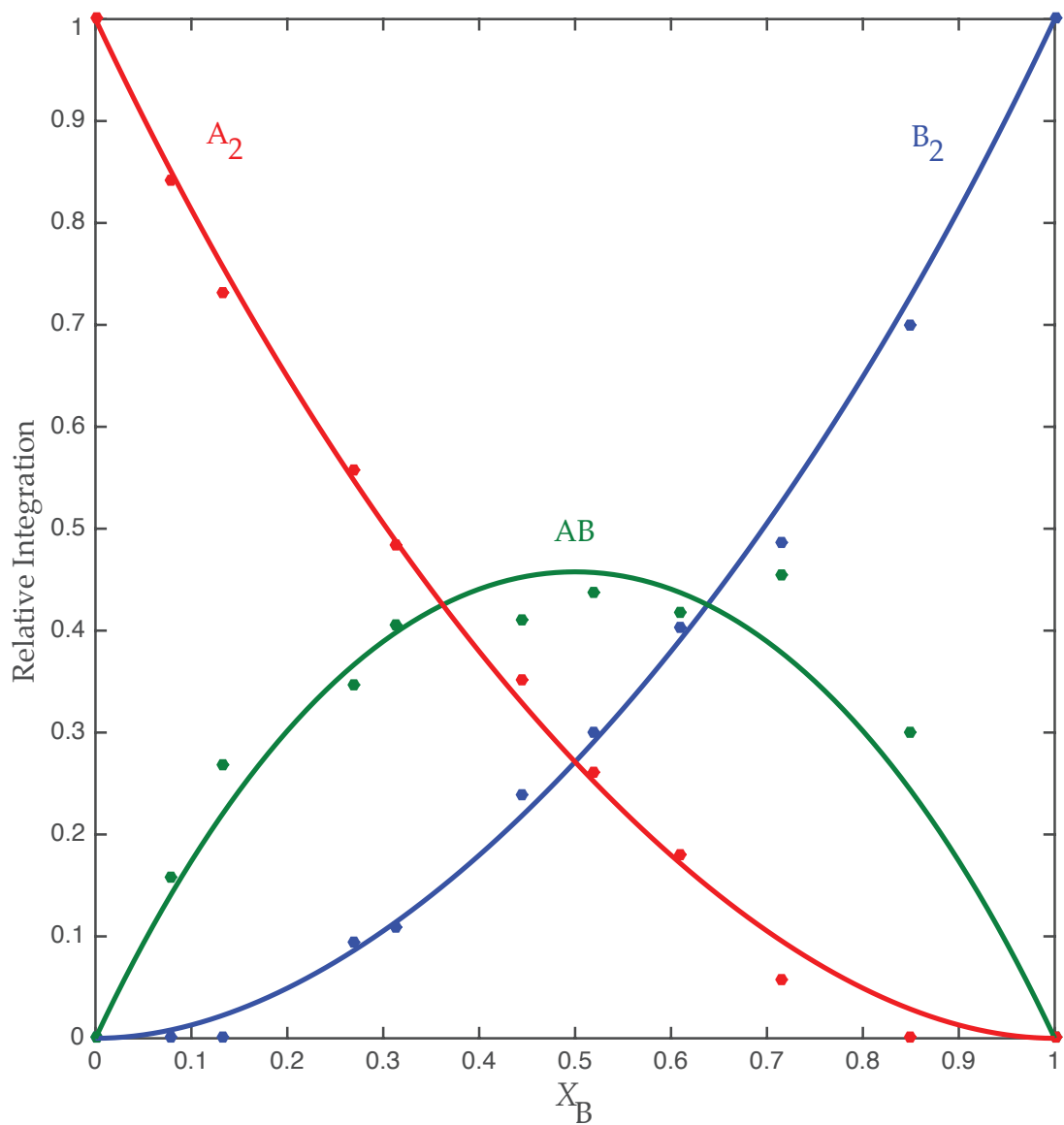
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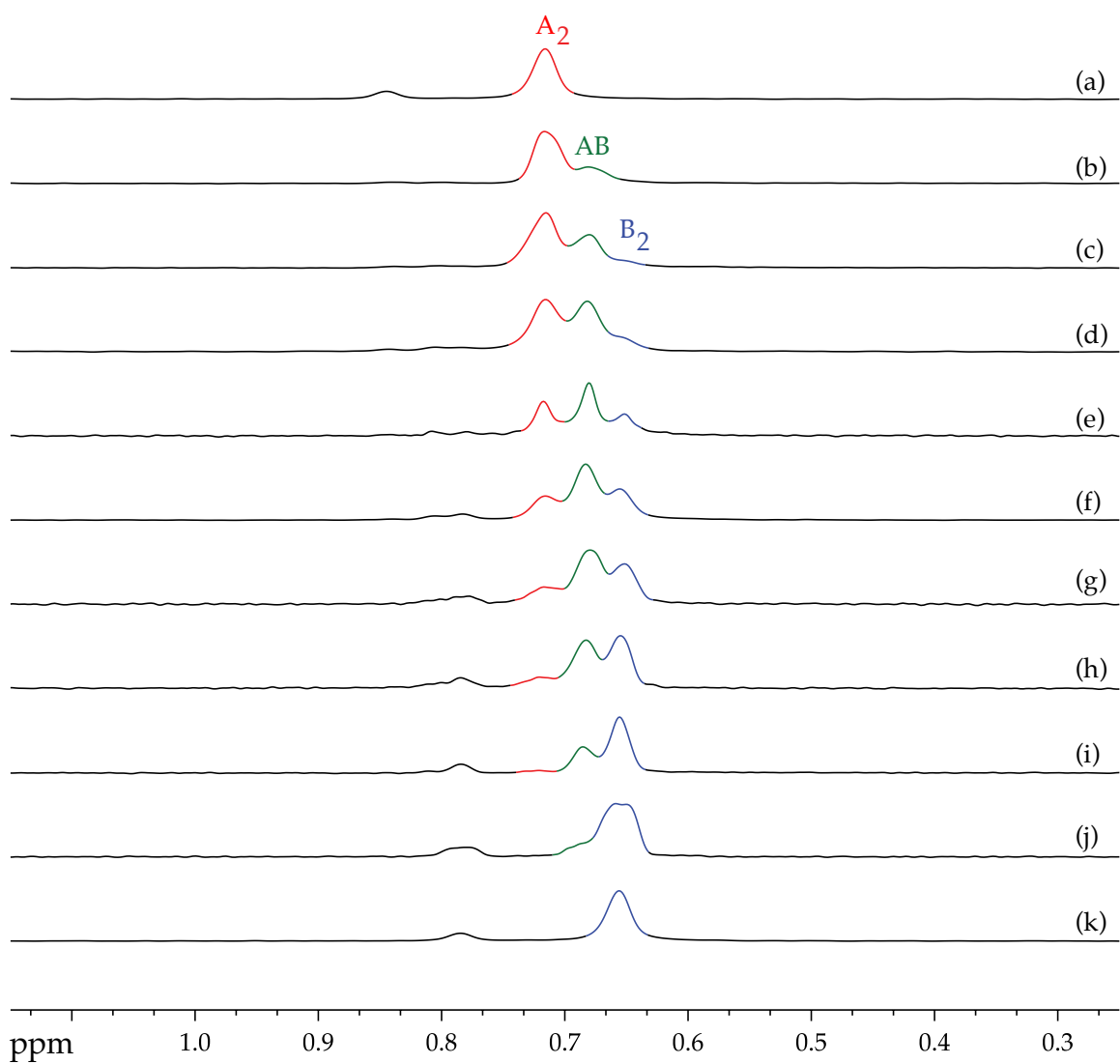
**Figure 1.**  $^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[^6\text{Li}]\mathbf{3d}$  (**A**) and  $[^6\text{Li}]\mathbf{3c}$  (**B**) in 12.3 M THF at  $-80\text{ }^\circ\text{C}$  with 0.13 M  $[^6\text{Li}]\text{LDA}$ . The measured mole fractions,  $X_B$ , for the tetramer are 0.00, 0.13, 0.24, 0.33, 0.42, 0.52, 0.55, 0.78, 0.89, and 1.00, respectively. The measured mole fractions for the dimer,  $X_B$ , (a)–(k) are 0.00, 0.08, 0.13, 0.27, 0.31, 0.44, 0.52, 0.61, 0.71, 0.85, and 1.00, respectively.



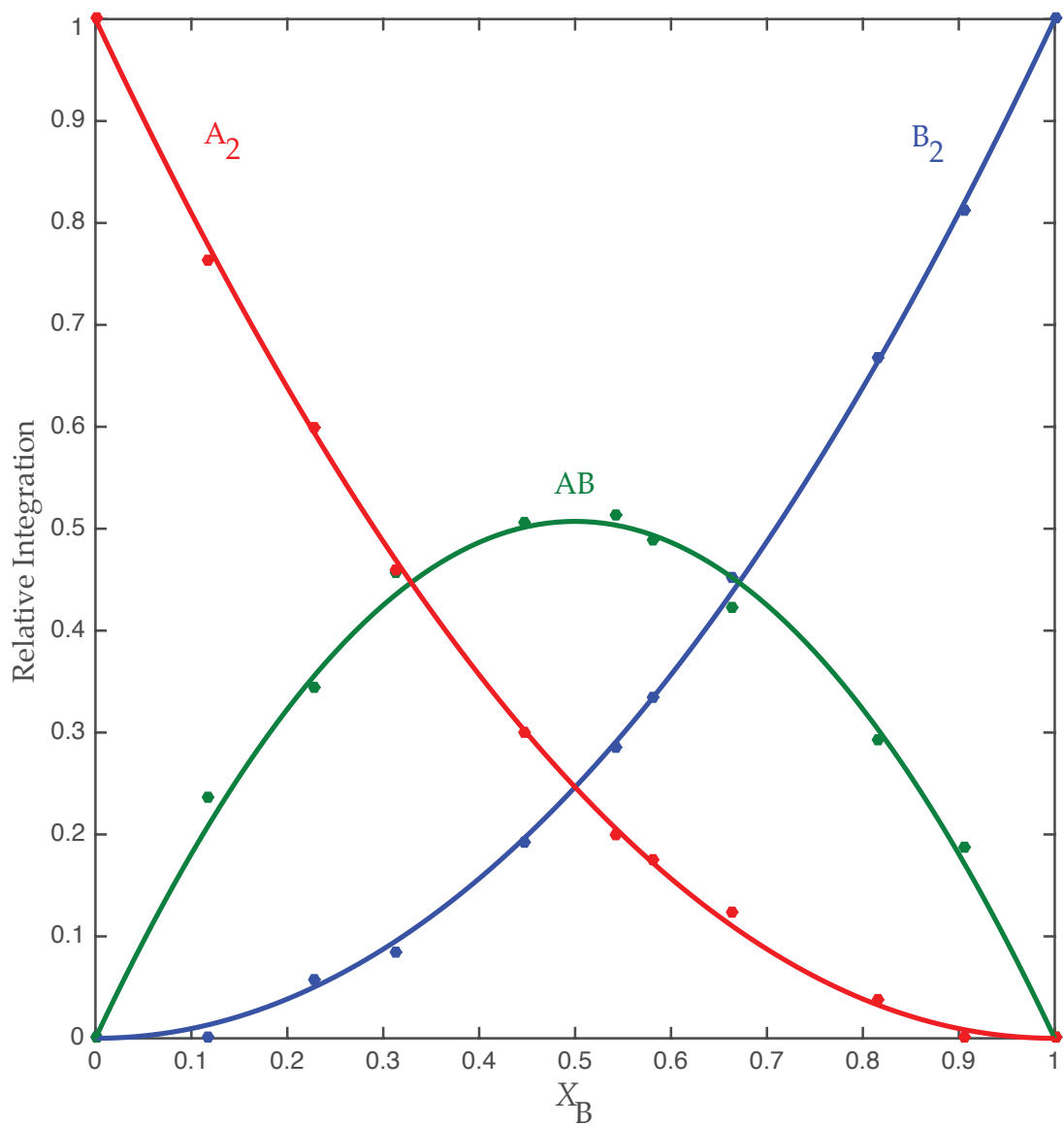
**Figure 2.** Job plot showing the relative integrations versus the measured mole fraction of tetramer for 0.10 M mixtures of [<sup>6</sup>Li]3d (**A**) and [<sup>6</sup>Li]3c (**B**) in 12.3 M THF at -80 °C.



**Figure 3.** Job plot showing the relative integrations versus the measured mole fraction of dimer for 0.10 M mixtures of [<sup>6</sup>Li]3d (**A**) and [<sup>6</sup>Li]3c (**B**) in 12.3 M THF at –80 °C.

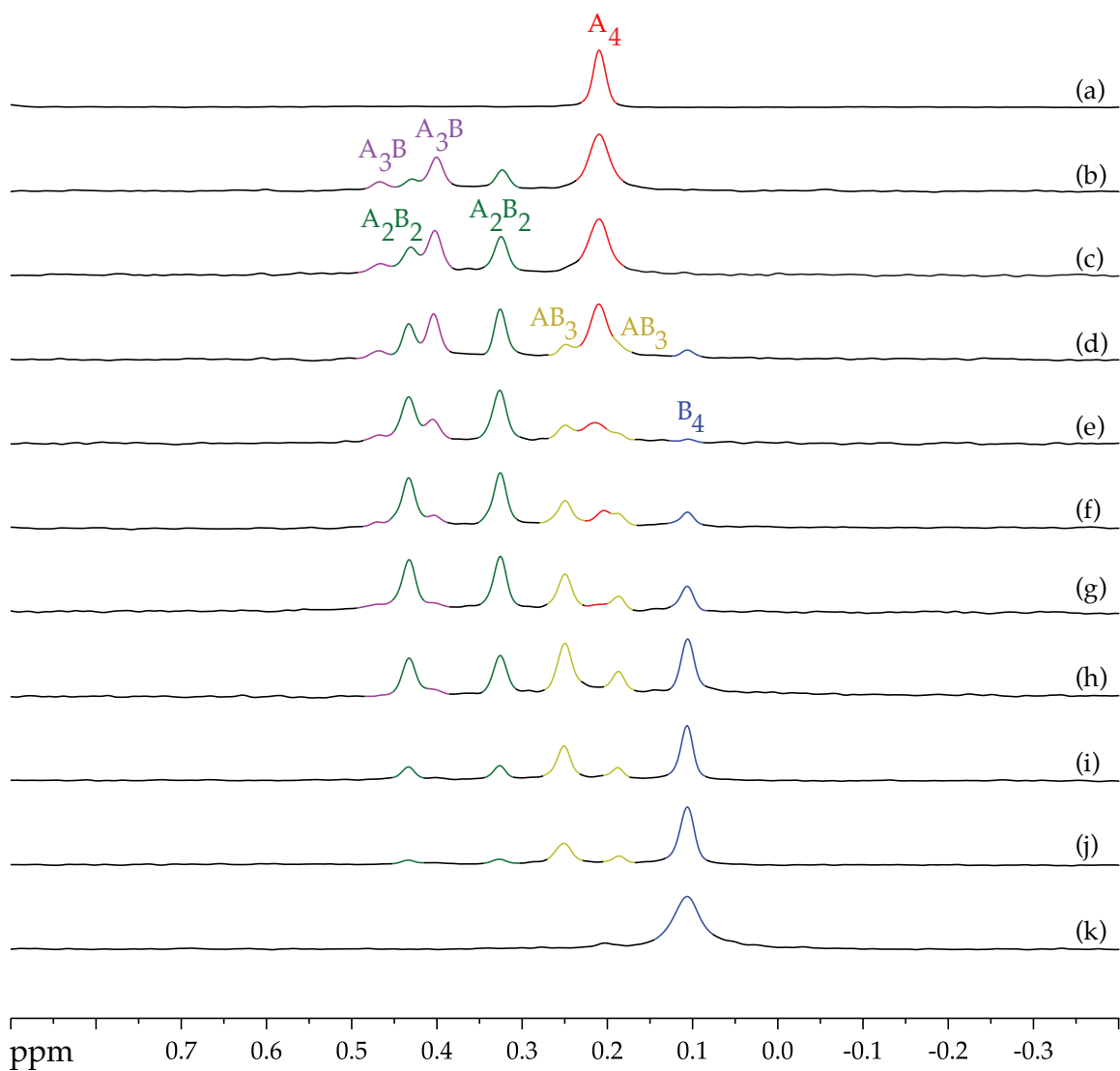


**Figure 4.**  ${}^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[{}^6\text{Li}]\mathbf{3f}$  (**A**) and  $[{}^6\text{Li}]\mathbf{3e}$  (**B**) in 1.0 M pyridine and THF at  $-80\text{ }^\circ\text{C}$  with 0.13 M  $[{}^6\text{Li}]\text{LDA}$ . The measured mole fractions,  $X_{\text{B}}$ , in (a)–(k) are 0.00, 0.12, 0.23, 0.31, 0.45, 0.54, 0.58, 0.66, 0.81, 0.91, and 1.00, respectively.

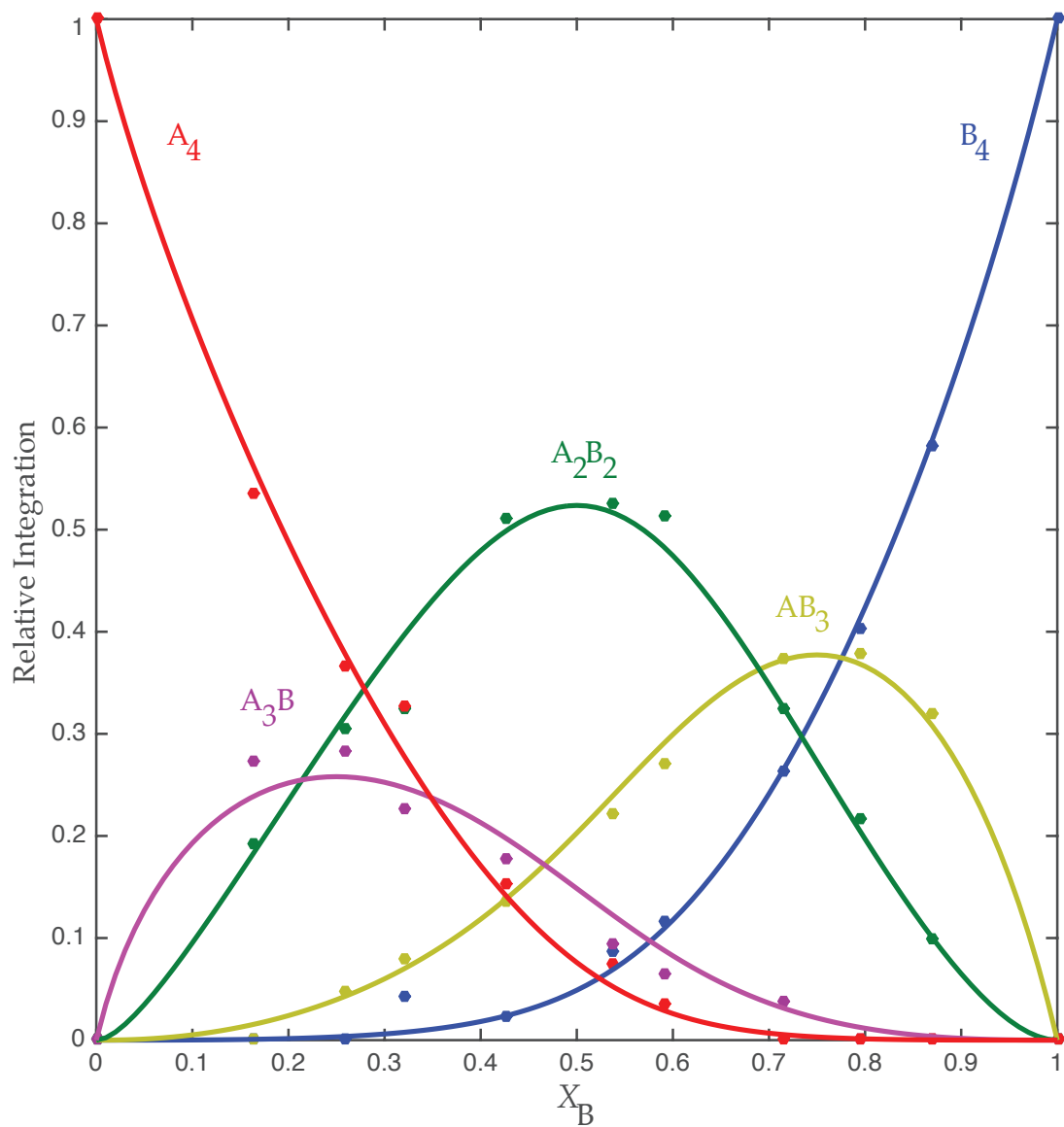


**Figure 5.** Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [ $^6\text{Li}$ ]3f (**A**) and [ $^6\text{Li}$ ]3e (**B**) in 1.0 M pyridine and THF at  $-80\text{ }^\circ\text{C}$ .

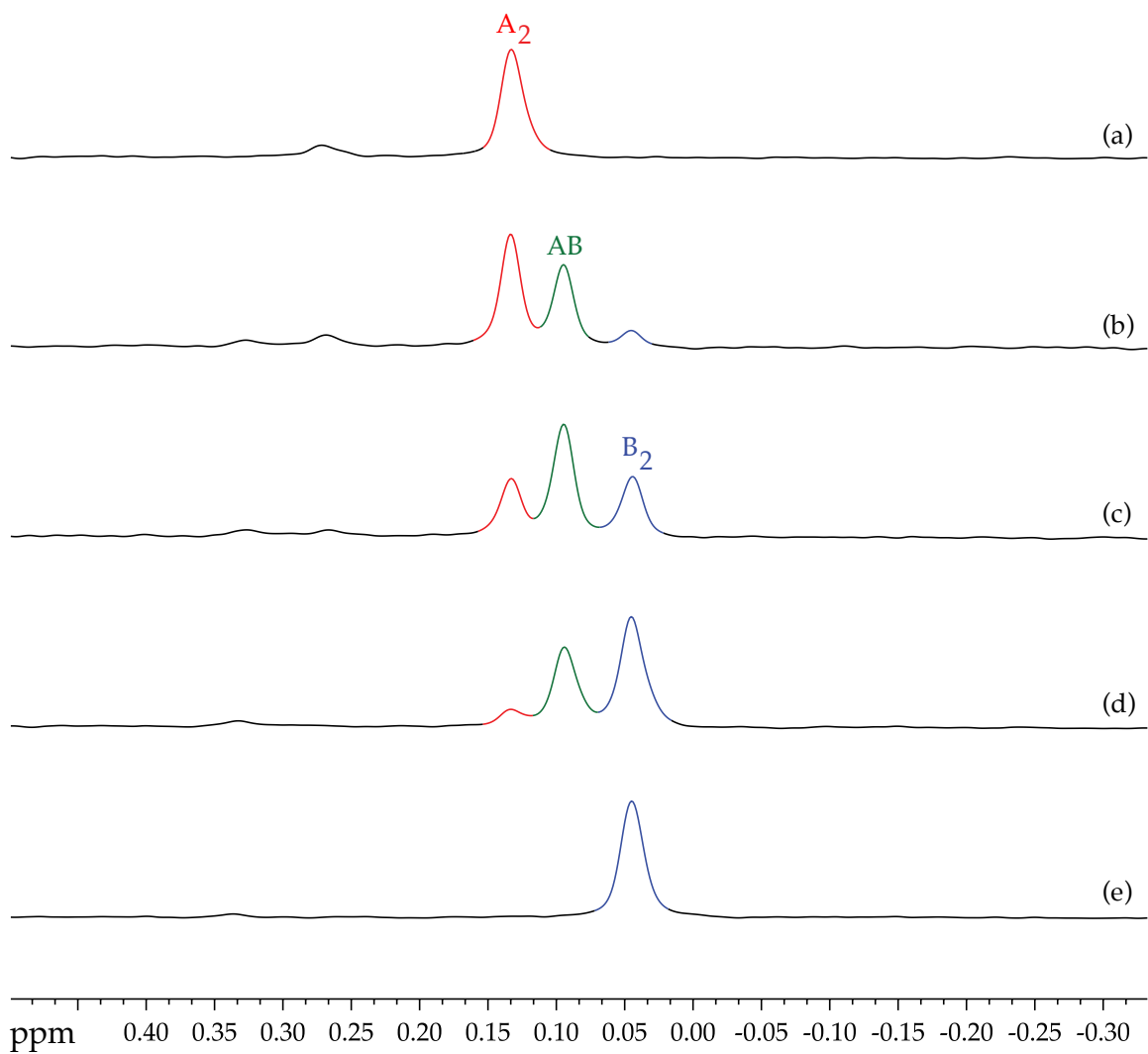




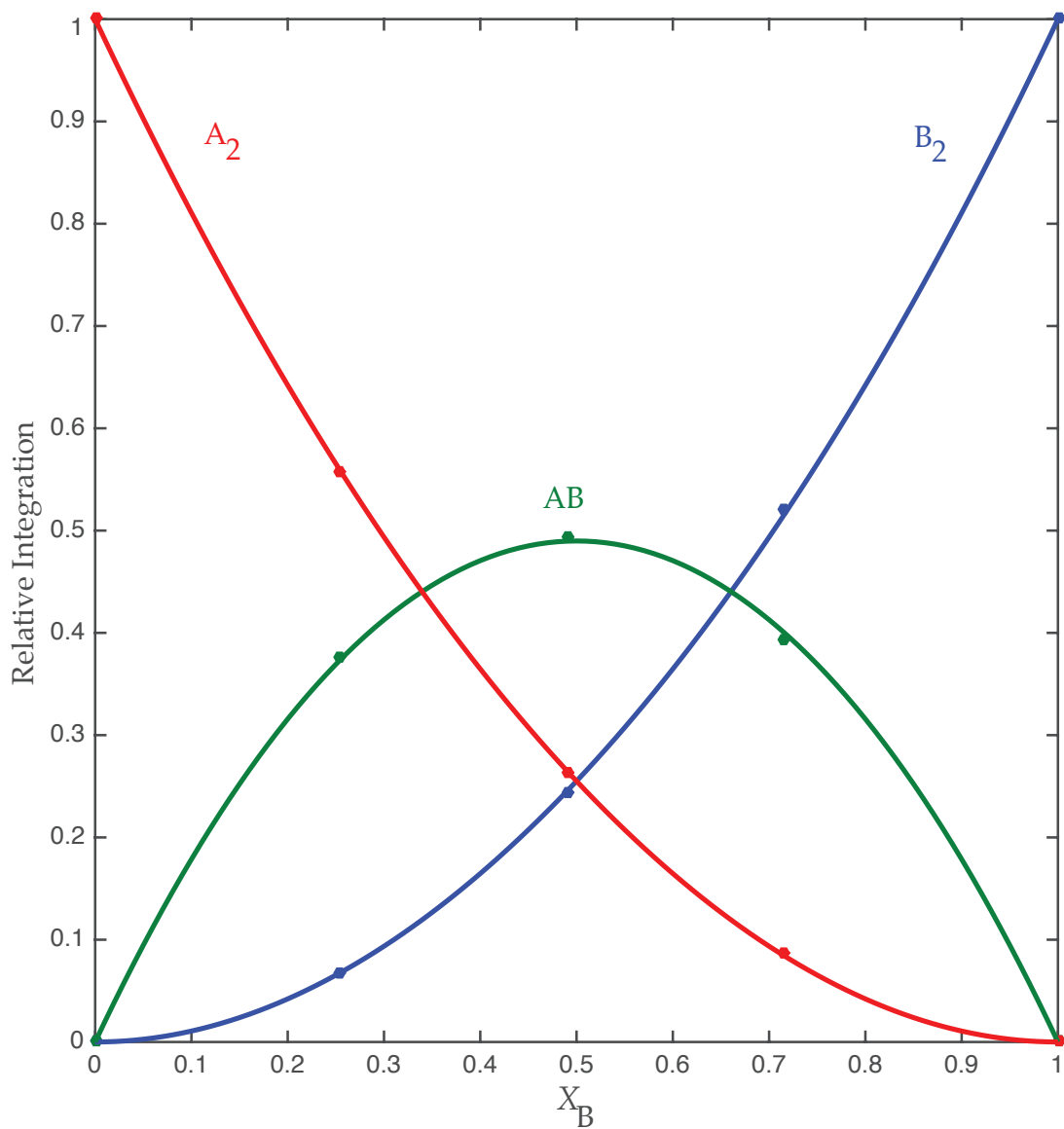
**Figure 6.**  $^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[\text{}^6\text{Li}]\mathbf{3c}$  (A) and  $[\text{}^6\text{Li}]\mathbf{3e}$  (B) in 1.0 M THF and toluene at  $-80\text{ }^\circ\text{C}$  with 0.13 M  $[\text{}^6\text{Li}]\text{LDA}$ . The measured mole fractions,  $X_B$ , in (a)–(k) are 0.00, 0.16, 0.26, 0.32, 0.43, 0.54, 0.59, 0.72, 0.80, 0.87, and 1.00, respectively.



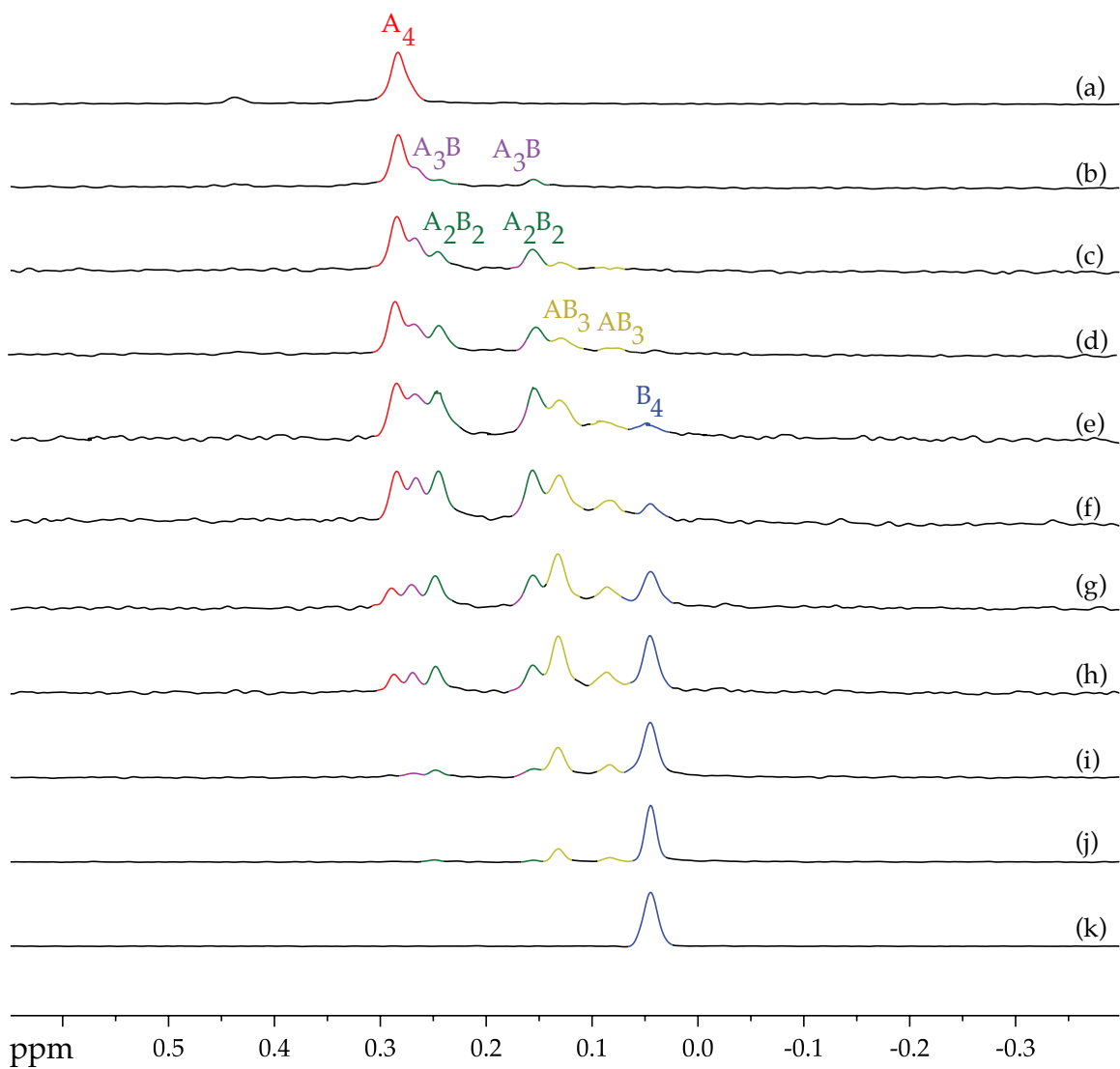
**Figure 7.** Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [<sup>6</sup>Li]**3c** (**A**) and [<sup>6</sup>Li]**3e** (**B**) in 1.0 M THF and toluene at  $-80\text{ }^{\circ}\text{C}$ .



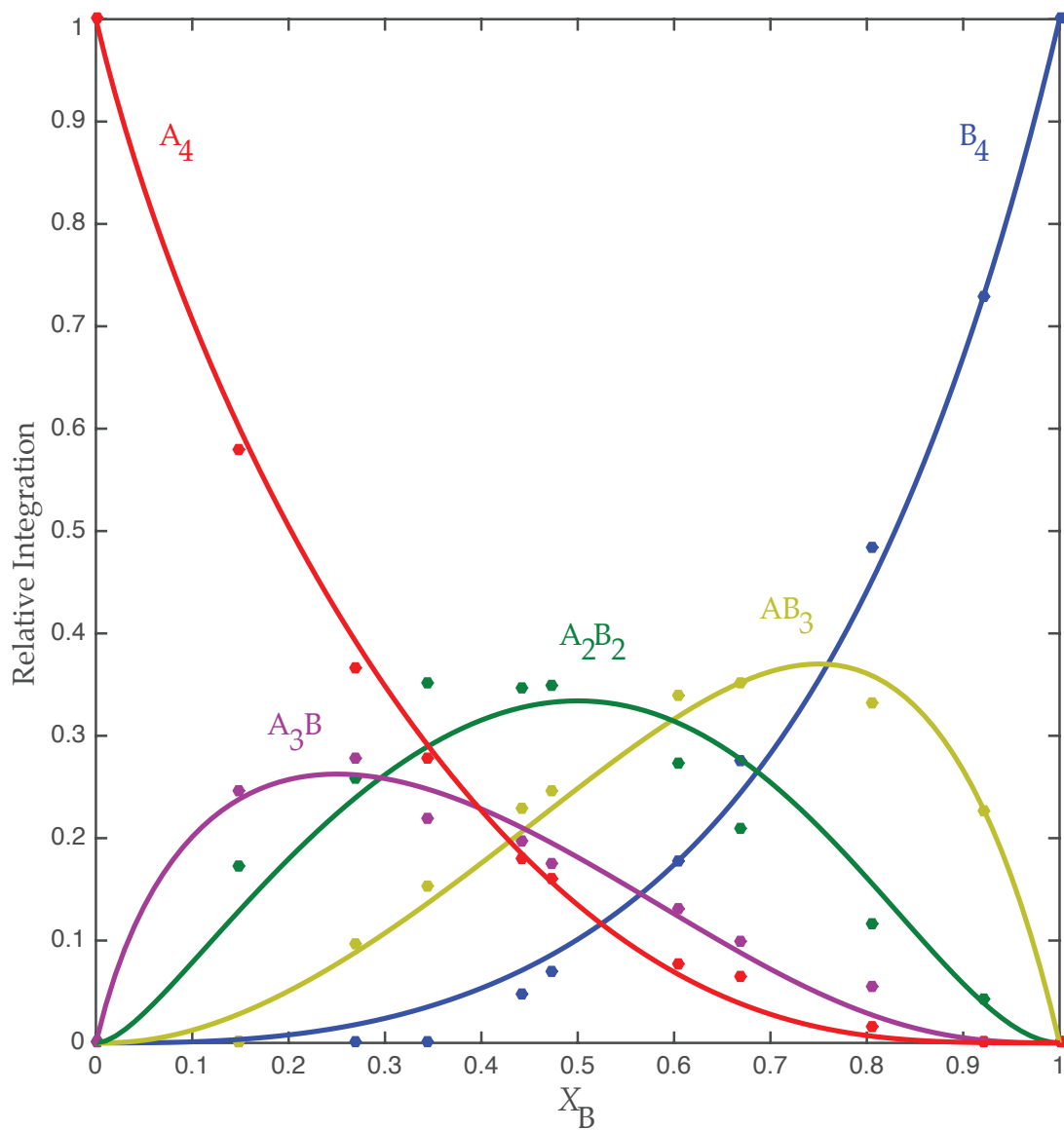
**Figure 8.**  $^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[^6\text{Li}]\mathbf{3e}$  (**A**) and  $[^6\text{Li}]\mathbf{3g}$  (**B**) in 12.3 M THF at  $-80\text{ }^\circ\text{C}$  with 0.13 M  $[^6\text{Li}]\text{LDA}$ . The measured mole fractions,  $X_{\text{B}}$ , in (a)–(e) are 0.00, 0.25, 0.49, 0.72, and 1.00, respectively.



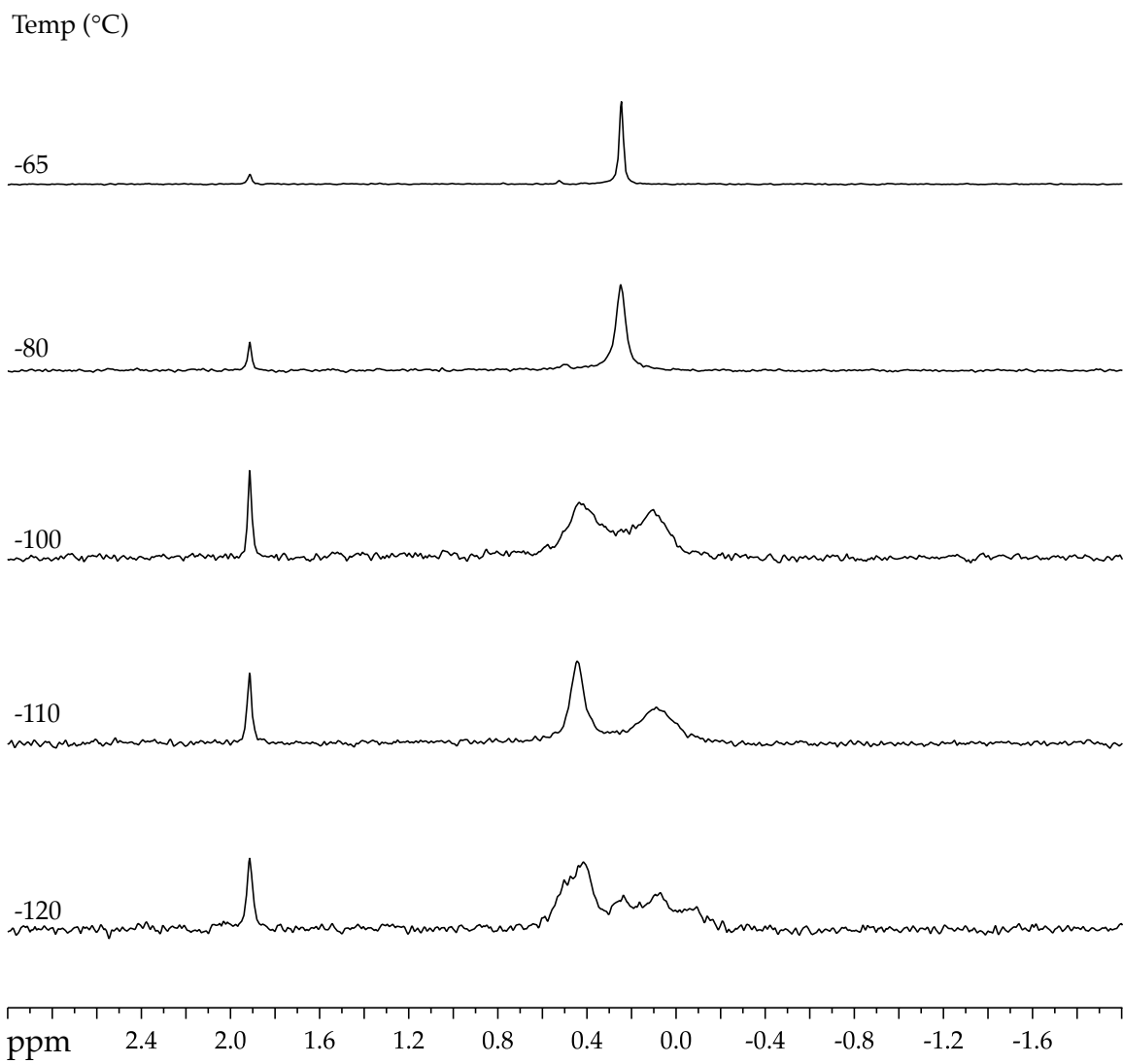
**Figure 9.** Job plot showing the relative integrations versus the measured mole fraction of **3** for 0.10 M mixtures of [<sup>6</sup>Li]**3e** (**A**) and [<sup>6</sup>Li]**3g** (**B**) in 12.3 M THF at -80 °C.



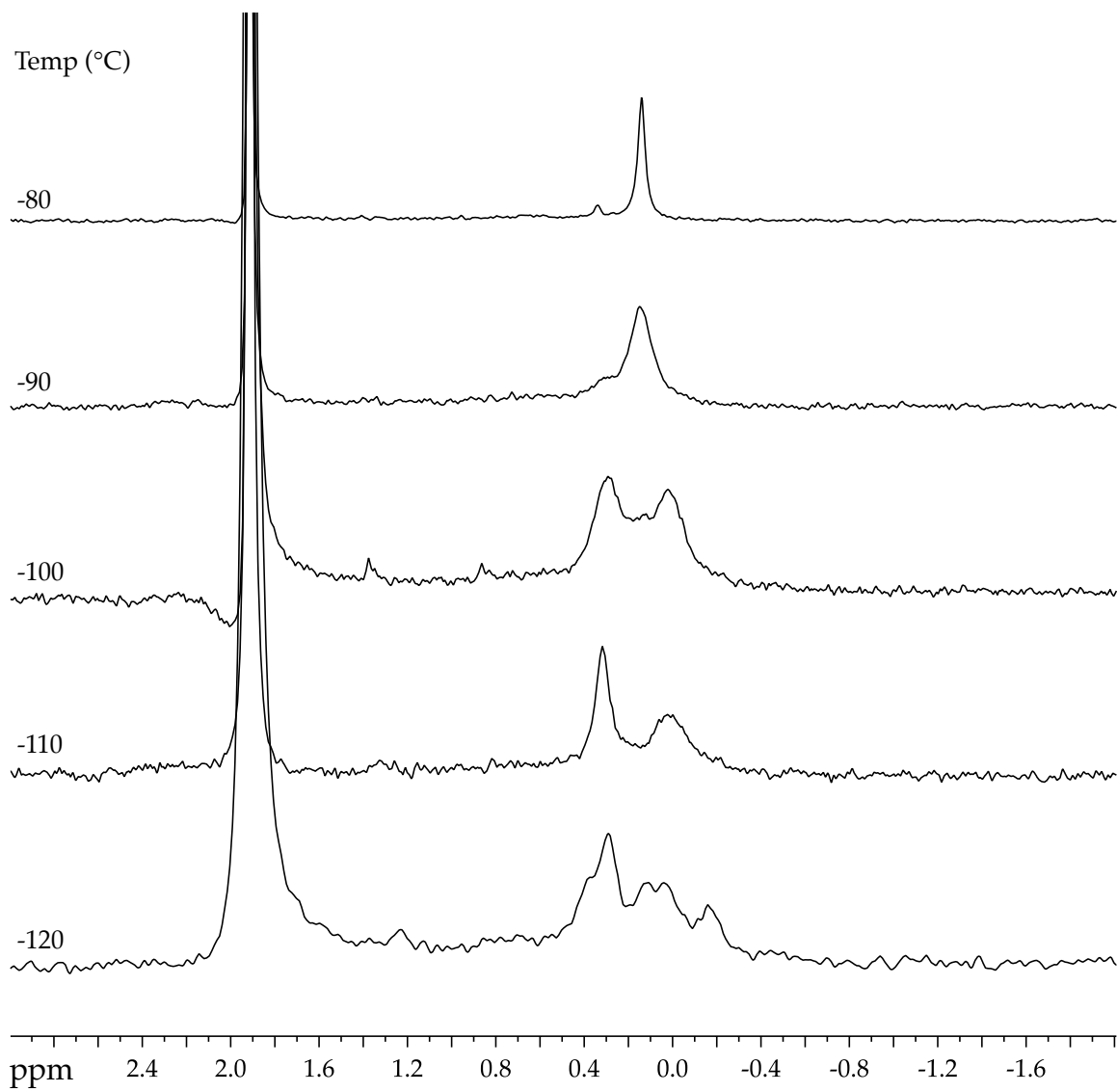
**Figure 10.**  $^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[\text{}^6\text{Li}]\mathbf{3a}$  (**A**) and  $[\text{}^6\text{Li}]\mathbf{3b}$  (**B**) in 12.3 M THF and toluene at  $-80\text{ }^\circ\text{C}$  with 0.13 M  $[\text{}^6\text{Li}]\text{LDA}$ . The measured mole fractions,  $X_B$ , in (a)–(k) are 0.00, 0.15, 0.27, 0.34, 0.44, 0.47, 0.60, 0.67, 0.80, 0.92, and 1.00, respectively.



**Figure 11.** Job plot showing the relative integrations versus the measured mole fractions of **3** for 0.10 M mixtures of [<sup>6</sup>Li]**3a** (**A**) and [<sup>6</sup>Li]**3b** (**B**) in 1.0 M THF and toluene at  $-80\text{ }^{\circ}\text{C}$ .

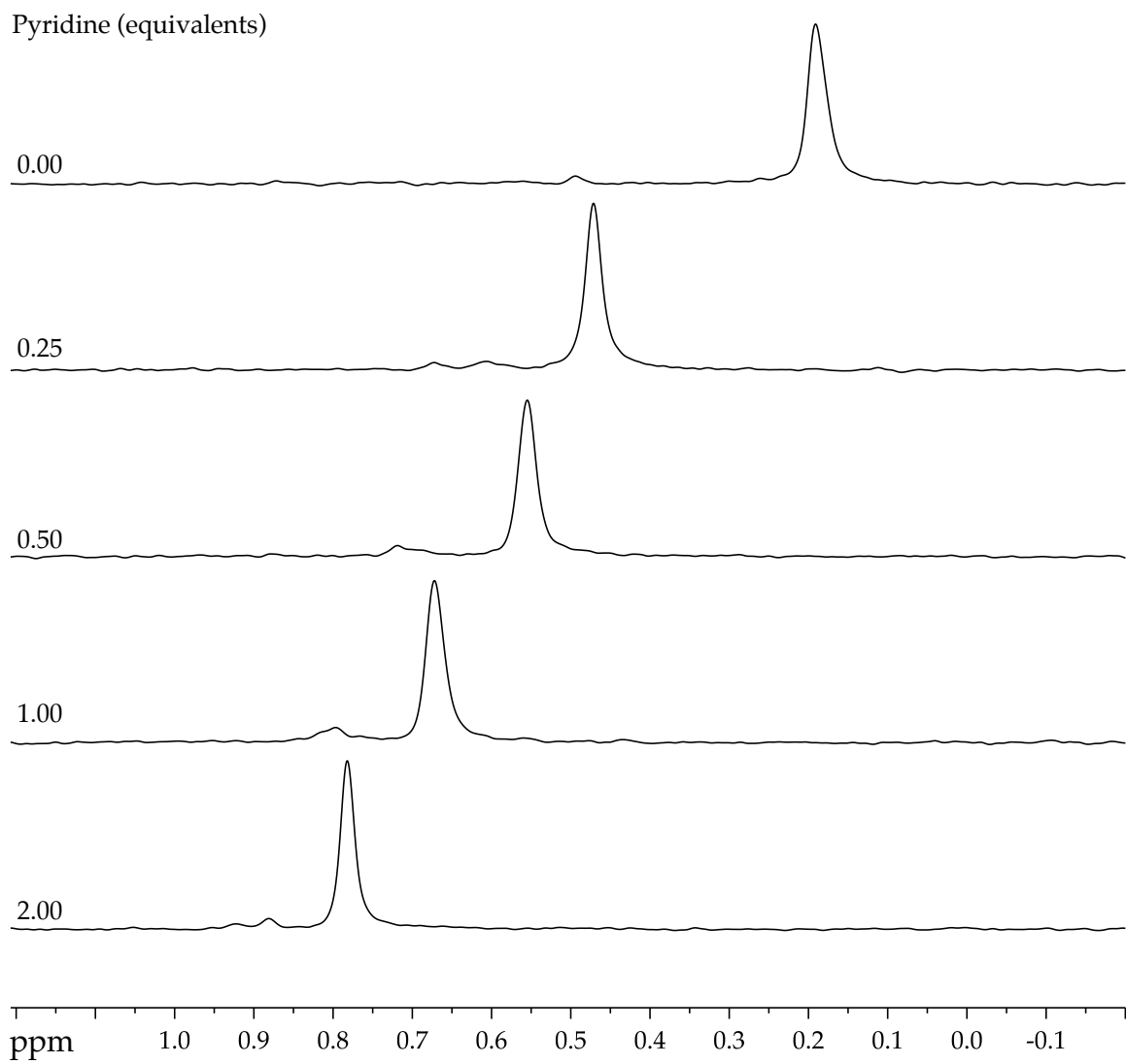


**Figure 12.**  $^6\text{Li}$  NMR spectra of a 0.10 M solution of  $[\text{}^6\text{Li}]\mathbf{3d}$  in 0.20 M THF and toluene with 0.11 M  $[\text{}^6\text{Li}]\text{LDA}$  and varying temperature.

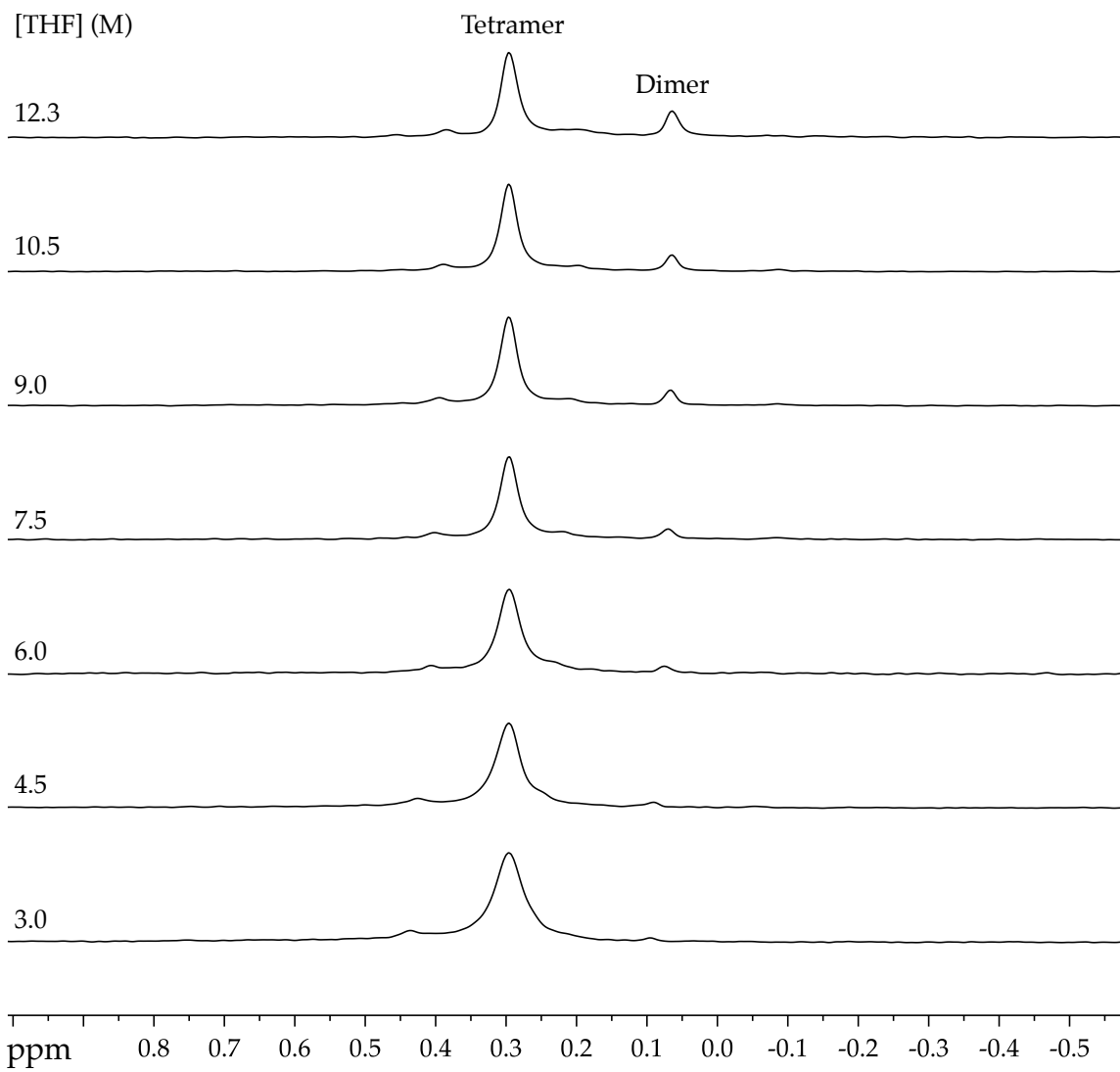


**Figure 13.**  $^6\text{Li}$  NMR spectra of a 0.10 M solution of  $[^6\text{Li}]\mathbf{3c}$  in 0.20 M THF and toluene with 0.11 M  $[^6\text{Li}]\text{LDA}$  and varying temperature.

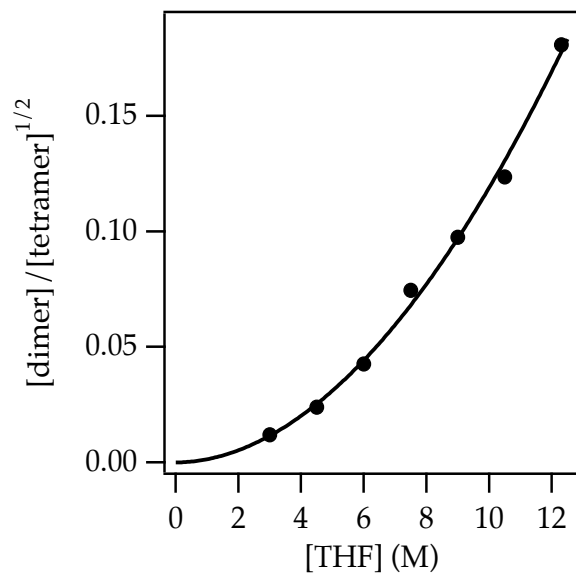




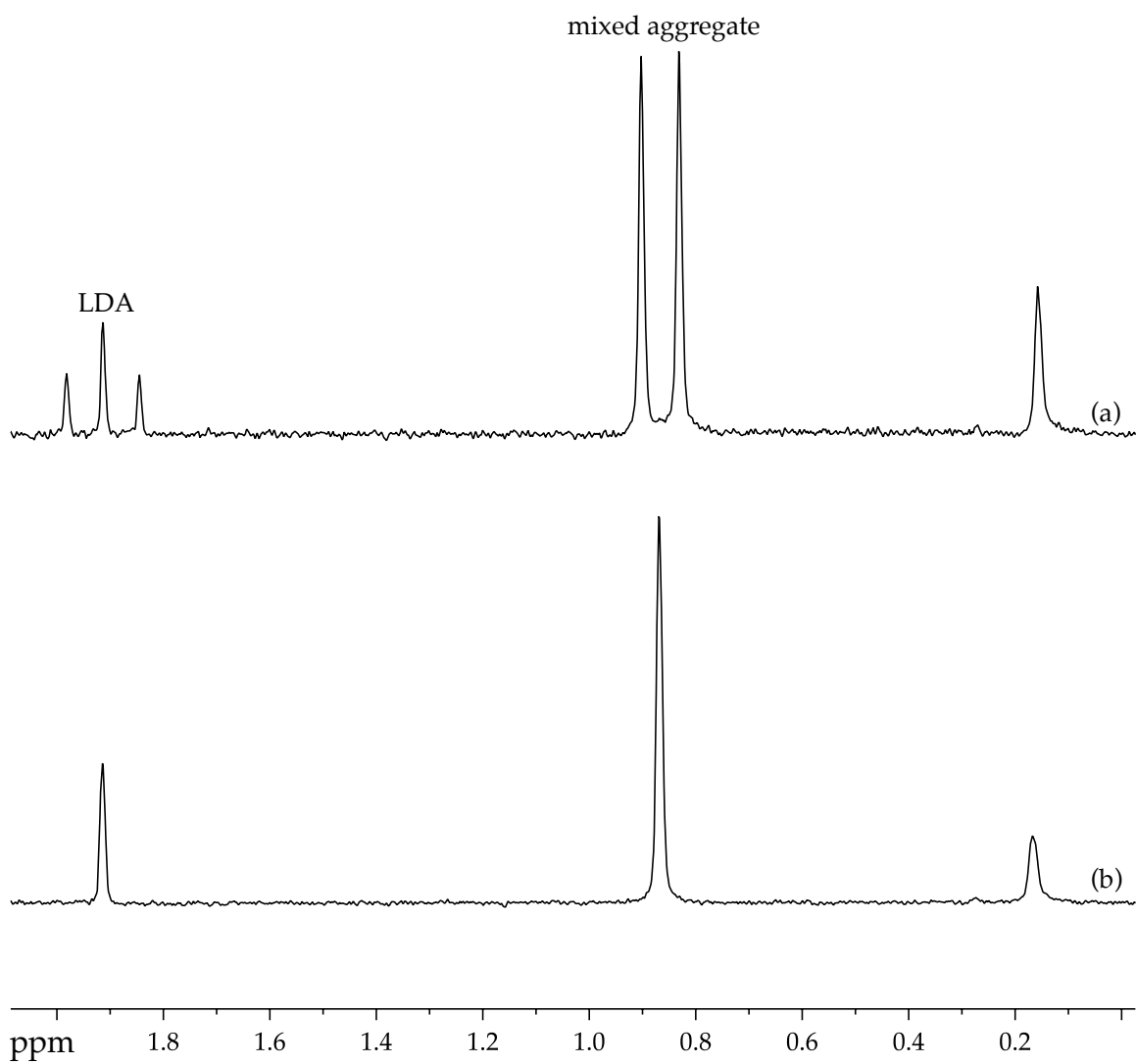
**Figure 14.**  $^6\text{Li}$  NMR spectra of 0.10 M solutions of  $[^6\text{Li}]\mathbf{3d}$  with varying concentrations of pyridine in 0.20 M THF and toluene at  $-80\text{ }^\circ\text{C}$  with 0.11 M  $[^6\text{Li}]\text{LDA}$ .



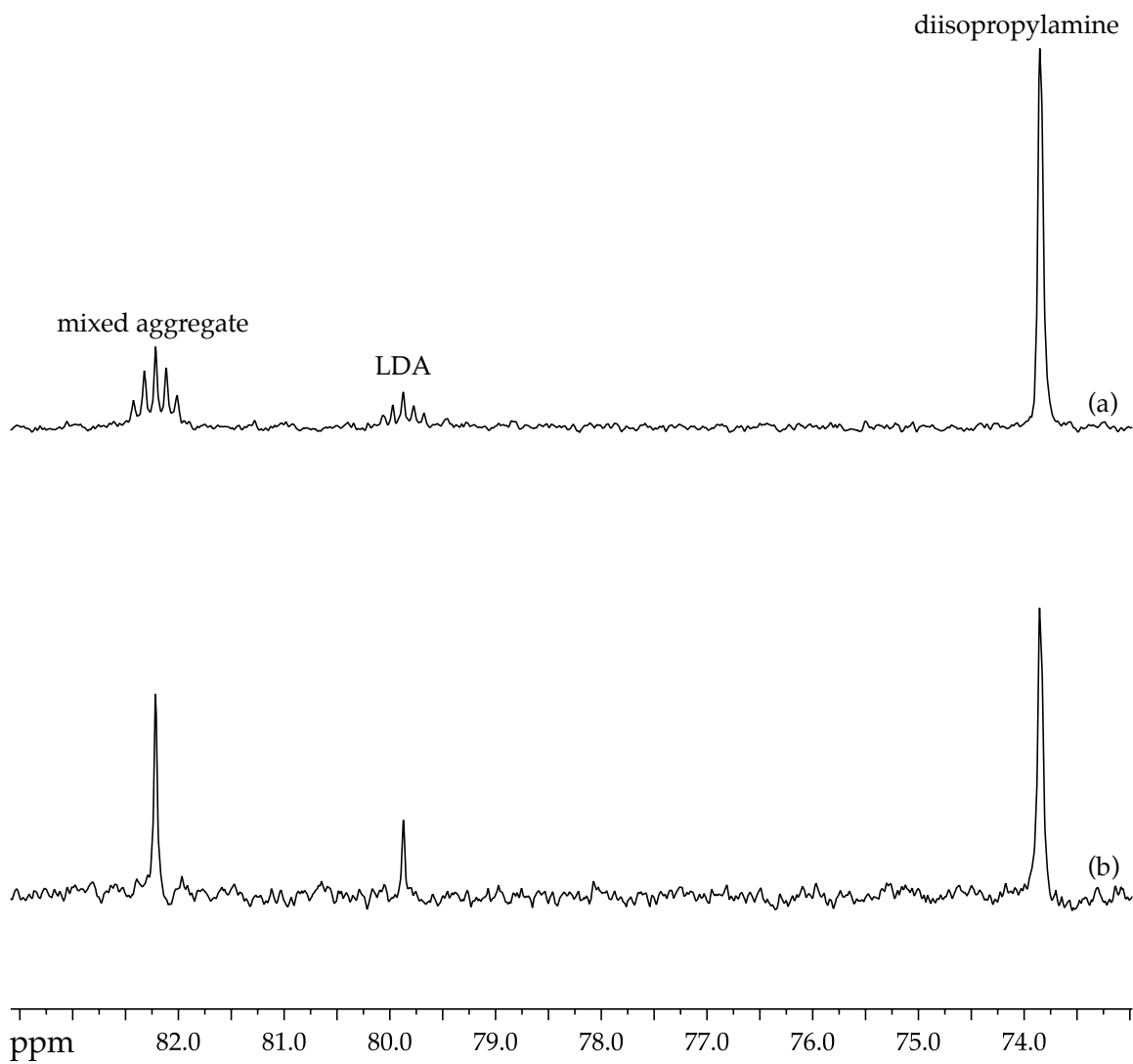
**Figure 15.**  ${}^6\text{Li}$  NMR spectra of 0.10 M solutions of  ${}^6\text{Li}$ 3d with varying concentrations of THF and toluene at  $-80\text{ }^\circ\text{C}$  with 0.11 M  ${}^6\text{Li}$ LDA.



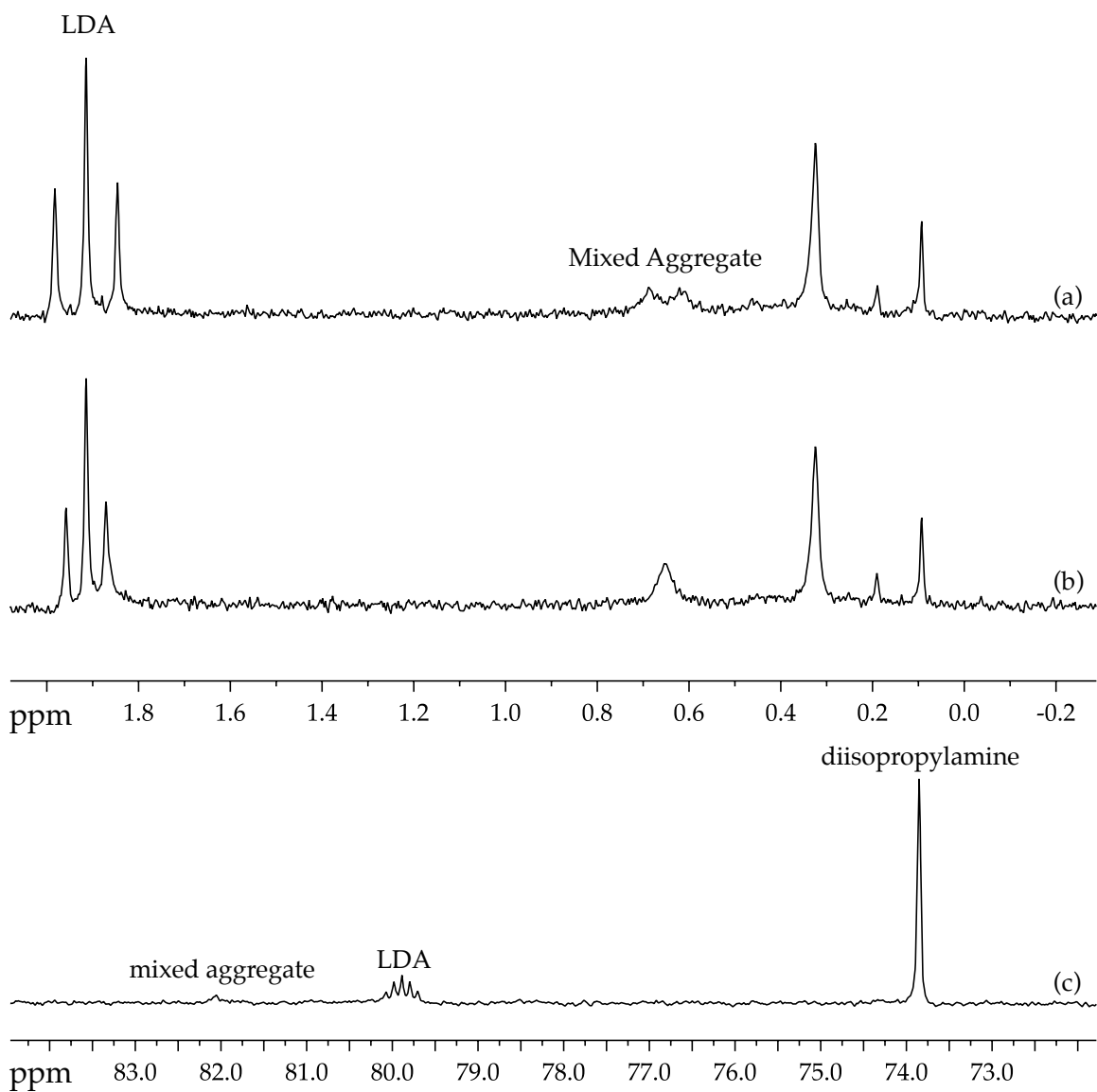
**Figure 16.** Plot of  $[\text{dimer}]/[\text{tetramer}]^{1/2}$  of  $[^6\text{Li}]\mathbf{3d}$  vs.  $[\text{THF}]$  in toluene at  $-80\text{ }^\circ\text{C}$ . The curve depicts an unweighted least-squares fit to  $y=k_{eq}[\text{THF}]^n$  [ $k_{eq} = (1.4 \pm 0.3) \times 10^{-3}$ ;  $n = 1.94 \pm 0.09$ ].



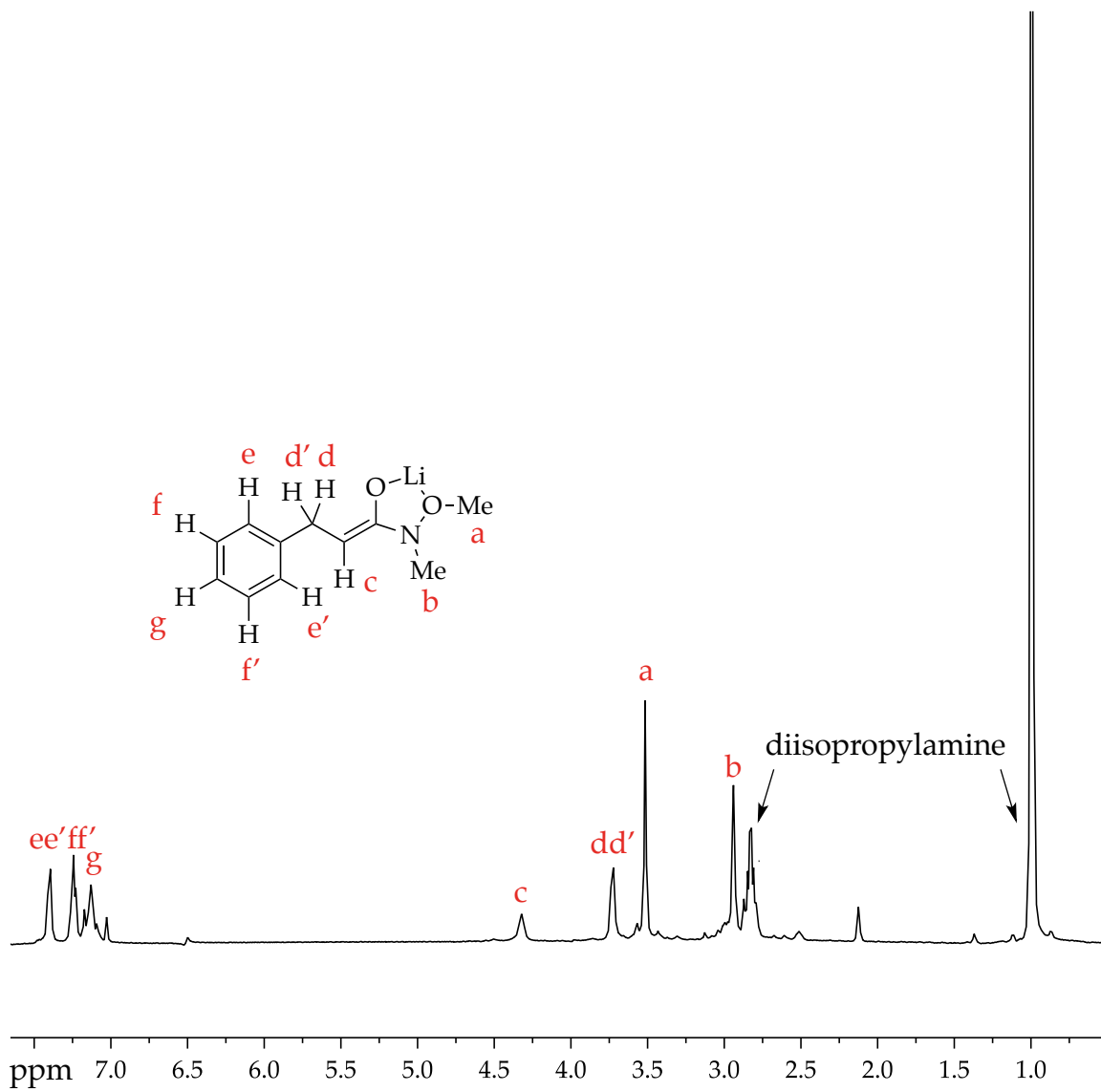
**Figure 17.**  ${}^6\text{Li}$  NMR spectra for 0.10 M solution of  $[{}^6\text{Li}]\mathbf{3g}$  in 12.3 M THF with 0.20 M  $[{}^6\text{Li}, {}^{15}\text{N}]\text{LDA}$  at  $-80\text{ }^\circ\text{C}$ : (a)  ${}^6\text{Li}$  spectrum; and (b)  ${}^6\text{Li}\{{}^{15}\text{N}\}$  spectrum.



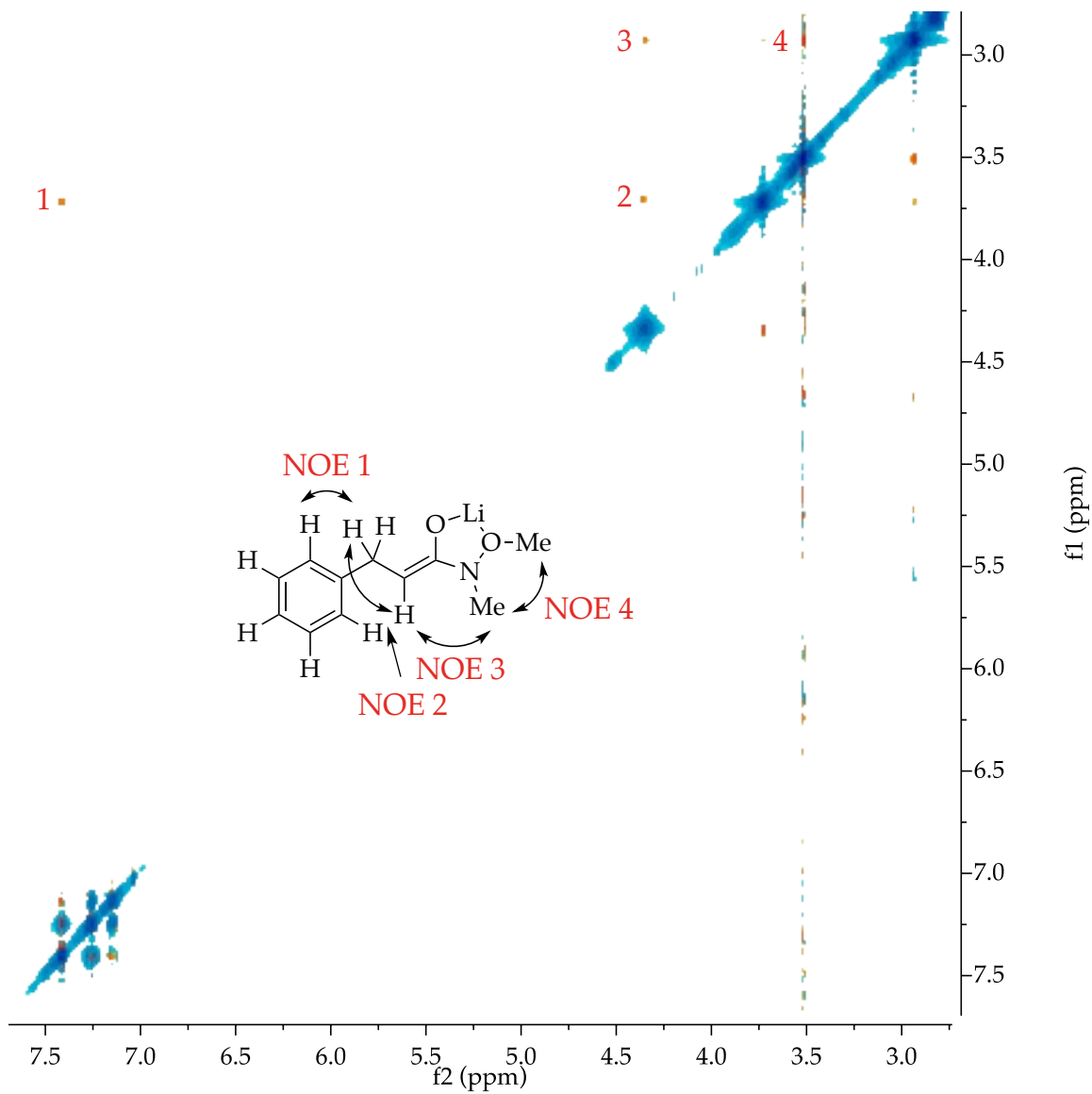
**Figure 18.**  $^{15}\text{N}$  NMR spectra for 0.10 M solution of  $[^6\text{Li}]\mathbf{3g}$  in 12.3 M THF with 0.20 M  $[^6\text{Li}, ^{15}\text{N}]\text{LDA}$  at  $-80\text{ }^\circ\text{C}$ : (a)  $^{15}\text{N}$  spectrum; and (b)  $^{15}\text{N}\{^6\text{Li}\}$  spectrum.



**Figure 19.**  $^6\text{Li}$  and  $^{15}\text{N}$  NMR spectra for 0.10 M solution of  $[^6\text{Li}]\mathbf{3d}$  in 12.3 M THF with 0.20 M  $[^6\text{Li},^{15}\text{N}]\text{LDA}$  at  $-80\text{ }^\circ\text{C}$ : (a)  $^6\text{Li}$  spectrum; (b)  $^6\text{Li}$  spectrum with  $^{15}\text{N}$  single-frequency decoupling on the mixed aggregate  $^{15}\text{N}$  resonance; and (c)  $^{15}\text{N}$  spectrum with single-frequency  $^6\text{Li}$  decoupling on the mixed aggregate  $^6\text{Li}$  resonance.

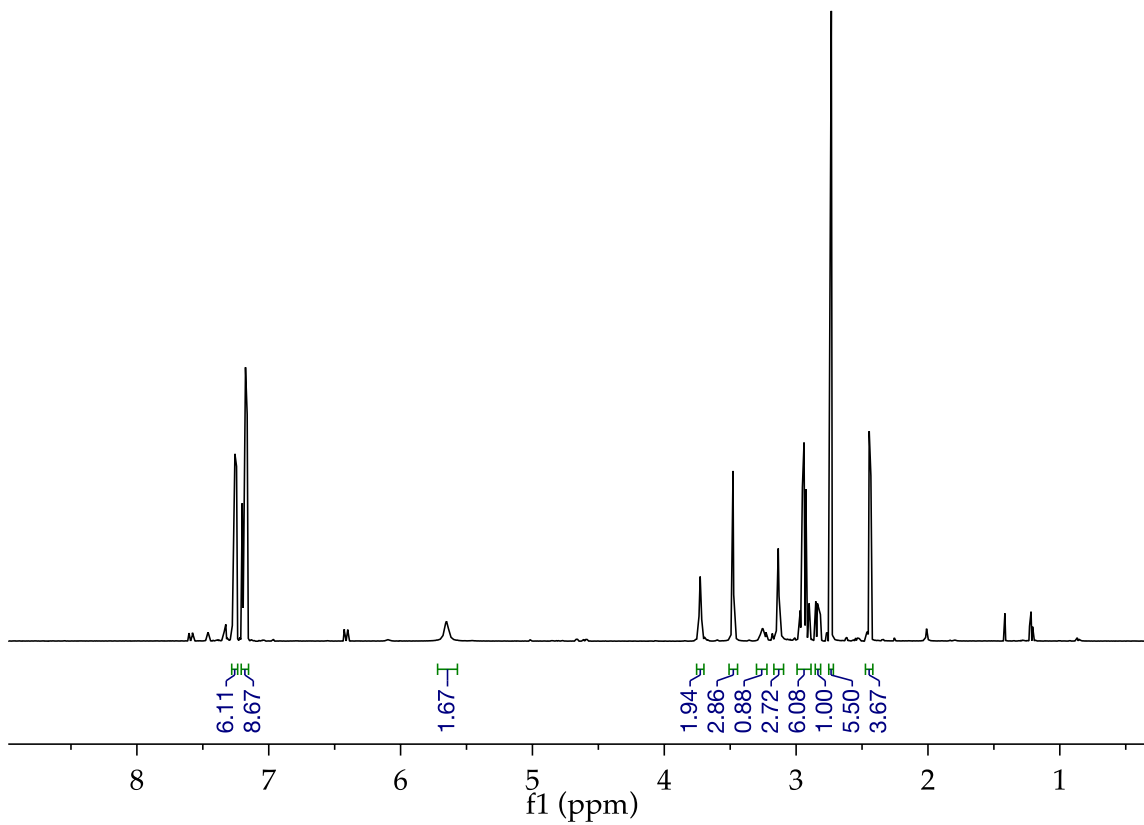


**Figure 20.** <sup>1</sup>H NMR spectrum for a 0.10 M solution of [<sup>6</sup>Li]**3d** in 0.50 M THF-*d*<sub>8</sub> and toluene-*d*<sub>8</sub> with 0.10 M [<sup>6</sup>Li]LDA at -65 °C.

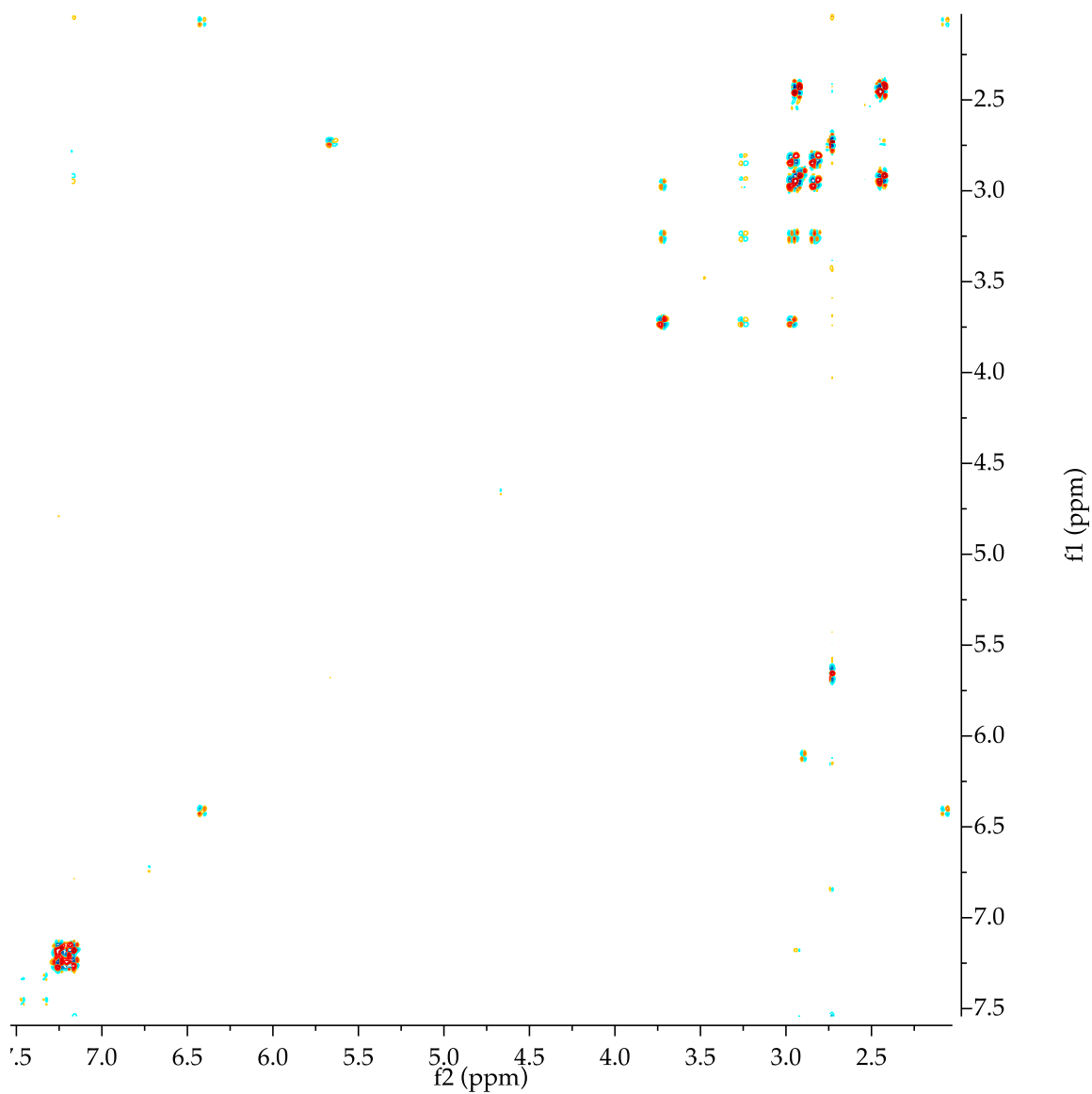


**Figure 21.** ROESY spectrum for a 0.10 M solution of [<sup>6</sup>Li]**3d** in 0.50 M THF-*d*<sub>8</sub> and toluene-*d*<sub>8</sub> with 0.10 M [<sup>6</sup>Li]LDA at -65 °C.

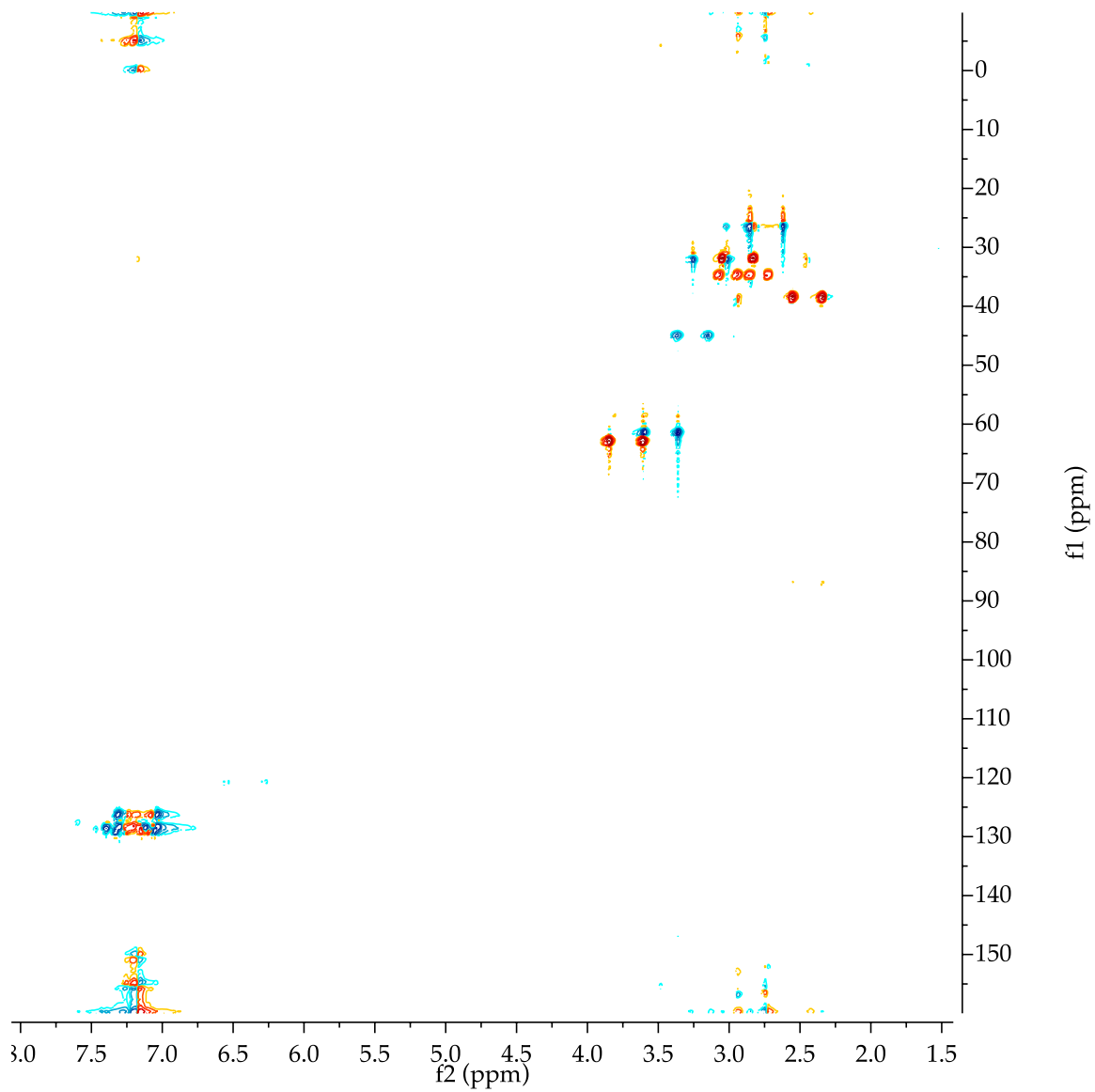




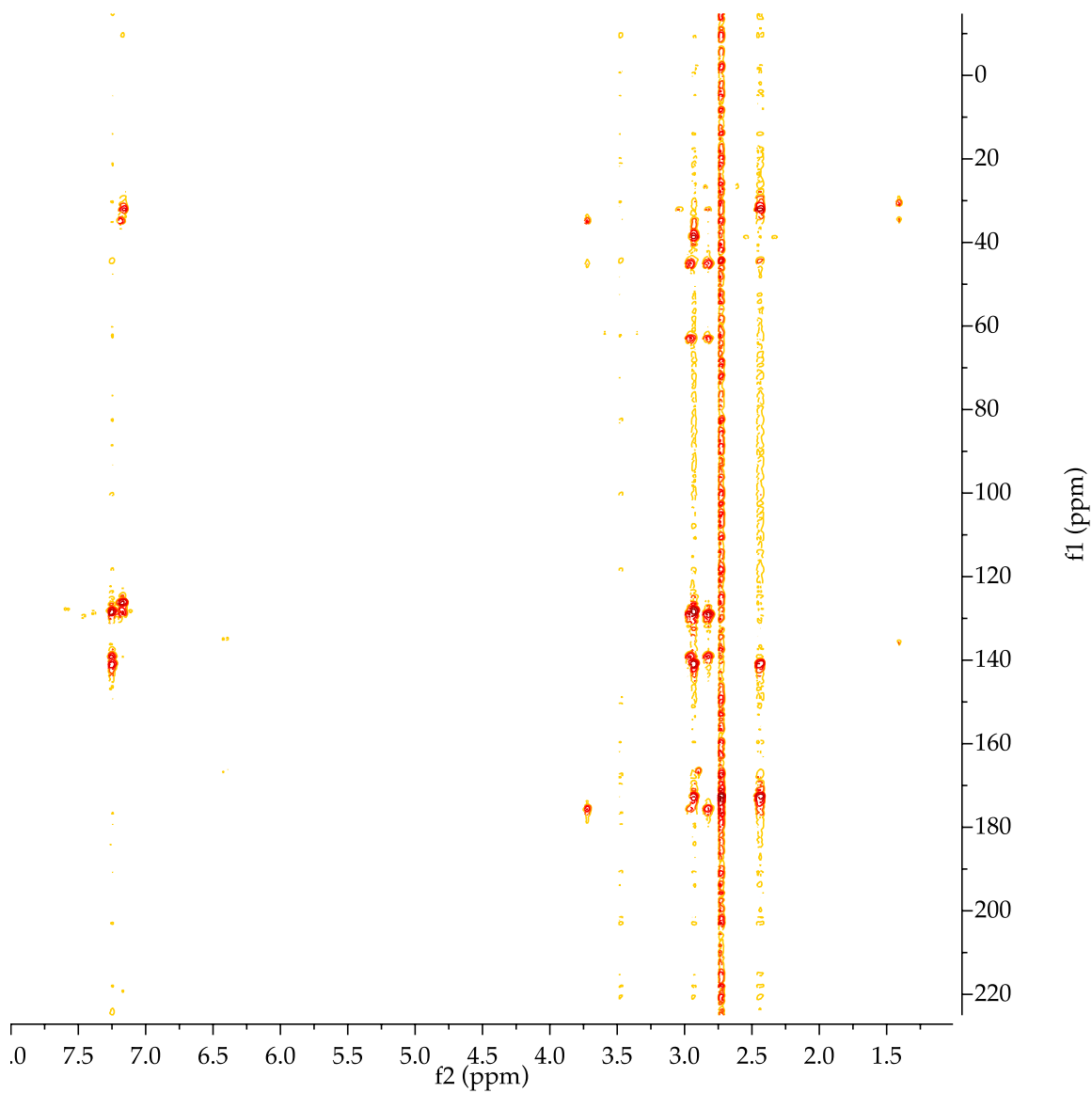
**Figure 22.**  $^1\text{H}$  NMR spectrum for a 2:1 mixture of *N*-methyl-3-phenylpropanamide to 2-benzyl-3-hydroxy-*N*-methoxy-*N*-methylpropanamide in chloroform-*d*.



**Figure 23.** COSY NMR spectrum for a 2:1 mixture of *N*-methyl-3-phenylpropanamide to 2-benzyl-3-hydroxy-*N*-methoxy-*N*-methylpropanamide in chloroform-*d*.



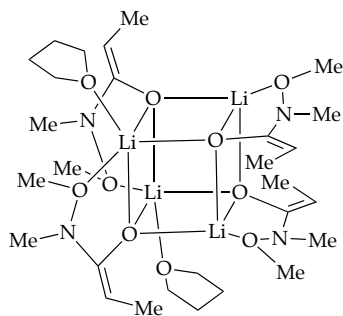
**Figure 24.** HSQC NMR spectrum for a 2:1 mixture of *N*-methyl-3-phenylpropanamide to 2-benzyl-3-hydroxy-*N*-methoxy-*N*-methylpropanamide in chloroform-*d*.



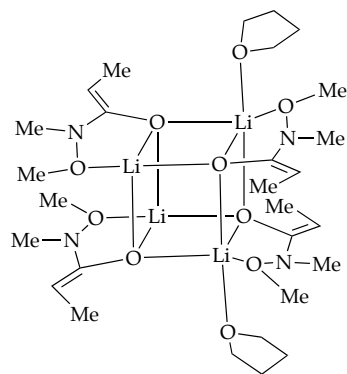
**Figure 25.** HMBC NMR spectrum for a 2:1 mixture of *N*-methyl-3-phenylpropanamide to 2-benzyl-3-hydroxy-*N*-methoxy-*N*-methylpropanamide in chloroform-*d*.

## Part 2: Computational Studies

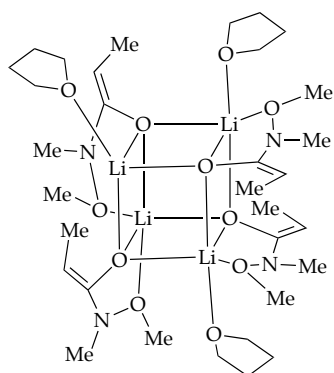
## Chart 2



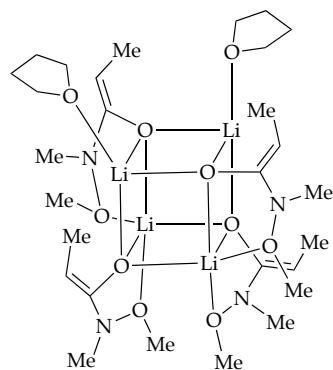
**1**



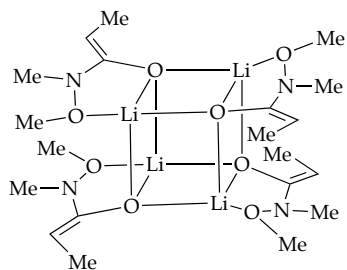
**2**



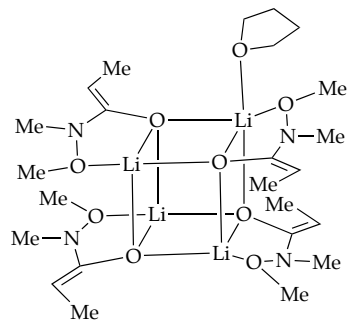
**3**



**4**

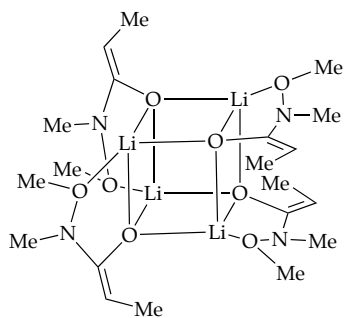


**5**

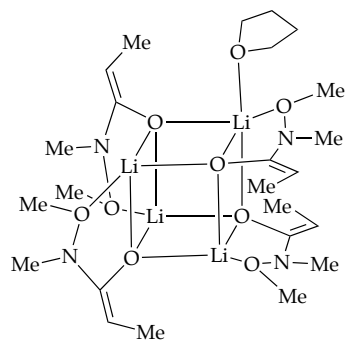


**6**

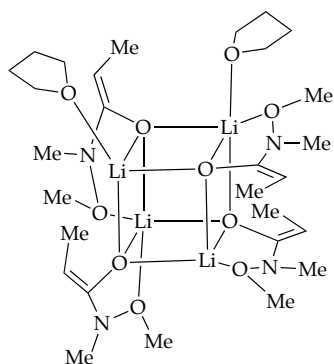
## Chart 2 (Continued)



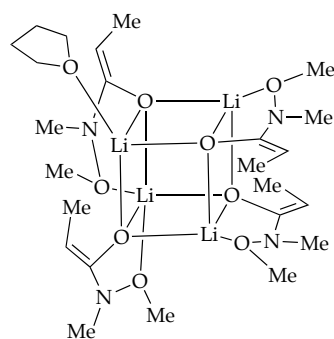
7



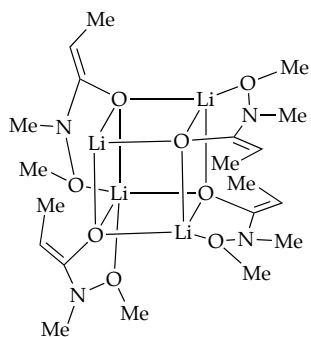
8



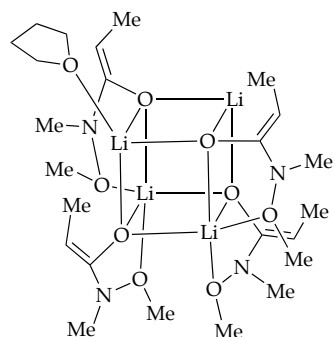
9



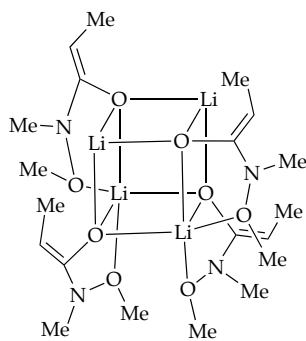
10



11

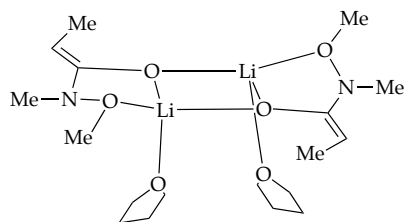


12

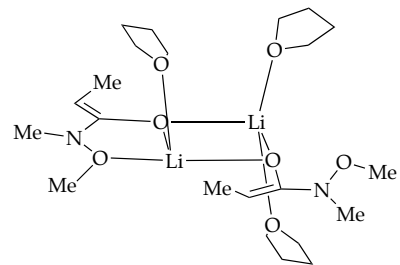


13

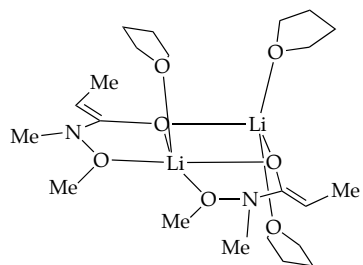
### Chart 3



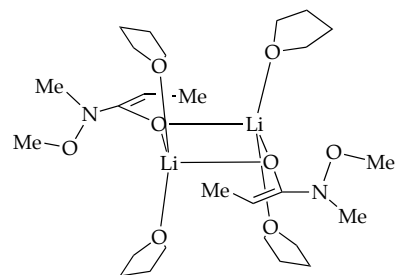
**14**



**15**

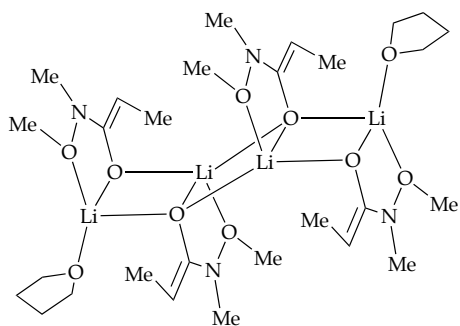


**16**

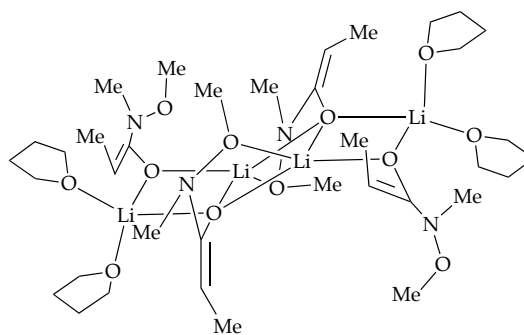


**17**

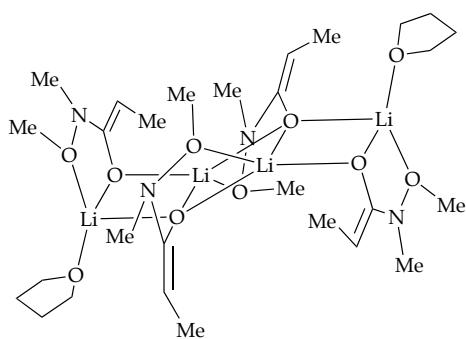
### Chart 4



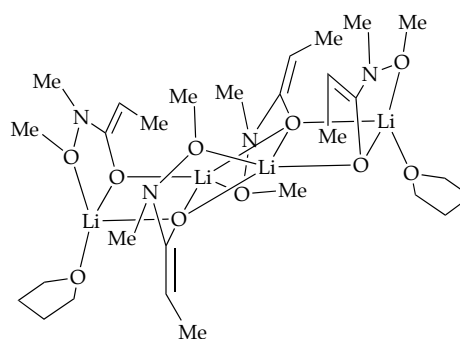
18



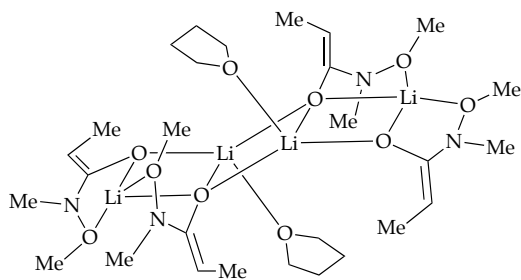
19



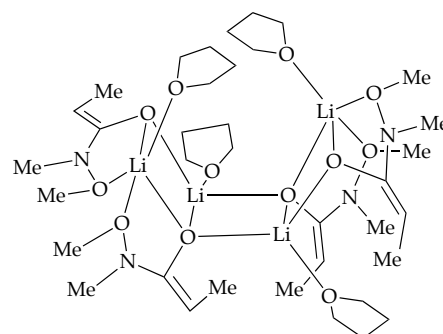
20



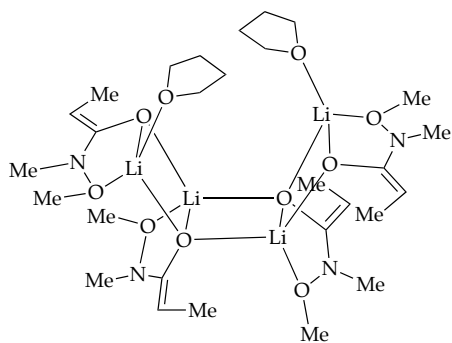
21



22



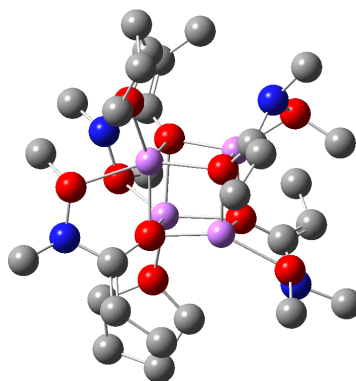
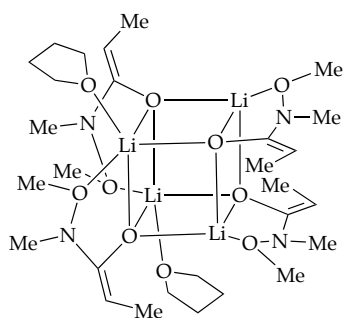
23



24



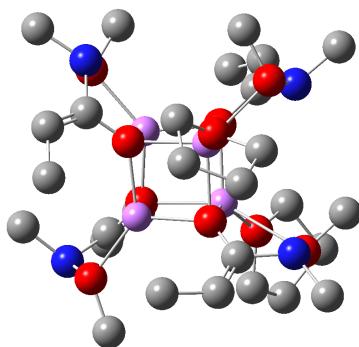
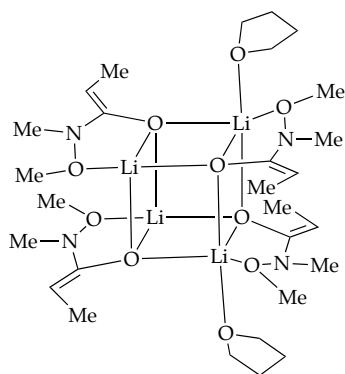
**Table 1.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the differentially solvated, tetra-internally chelated tetramers at  $-78\text{ }^{\circ}\text{C}$  with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



**1**  
 $G = -2101.382524$   
 $G_{\text{MP2}} = -2095.399303$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.65185700	2.26731300	3.70429200
Li	-2.61054300	0.30566400	1.02567400	H	-2.34498800	3.79470700	4.54370400
Li	-1.54517300	2.18073500	-0.57868900	H	-3.98102100	3.14785900	4.47654500
Li	-0.51109100	1.99587500	1.71403500	N	-3.41454900	4.15080500	0.16183700
O	-0.67828500	0.13776300	1.90532700	O	-2.23264500	4.14153300	-0.73067500
C	-0.61136300	-0.71697600	2.90984600	C	-2.58138600	4.50624100	-2.06547200
C	0.22179200	-0.66614300	3.98010000	H	-3.51657900	4.02602700	-2.36995500
H	0.11444200	-1.41048300	4.76239500	H	-2.66366300	5.59343000	-2.18060800
C	1.30512200	0.35736100	4.17784400	H	-1.75758900	4.15177800	-2.69155300
H	1.41096400	1.01138100	3.30787600	C	-3.87882700	5.52807900	0.30542100
H	1.10448700	1.00069000	5.04811900	H	-3.14180000	6.18702500	0.78675000
H	2.28395300	-0.11107100	4.36137600	H	-4.14263200	5.92960700	-0.67482800
N	-1.52926900	-1.81738600	2.74319900	H	-4.79150800	5.50448400	0.90340900
O	-2.86710900	-1.30140400	2.52531400	O	0.27438100	2.03827300	-0.11352300
C	-3.47673400	-0.75150600	3.70580000	C	1.34978600	2.79831200	-0.13974200
H	-2.78699900	-0.07952400	4.22835600	C	1.98285300	3.26645600	-1.24542400
H	-4.34124400	-0.19554600	3.33927200	H	2.82551200	3.94072000	-1.13556200
H	-3.81041700	-1.54286700	4.38745100	C	1.57827000	2.89698900	-2.64579600
C	-1.55141000	-2.91183800	3.69695000	H	0.79141900	2.13543600	-2.63575100
H	-1.74964200	-2.61418500	4.73884000	H	1.19517800	3.76225900	-3.20930800
H	-2.31777100	-3.62343800	3.37645600	H	2.42123800	2.50088400	-3.23133700
H	-0.57621800	-3.40369300	3.66156200	N	1.88218900	3.04063800	1.18179600
O	-2.34965500	2.35294700	1.17004500	O	0.82025000	3.48734300	2.07038000
C	-2.98473400	3.48603600	1.38405200	C	0.33893500	4.81694400	1.78734700
C	-3.30003500	4.00022400	2.60154400	H	0.13702900	4.93768800	0.71840600
H	-3.78152500	4.96706400	2.67951400	H	-0.59533300	4.90920800	2.34514300
C	-3.05680100	3.26597900	3.89127700	H	1.05659800	5.57062300	2.12959200

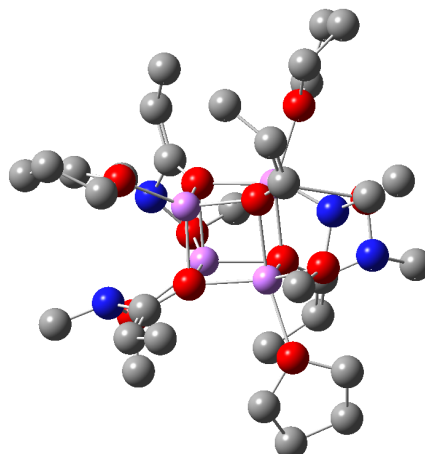
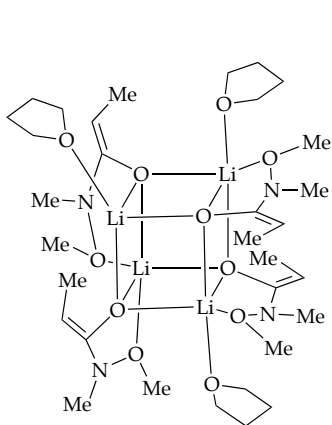
C	3.06604600	3.86466200	1.35839200	C	2.92260200	-0.41161100	0.96946600
H	3.27111000	3.93603400	2.42966100	C	4.29889400	-0.63203900	0.33792900
H	3.90179000	3.35495700	0.87289800	C	4.06032500	-0.16693300	-1.10701900
H	2.98664900	4.87769400	0.93425100	H	4.07830300	0.92730600	-1.16319800
O	-1.85826700	0.28828400	-0.80404500	H	4.78922100	-0.56461900	-1.82019800
C	-2.17697100	-0.48975200	-1.82094800	H	5.08680500	-0.07167000	0.85088400
C	-2.91604500	-0.12476800	-2.90255200	H	4.57067700	-1.69471800	0.35790900
H	-3.05765100	-0.81882700	-3.72116000	H	2.79972000	0.61300000	1.33495300
C	-3.59678400	1.20789100	-3.02844300	H	2.68968500	-1.10745400	1.78051700
H	-3.68469300	1.70005900	-2.05316400	H	2.64367200	-1.71339500	-1.73476500
H	-3.06896800	1.90000600	-3.70462400	H	2.08224300	-0.06117200	-2.07981000
H	-4.61398200	1.10385400	-3.43388700	C	-5.20441100	-1.09670300	0.23539900
N	-1.75791500	-1.85963300	-1.66010200	O	-4.67985900	0.12522200	0.80471100
O	-0.37865400	-1.86280100	-1.19741600	C	-5.59915200	1.21833000	0.57148200
C	-0.20567300	-2.92318100	-0.24927200	C	-6.71807500	0.65096100	-0.31044000
H	-0.85018900	-2.77271700	0.62175100	C	-6.70014600	-0.84231300	0.05207200
H	-0.40150000	-3.90027300	-0.70954700	H	-7.23900200	-1.01686100	0.99165500
H	0.84490300	-2.86678400	0.04305500	H	-7.14276500	-1.48093600	-0.71871000
C	-1.81957300	-2.72026700	-2.83693500	H	-7.68202200	1.13368600	-0.12105900
H	-1.28421500	-2.30272000	-3.70263700	H	-6.47411400	0.78478400	-1.37061600
H	-1.38929800	-3.69188000	-2.58391000	H	-5.98157500	1.55465000	1.54395900
H	-2.86840800	-2.87699200	-3.09913300	H	-5.05226200	2.04374100	0.10999500
C	2.64292300	-0.67680000	-1.37238300	H	-4.70689900	-1.28342200	-0.72414500
O	1.96698800	-0.63351100	-0.09619700	H	-4.96558700	-1.91011900	0.92426900



**2**  
 $G = -2101.383604$   
 $G_{\text{MP2}} = -2095.400534$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.99273900	0.15947300	2.22090300
Li	2.72022800	0.32518900	-0.67761000	C	2.79447900	0.65515000	3.20069100
Li	0.81474800	1.53568100	-2.06935400	H	2.82876300	0.15105900	4.16053100
Li	1.30797400	2.37528500	0.29300900	C	3.68968500	1.85094000	3.03679700
O	1.77418500	0.68541900	1.03078400	H	3.64294400	2.24164300	2.01550300

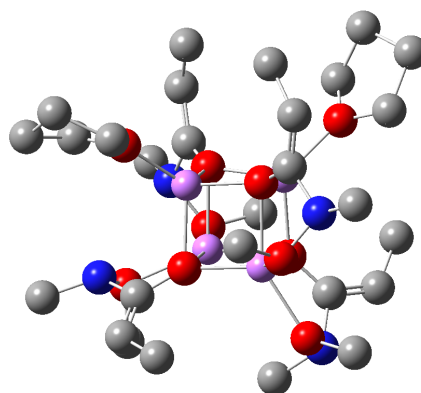
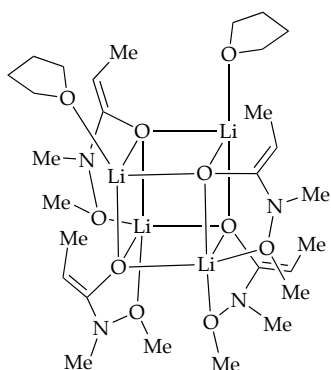
H 3.42137100 2.67048800 3.72092700 O 1.07650400 -0.30928700 -1.67149700  
H 4.74238700 1.61153600 3.24942400 C 1.02570700 -1.39048500 -2.43122400  
N 1.34430900 -1.11339700 2.38742900 C 0.38476700 -1.51912200 -3.62443200  
O -0.02660200 -1.05565500 1.94886200 H 0.47722300 -2.44926500 -4.17152100  
C -0.89624400 -0.33411400 2.83643300 C -0.53179000 -0.50196100 -4.24339800  
H -0.52945600 0.68167400 3.01569000 H -0.53856200 0.44558900 -3.69893400  
H -1.85166500 -0.29267100 2.31170600 H -0.25480100 -0.27602000 -5.28353200  
H -1.02281000 -0.86203300 3.78840500 H -1.57531000 -0.85361200 -4.27906100  
C 1.46594400 -1.85537000 3.62941900 N 1.64885700 -2.54498500 -1.83064200  
H 1.13074500 -1.31098800 4.52668500 O 2.96265300 -2.16096100 -1.34811300  
H 0.88454000 -2.77590700 3.52926500 C 3.18119200 -2.76863000 -0.07495100  
H 2.51849900 -2.11739400 3.76268500 H 2.46571700 -2.40139400 0.66761400  
O -0.37742900 1.90313200 -0.54311700 H 3.12654200 -3.86407800 -0.14058700  
C -1.26932600 2.84695500 -0.30753800 H 4.19903000 -2.48772200 0.20694200  
C -2.23226400 3.26412400 -1.16883600 C 1.83275900 -3.73220500 -2.65928400  
H -2.87063500 4.09773500 -0.90454100 H 2.38173400 -3.52606400 -3.59007700  
C -2.47315200 2.63789600 -2.51453900 H 2.38257000 -4.47737200 -2.07919200  
H -2.02014400 3.21658300 -3.33474700 H 0.85267400 -4.15036400 -2.90041600  
H -2.05608700 1.62771700 -2.56699800 O 4.72773800 0.13450400 -0.62716600  
H -3.54645700 2.56804000 -2.73819100 C 5.43649800 0.05793700 -1.88984100  
N -1.19100900 3.39243600 1.03650700 C 6.91806400 -0.15276800 -1.53586300  
O 0.20947000 3.82777800 1.22871800 O 4.72773800 0.13450400 -0.62716600  
C 0.57344800 3.72559200 2.60863700 C 5.43649800 0.05793700 -1.88984100  
H 1.59144700 4.11976600 2.66520900 C 6.91806400 -0.15276800 -1.53586300  
H -0.07560500 4.33979400 3.24225900 C 6.85286200 -0.72158800 -0.10815200  
H 0.55862700 2.68639000 2.95125500 C 5.65608600 0.03359800 0.46605200  
C -2.03255400 4.55191500 1.32182200 H 5.94523900 1.03947300 0.79889100  
H -1.83667600 4.89646300 2.33965300 H 5.14533000 -0.47205600 1.28959500  
H -1.87121800 5.38321600 0.62152900 H 7.77063800 -0.55758500 0.46496500  
H -3.07453200 4.22826000 1.27587300 H 6.64949200 -1.79888900 -0.13143400  
O 2.40940900 2.31063900 -1.24039000 H 7.45309800 0.80364000 -1.53589100  
C 3.00323600 3.17477200 -2.04751000 H 7.42170300 -0.81918800 -2.24239500  
C 4.22525000 3.74027800 -1.92305600 H 5.01542800 -0.78624400 -2.44497900  
H 4.54905700 4.38752000 -2.73296000 H 5.25736900 0.98477000 -2.44367200  
C 5.11480500 3.60977700 -0.72158700 O -1.81988400 -0.97780200 -0.22559700  
H 4.67029200 2.94150200 0.02054900 C -1.85951900 -2.40206700 -0.39958500  
H 6.10673500 3.20944000 -0.98126100 C -2.78325400 -2.63254300 -1.61030900  
H 5.29434700 4.58276600 -0.23963200 C -3.65161400 -1.34353100 -1.66958200  
N 2.23988500 3.62395600 -3.21522100 C -3.14992900 -0.50979000 -0.47671600  
O 1.47690400 2.47971300 -3.72663600 H -3.77114300 -0.69098600 0.41580300  
C 2.23775600 1.86558600 -4.76549700 H -3.09304300 0.56451100 -0.65628000  
H 2.37697200 2.56516200 -5.59638600 H -4.72342800 -1.55144400 -1.59249500  
H 3.21579100 1.54216300 -4.39077600 H -3.48308000 -0.80795700 -2.60806300  
H 1.66438500 0.99501000 -5.08829900 H -3.38503000 -3.53885600 -1.48961300  
C 1.22269900 4.62827800 -2.88948900 H -2.18853500 -2.73864500 -2.52119800  
H 1.74457400 5.48991600 -2.46559200 H -0.83295600 -2.74252300 -0.54428600  
H 0.71919400 4.93260000 -3.81139000 H -2.26854700 -2.86496900 0.51153100  
H 0.47060600 4.27476200 -2.16843500



**3**  
 $G = -2333.726142$   
 $G_{\text{MP2}} = -2327.092617$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-2.00065600	2.36010000	-2.97496900
Li	2.40143800	0.93934200	-1.05693400	C	-3.11891800	1.54287200	-3.34239700
Li	-0.00066400	1.47992500	-2.36464300	H	-2.76733800	0.93543000	-4.17708700
Li	0.63278100	2.69650500	-0.10870100	H	-3.43496000	0.89816900	-2.51343200
O	1.55318000	1.23934000	0.74001800	H	-3.96684300	2.15168200	-3.67730900
C	2.05998500	0.93423200	1.91783500	C	-3.34166200	4.05486600	-1.95910000
C	2.65225900	1.77135100	2.81069100	H	-3.20223700	4.56997300	-2.91371100
H	2.96196000	1.37386300	3.77163100	H	-4.33863200	3.58566300	-1.94594900
C	2.95013700	3.22363500	2.56560300	H	-3.30399500	4.79020100	-1.15181100
H	2.58850900	3.55102300	1.58731500	O	1.56691900	2.60759400	-1.80731500
H	2.48063000	3.86866600	3.32387400	C	1.89790200	3.44280100	-2.77427100
H	4.02899300	3.43987400	2.61101900	C	2.87531600	4.38753400	-2.74804500
N	2.00380100	-0.48186500	2.18639000	H	3.07446500	4.96345500	-3.64545100
O	0.65864700	-0.97155100	1.99497800	C	3.65748200	4.75555200	-1.51958100
C	-0.24356200	-0.59060400	3.04381400	H	3.32362000	4.17257500	-0.65728200
H	-0.17001900	0.48208500	3.25676700	H	4.73768700	4.57849900	-1.64066400
H	-1.23648300	-0.82902500	2.66063300	H	3.55345800	5.82268500	-1.26665300
H	-0.05745300	-1.16303300	3.96058200	N	1.02455100	3.34076000	-3.91293700
C	2.58913900	-1.03647600	3.39396000	O	0.78507800	1.96084200	-4.26113400
H	2.19003300	-0.62574500	4.33518800	C	1.94291900	1.28097800	-4.77341400
H	2.42640000	-2.11805700	3.37974800	H	2.80833300	1.44012500	-4.12213700
H	3.66409500	-0.84162600	3.36618900	H	1.67963400	0.22134600	-4.77488000
O	-0.98747300	1.64496700	-0.56260900	H	2.17670300	1.61575800	-5.79121300
C	-2.11949000	2.31863700	-0.60290300	C	1.24535900	4.13941400	-5.10343400
C	-3.08037300	2.37381500	0.35847700	H	2.23676100	4.00723600	-5.56760000
H	-4.00130700	2.90901100	0.15273300	H	0.46971800	3.87961100	-5.82821200
C	-2.93153800	1.77446400	1.72831600	H	1.13177600	5.19125000	-4.83001200
H	-3.52901400	0.85900700	1.86489500	O	0.27478000	4.53146100	0.53909600
H	-1.88774900	1.51291100	1.92374500	C	0.05625300	5.57264900	-0.45295900
H	-3.25591500	2.47220100	2.51401300	C	-0.75310600	6.67256100	0.25598300
N	-2.22857100	3.14044900	-1.78074200	C	-0.50937700	6.38457400	1.74733400

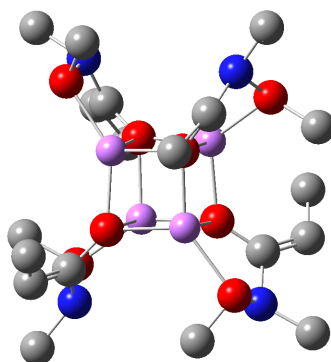
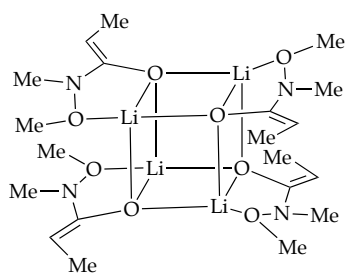
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H -1.42299500 4.40194600 1.73559300 C 5.24033400 1.36944100 -2.20798300  
H 0.14837200 4.44449400 2.58595500 C 6.68663300 1.68388300 -1.77532300  
H -1.30350100 6.76749500 2.39590400 C 6.67382700 1.39096500 -0.26448000  
H 0.44275900 6.81771400 2.07591900 C 5.24724800 1.78423400 0.11233700  
H -1.82029800 6.57605700 0.02461000 H 5.15648000 2.87216100 0.22908700  
H -0.43726500 7.67606600 -0.04497900 H 4.85474400 1.30335200 1.01114700  
H 1.03997300 5.91883500 -0.78072100 H 7.42943100 1.95686100 0.28947100  
H -0.46801200 5.13057500 -1.30429000 H 6.83926800 0.32363300 -0.07407400  
O 0.88890700 -0.23129200 -1.76496500 H 6.91827800 2.74017400 -1.95194300  
C 1.11933900 -1.33948600 -2.43804200 H 7.42212700 1.08597700 -2.32199300  
C 0.40859400 -1.78051500 -3.51383900 H 5.14330300 0.38357500 -2.67370800  
H 0.72969400 -2.66326500 -4.05146800 H 4.83210600 2.12952700 -2.88227600  
C -0.85855700 -1.12170000 -3.98201800 O -1.44188000 -1.50976400 0.11864400  
H -1.37727600 -0.64285700 -3.14439600 C -1.06450100 -2.89457200 0.08541700  
H -0.69782200 -0.34540000 -4.74762700 C -1.93103600 -3.51924000 -1.02209500  
H -1.54813500 -1.85619900 -4.41972100 C -3.16504600 -2.57758000 -1.10760500  
N 2.16490500 -2.16486300 -1.88581200 C -2.86059000 -1.47643400 -0.07286900  
O 3.32221200 -1.32939700 -1.61915400 H -3.35997900 -1.69287000 0.88512100  
C 3.91264600 -1.74558000 -0.38609600 H -3.12440000 -0.46394000 -0.38339700  
H 3.22334400 -1.58844700 0.44875300 H -4.10391300 -3.09112300 -0.87705600  
H 4.22686900 -2.79729700 -0.42988500 H -3.25669300 -2.15450600 -2.11190300  
H 4.79762300 -1.11737800 -0.26784400 H -2.20504800 -4.55250700 -0.78628800  
C 2.62844400 -3.29381800 -2.68555000 H -1.38194100 -3.51707700 -1.96695700  
H 2.95512200 -3.00054400 -3.69451000 H 0.00845400 -2.93681000 -0.10584200  
H 3.46276600 -3.77118900 -2.16597700 H -1.27485200 -3.34943100 1.06588500  
H 1.81935300 -4.02353300 -2.76380700



**4**  
 $G = -2101.388271$   
 $G_{\text{MP2}} = -2095.402722$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	3.14563700	-1.84112400	-3.34605600
Li	-1.54896200	-2.24769500	-0.09746700	H	2.37147200	-2.02173100	-4.09575400
Li	0.65122600	-2.21364800	-1.60971600	H	3.21981500	-0.76966900	-3.12771800
Li	0.83508600	-2.37821700	0.98694000	H	4.10489700	-2.20942000	-3.72856000
O	-0.72444600	-1.31592500	1.40606400	C	4.86071400	-2.45972200	-1.12988800
C	-1.32157400	-0.70256500	2.40932000	H	5.00518100	-3.47792200	-1.50285800
C	-1.82698600	-1.27075000	3.53415000	H	5.36799900	-1.75524500	-1.80759500
H	-2.23210000	-0.63133600	4.31171900	H	5.32420500	-2.37488000	-0.14348900
C	-1.87422600	-2.75221000	3.77928900	O	-0.07840400	-3.52015900	-0.30947600
H	-1.53481500	-3.30466400	2.89959900	C	-0.04783300	-4.75001500	-0.79387900
H	-1.23636800	-3.05346000	4.62496600	C	-0.42763600	-5.88585700	-0.14846800
H	-2.88942500	-3.09874600	4.02585700	H	-0.41644300	-6.82728300	-0.68702300
N	-1.45974700	0.71360200	2.17153200	C	-0.75784500	-5.94555700	1.31709000
O	-0.16450100	1.28274700	1.84487200	H	-0.59033700	-4.97564400	1.79332900
C	0.76967600	1.24125900	2.93340800	H	-1.80405300	-6.23114900	1.51086500
H	0.85486000	0.22838400	3.34131700	H	-0.13943900	-6.68872600	1.84369600
H	1.72312100	1.55151600	2.50560000	N	0.54853700	-4.82497800	-2.09570600
H	0.48391000	1.93801300	3.73019100	O	0.13125500	-3.74031200	-2.94507700
C	-2.15610700	1.55810600	3.12738900	C	-1.23271700	-3.83545900	-3.38303000
H	-1.74466000	1.53766700	4.14900100	H	-1.90608000	-3.99465200	-2.53552300
H	-2.13011900	2.58445300	2.75224300	H	-1.45583300	-2.87373900	-3.84723400
H	-3.19611100	1.22578400	3.16970500	H	-1.35451900	-4.64219000	-4.11547100
O	1.63240400	-1.02080000	-0.26034700	C	0.61081200	-6.07327500	-2.82920000
C	2.93177900	-0.97054800	-0.49053100	H	-0.36786300	-6.54657300	-3.01535200
C	3.76903100	0.08201000	-0.31514400	H	1.10442600	-5.87673300	-3.78434800
H	4.81210400	-0.03079400	-0.59251900	H	1.22565000	-6.77073900	-2.25523500
C	3.36701500	1.41704800	0.24328400	O	1.96304500	-3.22390200	2.33915300
H	3.75281900	2.23623800	-0.37933800	C	2.86596400	-4.28764500	1.93798200
H	2.27939700	1.52182000	0.27914300	C	4.06148900	-4.18435200	2.88764300
H	3.76180000	1.59088500	1.25770100	C	3.41763100	-3.61816800	4.16375100
N	3.43438000	-2.24030500	-0.96862300	C	2.38582000	-2.64450100	3.59097700
O	2.72245300	-2.58264900	-2.19192800	H	2.83062200	-1.66007300	3.39340100

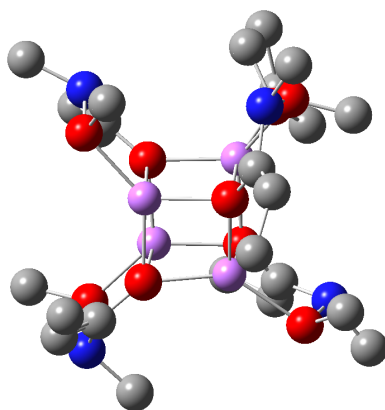
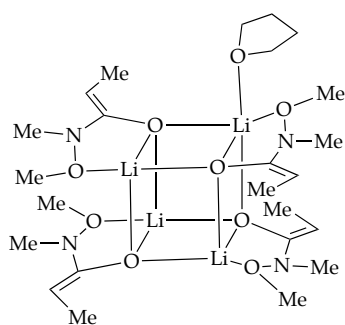
H	1.50124700	-2.51386900	4.22059800	H	-2.21569400	2.50381600	-0.89411600
H	4.13236800	-3.12506000	4.82956000	H	-0.82452400	3.04411200	0.09585400
H	2.91985600	-4.41594500	4.72771800	C	0.43257700	0.87497200	-3.28223200
H	4.80500300	-3.48118200	2.49353200	H	0.16237700	0.43116200	-4.24593500
H	4.55465200	-5.14867500	3.04305800	H	0.92180000	1.83735200	-3.45974800
H	2.33782500	-5.24198100	2.04708400	H	1.13282800	0.21491600	-2.75366700
H	3.11576500	-4.12828600	0.88635700	O	-3.38167400	-2.94038200	0.18480300
O	-1.00126700	-1.03714200	-1.52480100	C	-4.42233800	-2.18600800	0.85604600
C	-1.57233100	-0.12310300	-2.29302300	C	-5.49527900	-3.21209900	1.28133400
C	-2.78489300	-0.14248000	-2.89474700	C	-4.80149700	-4.57176600	1.06943700
H	-3.05177900	0.74565500	-3.45905700	C	-3.86445100	-4.26630600	-0.09483900
C	-3.77624800	-1.26970500	-2.86675700	H	-4.40794000	-4.26687900	-1.05284000
H	-3.49352700	-2.03592200	-2.14049100	H	-2.99320600	-4.92011400	-0.17521500
H	-4.77830800	-0.90664900	-2.59487500	H	-5.50423900	-5.38110800	0.84863100
H	-3.88637500	-1.75669300	-3.84886600	H	-4.21576000	-4.85167000	1.95182400
N	-0.80729100	1.09986500	-2.54339600	H	-6.37973300	-3.13270400	0.63963300
O	-0.37076000	1.59643400	-1.22908700	H	-5.82074000	-3.06091200	2.31460500
C	-1.14698300	2.74596100	-0.90388000	H	-3.95115400	-1.67957800	1.70240600
H	-0.95987500	3.55082300	-1.62404900	H	-4.81722300	-1.43431700	0.16332100



5  
 $G = -1636.692439$   
 $G_{MP2} = -1632.009189$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.75140500	-0.32042800	3.87907100
Li	-0.89160100	-1.64821300	-1.80919500	N	3.62984100	0.20024600	-0.47634800
Li	0.75070900	-2.49222700	0.00026400	O	3.62386000	-0.65220500	-1.66013800
Li	1.64235400	-0.84324000	-1.80895500	C	4.41364000	-1.85225200	-1.52231000
O	1.72367000	-0.86842200	0.22042600	H	4.27738500	-2.28862500	-0.52683500
C	2.92674300	-0.45768700	0.59664800	H	4.03683900	-2.54450100	-2.27795400
C	3.45264200	-0.54146800	1.84115600	H	5.47340100	-1.63812500	-1.69723600
H	4.47692800	-0.22456200	2.00649700	C	4.96201000	0.74076900	-0.26078200
C	2.68655400	-1.02718200	3.03953700	H	5.69938900	0.00374000	0.09306800
H	1.62765600	-1.16608200	2.79904700	H	5.30578600	1.17297100	-1.20370700
H	3.06903500	-1.98894900	3.41371800	H	4.88257600	1.53641900	0.48371500

O	0.76917400	-2.58807300	-1.94808700	O	-0.25512800	2.00056300	-0.14773700
C	1.27321900	-3.73390500	-2.37615600	C	0.86935400	2.56591600	0.54316700
C	1.99327100	-3.89486200	-3.51584400	H	1.80595800	2.19689400	0.11606900
H	2.41037200	-4.86459500	-3.75846500	H	0.84126000	3.66078900	0.50405500
C	2.16598100	-2.80846500	-4.54324500	H	0.76542100	2.24637800	1.58457100
H	1.49223000	-1.96641200	-4.35071800	C	-0.94193300	3.59854000	-1.73121000
H	3.19131700	-2.40668900	-4.57828100	H	-2.02515500	3.43240500	-1.63928400
H	1.94619200	-3.17797500	-5.55427600	H	-0.62293600	4.32632500	-0.98194700
N	0.91072000	-4.86879600	-1.56311800	H	-0.71891300	4.01321900	-2.71667600
O	1.00418400	-4.49259000	-0.14852400	O	-0.97273700	-1.62342600	0.22122100
C	-0.12046800	-5.05788700	0.54214200	C	-2.17563800	-2.03508000	0.59679800
H	-1.05696400	-4.68883900	0.11486200	C	-2.70170500	-1.95296400	1.84135600
H	-0.09238100	-6.15277400	0.50308900	H	-3.72582900	-2.27063800	2.00625300
H	-0.01675700	-4.73835400	1.58357300	C	-1.93606200	-1.46815700	3.04037300
C	1.69073400	-6.09047300	-1.73220200	H	-0.87749700	-1.32698300	2.79980100
H	2.77403500	-5.92457500	-1.64078100	H	-2.32014600	-0.50773100	3.41631700
H	1.37187800	-6.81804400	-0.98266500	H	-1.99941000	-2.17649000	3.87871300
H	1.46718900	-6.50531900	-2.71747800	N	-2.87835800	-2.69205300	-0.47703500
O	-0.01872800	0.09661200	-1.94789900	O	-2.87294100	-1.83791100	-1.65962900
C	-0.52370600	1.24221900	-2.37547900	C	-3.66325300	-0.63839400	-1.52016100
C	-1.24431200	1.40286900	-3.51485700	H	-3.52766100	-0.20377200	-0.52382600
H	-1.66240300	2.37228300	-3.75703300	H	-3.28623900	0.05531300	-2.27436200
C	-1.41670500	0.31636500	-4.54220700	H	-4.72285000	-0.85261700	-1.69597500
H	-0.73986000	-0.52373900	-4.35197100	C	-4.21018500	-3.23370800	-0.26218700
H	-2.44088600	-0.08861700	-4.57450900	H	-4.94806000	-2.49755300	0.09242500
H	-1.20092300	0.68703400	-5.55364700	H	-4.55360000	-3.66506300	-1.20563300
N	-0.16157000	2.37708600	-1.56226800	H	-4.13032000	-4.03014800	0.48141700

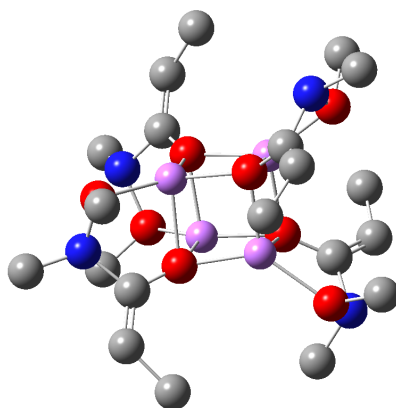
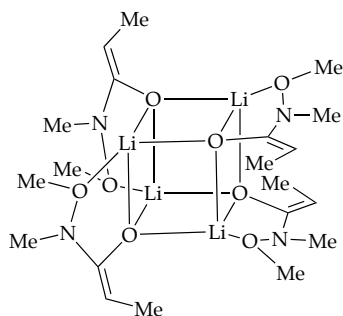


**6**  
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 $G_{MP2} = -1863.708802$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	-2.15376300	-1.28436000	-1.11653500
Li	-2.38005500	1.18646000	-0.54325200	Li	-2.36036300	-0.53936900	1.34837800



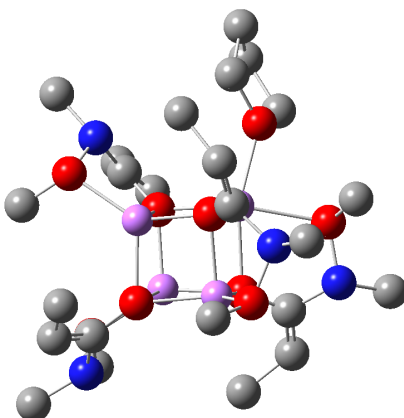
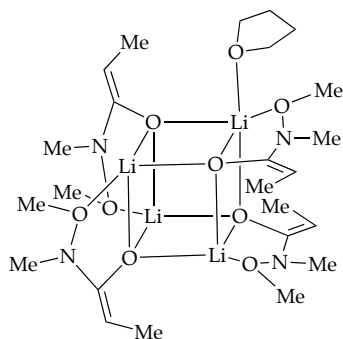
O -1.46265500 1.12184100 1.16148700 H -6.84627600 1.66103100 0.57150800  
C -0.98778600 2.14972200 1.84180500 N -4.89387900 -1.92568700 -1.16439800  
C -1.59193600 2.78411500 2.87858600 O -3.71373600 -2.17171500 -2.01776600  
H -1.06444600 3.57950000 3.39438600 C -4.10649800 -2.00176100 -3.37921000  
C -2.99751900 2.50087600 3.33138500 H -4.86696400 -2.74160600 -3.65024900  
H -3.48785900 1.77791500 2.67062400 H -4.49568700 -0.99193800 -3.54872300  
H -3.03635200 2.09714400 4.35505700 H -3.20274000 -2.15320400 -3.97484600  
H -3.61575400 3.41043900 3.33915500 C -4.83936100 -2.97843400 -0.14719900  
N 0.24855200 2.63850700 1.29471800 H -5.67124800 -2.80322300 0.54111100  
O 1.16402400 1.54997400 1.04883400 H -4.97735000 -3.94802500 -0.63356500  
C 1.73422400 0.98971700 2.24245700 H -3.89738000 -2.99235600 0.41928600  
H 0.95545500 0.72576100 2.96646900 O -1.10034500 0.25613800 -1.64686000  
H 2.25353100 0.09051400 1.90756500 C -0.98506900 0.80999100 -2.84141000  
H 2.45238800 1.67736600 2.70359400 C -0.66555800 0.15915900 -3.99092000  
C 0.93267800 3.76671600 1.90192100 H -0.65000400 0.69949100 -4.92916500  
H 1.18193900 3.63566900 2.96699900 C -0.25463500 -1.28544900 -4.04859900  
H 1.85069600 3.94706300 1.33636500 H -0.16307400 -1.71323200 -3.04547800  
H 0.28512500 4.64199000 1.80855600 H -0.96769000 -1.90814600 -4.61108000  
O -1.07837700 -1.68082200 0.44703200 H 0.71678300 -1.41245400 -4.55046100  
C -0.96716900 -2.81705100 1.11071100 N -1.12865300 2.24904800 -2.83909000  
C -0.83588800 -4.04878100 0.55531700 O -2.23894200 2.61158800 -1.95390600  
H -0.82285800 -4.92909300 1.18546300 C -1.89053000 3.81201600 -1.24714900  
C -0.71457800 -4.28180800 -0.92558400 H -0.97412500 3.66199400 -0.66946100  
H -1.66436500 -4.60431800 -1.37886200 H -1.77652500 4.65516700 -1.93834800  
H -0.40109500 -3.37228700 -1.44962200 H -2.73758300 4.01401300 -0.58436000  
H 0.02291800 -5.06430800 -1.15044200 C -1.38372900 2.89436900 -4.12400600  
N -0.91990600 -2.64127700 2.54881500 H -2.23148600 2.45062900 -4.66535900  
O -2.08823800 -1.81670800 2.91765100 H -1.57946700 3.95487600 -3.95240900  
C -1.75430500 -0.98167800 4.03085200 H -0.47998400 2.81792100 -4.73253300  
H -2.67211800 -0.43908500 4.27166800 O 1.85131600 -0.74297200 -0.53355400  
H -1.45654800 -1.57726900 4.90085100 C 2.55757300 -0.05977100 -1.60009800  
H -0.96092300 -0.27580500 3.76988200 C 3.57090200 -1.07240400 -2.16242900  
C -0.99027700 -3.85093100 3.36412200 C 2.99449300 -2.42567500 -1.71121500  
H -1.01331000 -3.56891900 4.41914200 C 2.38953000 -2.06578600 -0.35670200  
H -1.86750600 -4.47273700 3.13708700 H 3.16469800 -2.04547700 0.42582500  
H -0.07745600 -4.42545500 3.19239100 H 1.57472700 -2.71423900 -0.02915000  
O -3.55680600 -0.27202200 -0.11592300 H 3.74974300 -3.21482100 -1.64232300  
C -4.74748600 -0.58299700 -0.61619300 H 2.20827100 -2.75908700 -2.39746200  
C -5.84628200 0.19800700 -0.66682400 H 4.56133400 -0.91637800 -1.71869500  
H -6.71875400 -0.20934000 -1.16805800 H 3.67494200 -0.99059600 -3.24834900  
C -5.94841800 1.56553800 -0.05484800 H 1.81468700 0.24459400 -2.34375400  
H -5.07968200 1.78368000 0.57608800 H 3.03240500 0.83695800 -1.18893700  
H -6.01483400 2.35598400 -0.81782700



7  
 $G = -1636.688295$   
 $G_{\text{MP2}} = -1632.002899$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-4.33942600	2.44287100	0.10904400
Li	0.17257800	0.67107300	2.46572200	H	-3.81903400	2.82997100	-0.77175100
Li	-2.01994300	1.11069800	1.17597800	H	-5.42357500	2.48837300	-0.04350800
Li	-1.38826500	-1.29846100	1.87845100	H	-4.08869800	3.04093400	0.98981800
O	0.50147900	-1.09074800	1.64100700	C	-5.16547100	0.00450600	-1.27832700
C	1.58965300	-1.78003100	1.32540800	H	-5.73514800	-0.60809400	-0.56498000
C	2.02885300	-2.92351000	1.90269300	H	-5.69807800	0.93904200	-1.46406200
H	2.91701200	-3.40292100	1.50426100	H	-5.08583400	-0.51929100	-2.23260900
C	1.39276500	-3.57176400	3.09910100	O	-1.63788800	0.36641900	2.92057800
H	0.46489000	-3.06663700	3.37918500	C	-2.52215200	0.16827100	3.89176900
H	1.15036200	-4.62567000	2.90189900	C	-3.33673400	1.08102900	4.45962100
H	2.05676800	-3.56526200	3.97696800	H	-4.04235400	0.72087500	5.20194800
N	2.35637700	-1.13045400	0.28834900	C	-3.30017200	2.55338000	4.16617300
O	1.51057700	-0.92052800	-0.88696900	H	-2.45653800	2.80880500	3.51504800
C	1.19674000	-2.12606000	-1.61063600	H	-4.22395100	2.90143900	3.67896800
H	0.90581000	-2.92809500	-0.92444500	H	-3.19575800	3.14559900	5.08610900
H	0.35606400	-1.86699200	-2.25838000	N	-2.60279800	-1.18357700	4.43130900
H	2.04526300	-2.44410200	-2.22541900	O	-2.54064700	-2.11795800	3.29414400
C	3.65021900	-1.65161900	-0.11772700	C	-3.84675000	-2.65667900	3.08491400
H	3.63642600	-2.69222400	-0.47704300	H	-4.56780600	-1.85795300	2.88206300
H	4.04136800	-1.00317600	-0.90609900	H	-3.76591700	-3.31055700	2.21238300
H	4.31526700	-1.59571300	0.74731200	H	-4.16602700	-3.23142100	3.96054600
O	-1.86102900	-0.51289300	0.13605800	C	-1.45388900	-1.52924900	5.27053500
C	-2.98151200	-0.83925700	-0.48900900	H	-1.46930800	-0.85376600	6.13024100
C	-3.33352600	-2.09515000	-0.86221300	H	-1.56471200	-2.55847500	5.62234700
H	-4.29609400	-2.27358600	-1.32436200	H	-0.49066400	-1.42758400	4.74904800
C	-2.42883900	-3.28929200	-0.73513200	O	-0.17582100	1.69685500	0.84987300
H	-1.49166600	-3.03301000	-0.23149500	C	0.41162800	2.88369100	0.91687000
H	-2.90093800	-4.10320600	-0.16530200	C	-0.02417400	4.01386600	0.30702400
H	-2.16798200	-3.71583600	-1.71605000	H	0.49618600	4.94888200	0.47178100
N	-3.80962200	0.30060800	-0.82351300	C	-1.13830400	4.03866700	-0.70091500
O	-3.90598300	1.11380000	0.40856400	H	-1.45442700	3.02442600	-0.96665100

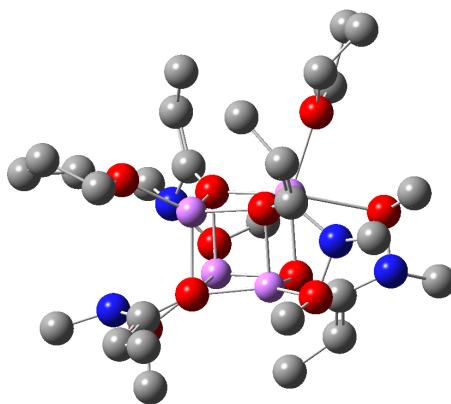
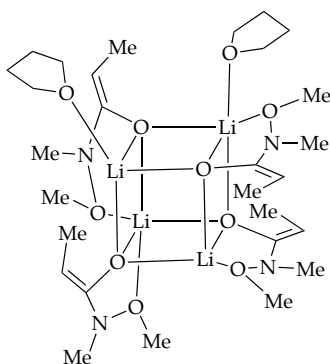
H	-2.02397300	4.58621700	-0.34343400	H	3.63111600	1.97508400	3.14709900
H	-0.82365900	4.53741100	-1.62906300	H	2.64257500	0.66793200	3.84233700
N	1.67390200	2.88087000	1.61836000	C	2.19924000	4.17271100	2.05171500
O	1.56367100	2.04318300	2.81854700	H	1.46919100	4.76217100	2.62476600
C	2.78550000	1.30282700	2.96219800	H	3.08709000	4.00254900	2.66435100
H	2.96841900	0.69811700	2.06977300	H	2.50793900	4.73261000	1.16642900



8  
 $G = -1636.688295$   
 $G_{\text{MP2}} = -1632.002899$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	4.73521600	-0.29519800	-0.77609300
Li	1.99948300	-1.76549500	-0.29452200	C	5.48724700	-0.47024300	-1.89287200
Li	2.60670200	0.49348800	0.78546400	H	6.54620300	-0.24552500	-1.87365100
Li	2.03863400	0.43920400	-1.72269300	C	4.95032900	-1.01325100	-3.18798900
O	0.77778800	-0.97107300	-1.64716700	H	3.86501400	-1.14349900	-3.14921100
C	0.36915600	-1.93791200	-2.45336800	H	5.17385800	-0.34344800	-4.03115700
C	-0.07222400	-1.80464900	-3.72796000	H	5.39104000	-1.98857400	-3.44600900
H	-0.32360300	-2.69565500	-4.29403000	N	5.34672600	0.08570200	0.48486300
C	-0.27246900	-0.48507300	-4.41856900	O	4.52848200	1.22262800	0.98029400
H	-0.02948200	0.35059200	-3.75592100	C	4.87255400	1.57400900	2.32083300
H	0.36085400	-0.39322300	-5.31329800	H	5.03528000	0.67967400	2.92969500
H	-1.31033900	-0.35287000	-4.75992900	H	5.75917500	2.21763300	2.35343300
N	0.36902000	-3.22510100	-1.79903800	H	4.01822800	2.13709500	2.70743900
O	1.69385800	-3.49918500	-1.24833700	C	6.74303100	0.50672900	0.42408700
C	2.67844000	-3.84763200	-2.23931100	H	6.91624400	1.34442200	-0.26747600
H	2.62388900	-3.17030000	-3.09732400	H	7.08580100	0.78086500	1.42346100
H	3.64535800	-3.73957900	-1.74273400	H	7.32812300	-0.35779200	0.10566600
H	2.55099600	-4.88472500	-2.56756800	O	1.35862300	1.51599300	-0.21164500
C	-0.15249500	-4.40286600	-2.46945400	C	1.24843600	2.78167800	-0.56604400
H	0.34012100	-4.64878700	-3.42312000	C	1.08457200	3.84252600	0.26385000
H	-0.05585900	-5.25057500	-1.78557900	H	1.07630200	4.84643900	-0.14719400
H	-1.21287300	-4.22758600	-2.66612400	C	0.90349400	3.71019200	1.75092200
O	3.43096800	-0.48278100	-0.68937400	H	0.81932500	2.65832000	2.04346900

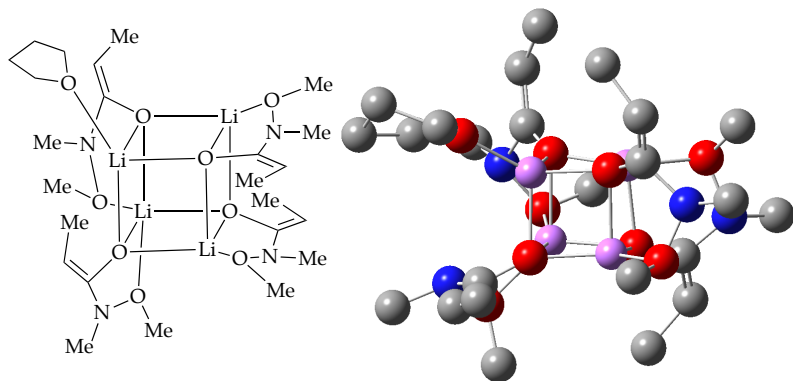
H	1.74613900	4.14430500	2.31123400	C	-2.01484800	-2.04698000	0.47025500
H	0.00123800	4.22955000	2.10614900	H	-1.34244400	-2.67610700	-0.11956300
N	1.23741400	2.94768600	-2.00113700	H	-2.72217800	-2.66880400	1.03406300
O	2.36067400	2.23220900	-2.59033900	H	-2.57149900	-1.36387400	-0.17464900
C	3.64581600	2.82510000	-2.31000600	C	-1.21296700	-2.33330700	3.40245600
H	3.73815800	3.06650700	-1.24638600	H	-1.38480700	-1.45258200	4.03917100
H	4.38059500	2.06124000	-2.57219600	H	-2.17596500	-2.74838000	3.09672800
H	3.80037300	3.72104500	-2.92092000	H	-0.68497200	-3.09921800	3.97474700
C	1.12292600	4.27271300	-2.58734200	O	-1.76413900	1.00346700	-0.41682700
H	1.16077100	4.16533400	-3.67442300	C	-2.40758000	1.75559100	0.63369600
H	0.14757700	4.67731600	-2.30650000	C	-2.76976300	3.09894400	0.00350300
H	1.89847200	4.98416500	-2.26410300	C	-3.11070900	2.68378300	-1.43616500
O	1.36266700	-0.90446500	1.27524800	C	-2.08103100	1.58020600	-1.70875900
C	0.83146800	-1.36867000	2.39636000	H	-1.15456900	1.97497300	-2.13683100
C	1.42045600	-1.34387500	3.61846500	H	-2.46184200	0.78440000	-2.35651700
H	0.87405400	-1.68574200	4.48805100	H	-3.03569900	3.50604300	-2.15446500
C	2.84873200	-0.93498100	3.83923900	H	-4.13124800	2.28501100	-1.48652300
H	3.42203300	-0.98488400	2.90623000	H	-1.89581000	3.75969500	0.01281500
H	2.94908200	0.08626600	4.24137300	H	-3.59536500	3.59844500	0.52014900
H	3.34504700	-1.59901200	4.56052500	H	-3.30081700	1.21126300	0.97060000
N	-0.43253000	-2.02959700	2.20812000	H	-1.71115300	1.83257400	1.47198400
O	-1.26281500	-1.19799200	1.34606300				



**9**  
 $G = -2101.377355$   
 $G_{Mr2} = -2095.394390$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.06669300	-4.58580500	-1.94278800
Li	-1.37442000	-0.08247200	-2.27559500	C	-0.88553300	-4.36227500	0.04296000
Li	-2.23173600	1.68214100	-0.43727500	H	-1.27298400	-3.54645900	0.65998900
Li	-2.51560800	-0.97868300	-0.07520300	H	-1.70067500	-5.08767800	-0.10120400
O	-0.90155000	-1.52995200	-0.98671400	H	-0.11216400	-4.88615200	0.62508400
C	-0.37252500	-2.54509800	-1.64212600	N	0.31372200	-2.11963500	-2.84035400
C	-0.35940500	-3.85038300	-1.26817700	O	-0.59062100	-1.34554900	-3.68093100

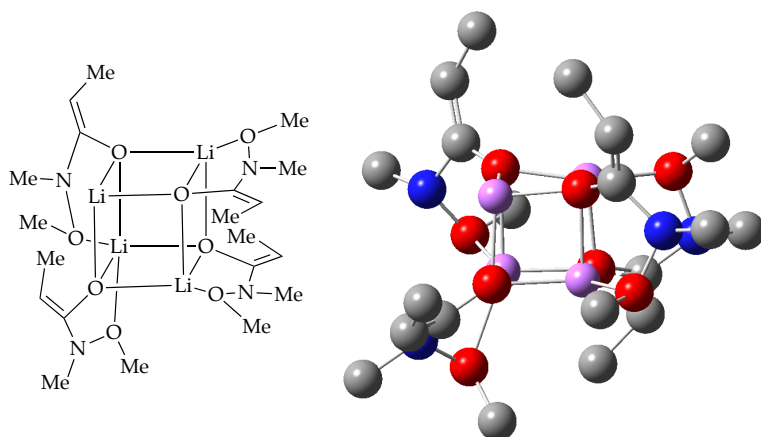
C	-1.52515400	-2.15363300	-4.41617900	O	-3.90192800	-2.06006200	0.81905200
H	-2.00600200	-2.88864000	-3.76189400	C	-4.72504000	-1.38982000	1.81601700
H	-2.27069600	-1.45799400	-4.80540700	C	-6.05505200	-2.15752900	1.85143000
H	-1.03181700	-2.66050100	-5.25250200	C	-5.67659600	-3.53293200	1.27744700
C	1.08130600	-3.05798200	-3.63868700	C	-4.63879900	-3.14854300	0.22605600
H	0.51170000	-3.91965500	-4.02046200	H	-5.11624800	-2.80204900	-0.69989900
H	1.51275600	-2.51033000	-4.48129500	H	-3.92380300	-3.94033700	-0.01014800
H	1.89257200	-3.43607700	-3.01180100	H	-6.52807200	-4.07311300	0.85216500
O	-3.15878100	0.16511700	-1.59123200	H	-5.21963800	-4.16288100	2.04991700
C	-4.46750900	0.32886000	-1.65767000	H	-6.79731100	-1.67432500	1.20557400
C	-5.33850100	-0.31778400	-2.47350200	H	-6.47348800	-2.21130500	2.86103500
H	-6.38047600	-0.01648400	-2.47445900	H	-4.18876300	-1.43897900	2.76750800
C	-4.95284200	-1.44361600	-3.38956200	H	-4.83395100	-0.34259300	1.52233300
H	-4.78612700	-1.11346700	-4.42811700	O	-0.50717700	1.39642000	-1.44801300
H	-4.02982200	-1.92251100	-3.04941800	C	0.40352600	2.26014900	-1.86198200
H	-5.73543100	-2.21343500	-3.43346500	C	0.15783300	3.54994700	-2.21531900
N	-4.95302900	1.24166900	-0.65420000	H	0.97547400	4.20711800	-2.47952200
O	-4.25019700	2.50424500	-0.74145500	C	-1.23356800	4.10248700	-2.34576400
C	-4.62341600	3.28070600	-1.88923300	H	-1.92545200	3.33905200	-2.72136700
H	-3.96172400	4.14668000	-1.87557100	H	-1.64899600	4.47422000	-1.39467200
H	-4.48492300	2.71206000	-2.81608200	H	-1.25809300	4.94264700	-3.05110800
H	-5.66168500	3.62351300	-1.81669000	N	1.72274500	1.70968100	-2.02126800
C	-6.37684300	1.46080600	-0.46877100	O	2.04329700	0.90112300	-0.85489300
H	-6.49978500	2.18994100	0.33666600	C	2.76965000	-0.24790600	-1.29849200
H	-6.91493300	1.81642700	-1.36180400	H	2.15838600	-0.84052700	-1.98466700
H	-6.82489900	0.51316700	-0.16016000	H	3.71302400	0.03904000	-1.78150900
O	-1.68750500	0.38711100	1.01570800	H	2.99423400	-0.81321800	-0.39280900
C	-1.90789300	0.92478400	2.20165900	C	2.82065600	2.65028600	-2.21413000
C	-1.73465300	0.33566100	3.41487500	H	2.87187900	3.42011100	-1.42925300
H	-1.90165400	0.91980500	4.31350100	H	3.76111400	2.09483500	-2.23121700
C	-1.40590600	-1.11833000	3.60349800	H	2.69873400	3.13124000	-3.18710400
H	-1.35328200	-1.63323100	2.64033100	O	1.28105000	-0.81023000	1.43388000
H	-0.44134900	-1.26922600	4.11282900	C	1.93605000	0.00673300	2.43237700
H	-2.15687300	-1.63430500	4.22247100	C	2.77607300	-0.95289400	3.29472600
N	-2.48183000	2.24025900	2.11167700	C	2.92410700	-2.19004100	2.39239400
O	-1.82219300	3.03139600	1.10261000	C	1.58472100	-2.19803400	1.65767700
C	-0.46628300	3.38216200	1.42586800	H	0.79792000	-2.65401200	2.27244200
H	0.10408000	2.49853600	1.73120700	H	1.59776700	-2.69489400	0.68447700
H	-0.04614800	3.78509900	0.50198800	H	3.10403700	-3.11293400	2.95249100
H	-0.43495300	4.13833900	2.21926100	H	3.74984400	-2.05545400	1.68296800
C	-2.73696500	3.03129300	3.30068700	H	2.23627800	-1.21718500	4.21093700
H	-1.84993900	3.21080100	3.93027700	H	3.73570900	-0.51573300	3.58668000
H	-3.15366300	3.98943400	2.98060100	H	2.55347400	0.73894500	1.90034000
H	-3.48443500	2.50714100	3.90118900	H	1.16920700	0.53382300	3.00895600



**10**  
 $G = -1869.038732$   
 $G_{MP2} = -1863.701458$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.00676900	-1.67362200	2.81006000
Li	0.94883900	2.45458000	0.76037500	H	-0.58527100	-0.04447800	3.28442600
Li	1.38053400	1.62512200	-1.58593100	H	-1.66303400	-1.47030400	3.43354500
Li	-1.03685800	2.33512500	-1.01175100	C	-3.57842400	-0.43418800	1.87554800
O	0.62044400	3.33143400	-1.01925600	H	-3.69495900	-1.46709800	1.53766400
C	1.14476900	4.54578300	-1.00848200	H	-3.61255100	-0.40670700	2.97620900
C	0.82282800	5.57934800	-1.82386700	H	-4.41379800	0.15834700	1.49457700
H	1.29412200	6.54357700	-1.66394400	O	-0.26963400	0.77618600	-1.88104100
C	-0.12362500	5.46879000	-2.98565400	C	-0.67967800	-0.16522300	-2.71687800
H	-0.46517000	4.43774900	-3.11820500	C	-0.89626500	-0.02412200	-4.04745800
H	-1.01483500	6.10153200	-2.85347100	H	-1.17104200	-0.89414600	-4.63445700
H	0.34434000	5.79137100	-3.92737200	C	-0.79940200	1.28666800	-4.77750900
N	2.22689300	4.65829900	-0.06209000	H	-0.58079800	2.10668000	-4.08640300
O	1.78176000	4.23401100	1.26022600	H	-0.00648500	1.27556400	-5.54079600
C	0.94002300	5.19466100	1.92157300	H	-1.73168600	1.53637500	-5.30651700
H	0.14826300	5.54769000	1.25187100	N	-0.96453500	-1.39980900	-2.03711900
H	0.50144600	4.66498100	2.76935500	O	0.12942000	-1.74771200	-1.15260700
H	1.52732200	6.04289600	2.28917800	C	1.34833100	-2.08846700	-1.83630600
C	3.01643800	5.87329600	0.03230700	H	1.59501400	-1.34039800	-2.59769400
H	2.44026900	6.78492600	0.25580700	H	2.12034200	-2.08899000	-1.06411600
H	3.77186100	5.72440700	0.80853800	H	1.27543100	-3.08043400	-2.29699400
H	3.52114200	6.01514400	-0.92632600	C	-1.41051100	-2.56496300	-2.77915100
O	-0.82752300	1.74540300	0.87890800	H	-0.72625600	-2.88796200	-3.58022300
C	-1.91714100	1.43229000	1.55896200	H	-1.54635700	-3.38349600	-2.06793500
C	-2.65242200	2.24849900	2.35480700	H	-2.37733000	-2.32534300	-3.22884500
H	-3.48130500	1.83050200	2.91580900	O	-2.84185400	2.76277000	-1.61299200
C	-2.40606400	3.72274200	2.50005700	C	-3.73300000	1.62793800	-1.79900700
H	-1.92525900	3.98238300	3.45724100	C	-5.13913900	2.16637000	-1.52563200
H	-1.75710800	4.08919600	1.69901700	C	-5.01271100	3.64192600	-1.93793700
H	-3.34354300	4.29577400	2.46391900	C	-3.60082200	3.98096700	-1.45922800
N	-2.35634000	0.08790800	1.28913300	H	-3.59521600	4.27383100	-0.40150300
O	-1.26692200	-0.84817800	1.47020900	H	-3.10921500	4.76120600	-2.04674900
C	-0.86792700	-1.00556700	2.84023700	H	-5.77297300	4.28620300	-1.48602200

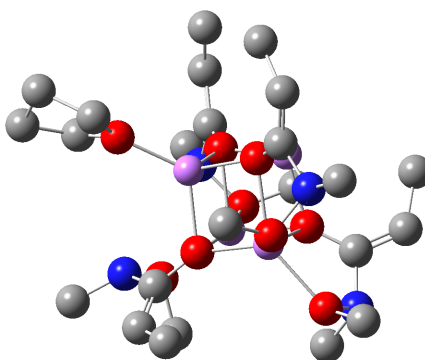
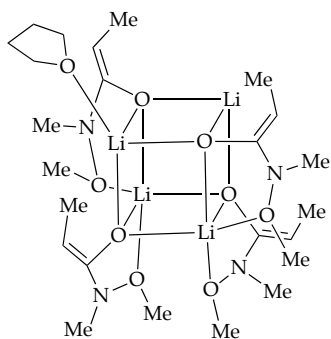
H	-5.08214100	3.74279900	-3.02757800	H	3.35710200	-1.52274300	2.86166700
H	-5.37589100	2.09154300	-0.45769400	N	3.98921200	1.07501200	-0.75491100
H	-5.90788900	1.62489200	-2.08519400	O	3.30801100	1.32534100	-2.03377500
H	-3.61685400	1.27273700	-2.82884100	C	3.75393900	2.58381000	-2.55955700
H	-3.41771100	0.83777900	-1.11305200	H	3.62361100	3.37044600	-1.81221200
O	1.85246200	0.87155500	0.14725500	H	4.80115400	2.53068100	-2.87960800
C	3.07754800	0.37436500	0.12224300	H	3.12974000	2.77244700	-3.43838700
C	3.52733900	-0.64418400	0.89899900	C	5.25221600	0.41185400	-1.06402400
H	4.52937700	-1.03037500	0.76471600	H	5.12078900	-0.61192300	-1.44353000
C	2.71615400	-1.23201400	2.01928200	H	5.79251000	1.00418300	-1.80528100
H	1.98382600	-0.50784400	2.39102600	H	5.85509000	0.38912200	-0.15384200
H	2.15927000	-2.13627700	1.72193600				



**11**  
 $G = -1636.679283$   
 $G_{\text{MP2}} = -1631.994016$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.54970500	3.04378900	-1.05265900
Li	-2.54768400	0.61893200	-0.53421500	C	-6.57883600	0.58671400	-0.33104800
Li	-2.12833800	-1.44411600	0.90728000	H	-6.98876800	1.51766100	0.09035300
Li	-1.73594800	0.83752300	1.90853800	H	-6.75254500	0.57161000	-1.41014100
O	-3.32692300	0.08770400	1.24634200	H	-7.10495700	-0.25665200	0.12237400
C	-4.62272300	0.36425600	1.23362600	O	-1.19423300	1.71261000	0.33475700
C	-5.42005800	0.52701300	2.31582500	C	-0.34895700	2.73315900	0.24657000
H	-6.45660000	0.81285900	2.17125600	C	-0.59253700	4.01864800	0.59566100
C	-4.96586100	0.29625900	3.72983300	H	0.17441100	4.76513100	0.41931900
H	-3.96371300	-0.14432100	3.75447800	C	-1.84630800	4.48665600	1.27932700
H	-4.93361600	1.22908300	4.31313600	H	-2.41070400	5.20649700	0.66731400
H	-5.64182900	-0.38205900	4.26938300	H	-2.51709500	3.64849700	1.49435300
N	-5.15742400	0.39063800	-0.10383300	H	-1.62827700	4.99544200	2.22978000
O	-4.38012700	1.30798000	-0.93210000	N	0.95543600	2.31137300	-0.18070100
C	-4.60106600	2.69871800	-0.62819700	O	0.86460600	1.46668700	-1.35238000
H	-4.58657000	2.86753300	0.45317600	C	0.29885900	2.12163400	-2.49684600
H	-3.77339200	3.23655500	-1.09525600	H	0.21428000	1.34542600	-3.25849900

H	-0.69159300	2.53010800	-2.26842300	H	2.94933700	-2.25311800	2.77828600
H	0.95440500	2.92065800	-2.86072300	H	3.62328500	-0.82909900	1.92876200
C	2.04026200	3.26642000	-0.32284400	H	2.91825300	-0.64839700	3.54992800
H	2.92509600	2.71892300	-0.65521100	O	-1.50467700	-0.96180400	-0.88559200
H	1.83423100	4.08922300	-1.02583100	C	-1.59005700	-2.03268900	-1.66412900
H	2.23976700	3.69366700	0.66260700	C	-0.71851400	-2.38880300	-2.64165800
O	-0.73448500	-0.73043000	1.96884600	H	-0.88140400	-3.31212000	-3.18303600
C	0.32298200	-1.14946700	2.65175300	C	0.43497800	-1.55032000	-3.11561000
C	0.30357600	-1.76936300	3.85532300	H	0.22234700	-1.05856600	-4.07904800
H	1.23605500	-2.11721700	4.28690500	H	0.70174900	-0.76977400	-2.39975700
C	-0.94166600	-1.97437900	4.67145300	H	1.33043100	-2.16572000	-3.27894000
H	-1.81533900	-1.54599100	4.16966200	N	-2.78598600	-2.81577400	-1.44120900
H	-1.14967900	-3.04106100	4.84259300	O	-2.91187500	-3.04618900	0.00811900
H	-0.86443800	-1.51058800	5.66617000	C	-4.30322300	-3.05422000	0.36131600
N	1.55669000	-0.80236200	2.00172800	H	-4.78766700	-2.14210800	0.00501100
O	1.51634700	-1.21009900	0.60811100	H	-4.80630700	-3.94009900	-0.04336600
C	1.46340500	-2.63627100	0.41613300	H	-4.32851100	-3.10628500	1.45388300
H	0.74602100	-3.09371000	1.10604600	C	-2.86189000	-4.12358400	-2.08483000
H	1.12518000	-2.78259400	-0.61107200	H	-1.99661200	-4.76474100	-1.86306400
H	2.45338400	-3.08481600	0.55578100	H	-3.77479400	-4.62560600	-1.75764400
C	2.82924400	-1.17336200	2.59581900	H	-2.93723100	-3.96773400	-3.16306500

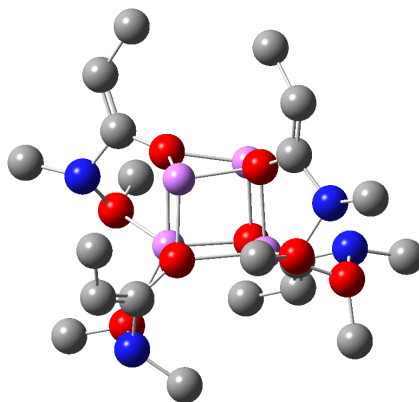
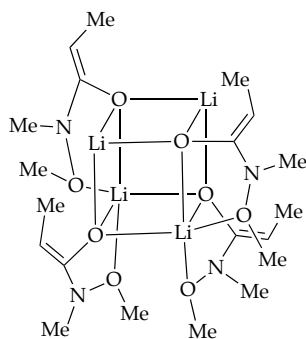


**12**  
 $G = -1869.034498$   
 $G_{\text{MP2}} = -1863.694701$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.51665000	2.87655200	-3.90813500
Li	-1.09869800	-0.66614000	-2.33833600	H	-2.19902000	2.06843800	-3.63031500
Li	-2.03271100	-1.96997400	-0.28834200	H	-2.08324600	3.81900000	-3.86664100
Li	-2.57799800	0.58278300	-0.71121100	H	-1.23637900	2.73295900	-4.96260700
O	-0.92001500	1.04901200	-1.61081300	N	1.14614800	1.98333400	-1.28616200
C	-0.10222800	2.01190600	-2.00646300	O	0.88787600	1.99449200	0.14532700
C	-0.31958200	2.90527500	-3.00107600	C	0.24193400	3.19205100	0.60388100
H	0.41839900	3.67822300	-3.18767200	H	-0.67189600	3.39036500	0.03388800



H	-0.00455500	3.00354800	1.64889200	H	-2.63587000	-5.17214600	-2.67136700
H	0.91453900	4.05487300	0.53758800	C	-5.06925400	-3.92192300	-2.07798400
C	2.20355600	2.92516700	-1.61413000	H	-4.88601000	-4.34438500	-3.07953300
H	1.91427400	3.98522900	-1.54018500	H	-5.10288800	-4.73242400	-1.34542600
H	3.04477500	2.73498300	-0.94308100	H	-6.03890900	-3.41844600	-2.08908100
H	2.51967800	2.72422100	-2.64043400	O	-4.14608200	1.70517100	-0.49308800
O	-1.70244000	-0.29834100	0.86209300	C	-5.41834200	1.04450900	-0.25989000
C	-2.29350800	-0.41013100	2.03953500	C	-6.32872100	2.12866500	0.31690600
C	-1.87955500	0.08557800	3.23124100	C	-5.80406000	3.39440600	-0.38035900
H	-2.46652600	-0.13483900	4.11679500	C	-4.29482400	3.13851400	-0.41637600
C	-0.65953700	0.93630600	3.43686400	H	-3.80350300	3.49347900	0.49921200
H	-0.06904100	0.57663700	4.29083700	H	-3.79434900	3.58408300	-1.28111700
H	-0.00661300	0.91812600	2.56019800	H	-6.05738200	4.31923900	0.14661200
H	-0.90674800	1.98804300	3.65488800	H	-6.20484600	3.46193700	-1.39859200
N	-3.53005300	-1.15319200	1.94181400	H	-6.19316700	2.20728800	1.40237500
O	-3.23098400	-2.47296900	1.40140000	H	-7.38699800	1.93396900	0.11870500
C	-2.58137600	-3.35434000	2.33067300	H	-5.79083200	0.66338900	-1.21821700
H	-2.23066600	-4.19331600	1.72480700	H	-5.23024700	0.20291600	0.41105200
H	-1.73608400	-2.86036100	2.82362500	O	-0.17674500	-1.76626500	-1.14504300
H	-3.28392100	-3.72946800	3.08385800	C	1.04532600	-2.27075600	-1.21228900
C	-4.42101900	-1.26261600	3.08372800	C	1.70453800	-2.71606700	-2.30518500
H	-5.28011100	-1.86933800	2.78337200	H	2.72545100	-3.05343300	-2.15830400
H	-3.97002400	-1.70233000	3.98717800	C	1.14347500	-2.76595500	-3.69756700
H	-4.76698200	-0.25597400	3.33201500	H	0.06406400	-2.57168700	-3.70898400
O	-2.86817400	-1.01985900	-1.83957800	H	1.61978000	-2.02820200	-4.36156900
C	-3.80468800	-1.77647300	-2.39621800	H	1.29722700	-3.74819000	-4.16638200
C	-4.51724100	-1.48296800	-3.51227300	N	1.78824400	-2.34848600	0.03986900
H	-5.20272700	-2.22321700	-3.91107900	O	1.71577000	-1.00520300	0.63851900
C	-4.45493900	-0.16006300	-4.22294500	C	3.02507600	-0.44244600	0.62636300
H	-3.88358100	0.56914500	-3.64093500	H	3.70620600	-1.03958200	1.24360200
H	-3.98049400	-0.23570600	-5.21363300	H	3.41263600	-0.38120700	-0.39644400
H	-5.45783200	0.25814900	-4.39453900	H	2.91796400	0.56192100	1.04207600
N	-4.07621500	-2.96226300	-1.63518400	C	1.17159700	-3.23354900	1.02526500
O	-2.84509800	-3.62978600	-1.26756900	H	1.16110500	-4.24115800	0.59706200
C	-2.15654900	-4.23172700	-2.37496000	H	1.78358300	-3.24027500	1.93185200
H	-2.12115100	-3.54956500	-3.23097700	H	0.14717400	-2.93719600	1.28807300
H	-1.14241500	-4.42538700	-2.02088200				

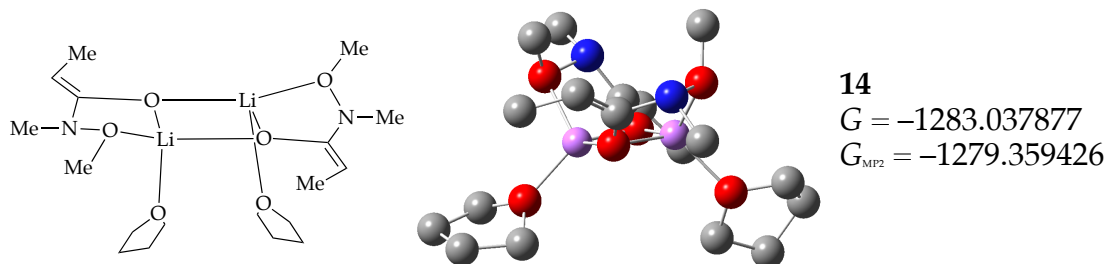


**13**  
 $G = -1636.672205$   
 $G_{MP2} = -1631.987499$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-4.16437800	2.61246600	0.08512400
Li	-1.41280300	-2.30783900	0.16024500	H	-4.51889200	2.24330700	1.05064600
Li	-2.87839100	-0.12293600	0.15181600	H	-3.21267100	3.14293600	0.20549700
Li	-1.62454000	-0.97908700	-1.89662200	H	-4.91703200	3.28961400	-0.33427600
O	-0.14282900	-1.88233700	-1.15952600	C	-3.99515000	2.62487600	-2.80541000
C	1.09439200	-2.34594300	-1.27522600	H	-5.02924300	2.28581100	-2.91106700
C	1.48267200	-3.45467800	-1.94630100	H	-3.99204900	3.65836500	-2.42486300
H	2.53999600	-3.68950600	-2.00780400	H	-3.51984500	2.62098100	-3.78951300
C	0.53487500	-4.41743200	-2.60230900	O	-2.94540900	-1.86387900	-0.85719900
H	-0.50447200	-4.11940200	-2.43817600	C	-4.17213000	-2.37604100	-0.78640000
H	0.69595300	-4.47322100	-3.68916800	C	-4.56029900	-3.58293400	-1.26343200
H	0.65644700	-5.44092600	-2.21847000	H	-5.57468400	-3.91955700	-1.07833900
N	2.03433700	-1.55587400	-0.52097300	C	-3.69449900	-4.47040800	-2.11230900
O	1.92338200	-0.15590900	-0.90683000	H	-2.76567100	-3.96303100	-2.39050500
C	2.24542600	0.09357100	-2.28437000	H	-3.41792700	-5.40421700	-1.59958800
H	1.64389400	-0.53411300	-2.95014400	H	-4.20533900	-4.76650000	-3.03978600
H	2.00836500	1.14506000	-2.44747700	N	-5.11442600	-1.46669300	-0.20731700
H	3.31064400	-0.07517200	-2.47775100	O	-4.59425200	-0.89441400	1.01806300
C	3.43358700	-1.94741200	-0.45811200	C	-4.52267000	-1.82559100	2.11011400
H	3.93101600	-2.03094000	-1.43660600	H	-4.12073500	-2.78818100	1.77553200
H	3.96263100	-1.21136800	0.15198500	H	-3.84297600	-1.37821400	2.83754500
H	3.48382300	-2.91892200	0.03910800	H	-5.51010900	-1.97545700	2.56166300
O	-1.40072300	0.74689500	-1.09279000	C	-6.50864100	-1.83550100	-0.05445000
C	-1.89553900	1.83742500	-1.66293600	H	-6.68017500	-2.73943800	0.55273600
C	-1.24458000	2.98620000	-1.95954600	H	-7.03166200	-0.99064400	0.40082000
H	-1.81049200	3.80123900	-2.39924900	H	-6.91978200	-2.00607900	-1.05213900
C	0.22242000	3.22628500	-1.74622200	O	-1.37147500	-0.85807300	1.33558000
H	0.39617500	4.20418900	-1.27711300	C	-0.83306300	-0.70543100	2.53744500
H	0.65972100	2.46801500	-1.09064800	C	-0.70240400	-1.62869400	3.51550600
H	0.79146500	3.23160500	-2.68971800	H	-0.19141600	-1.31462200	4.41986500
N	-3.29186200	1.66184800	-1.97680800	C	-1.18978600	-3.04753200	3.44456000
O	-4.00963300	1.43660400	-0.72533600	H	-1.81341300	-3.22157500	2.55929800

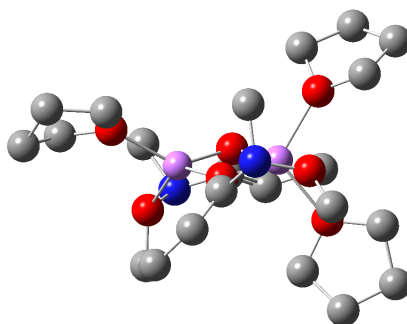
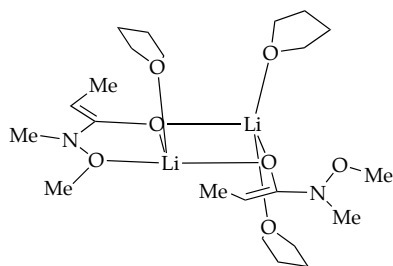
H	-0.35718200	-3.76627300	3.40914600	H	2.18754000	-0.09415100	2.63413200
H	-1.79521300	-3.31790400	4.32116700	H	2.59605600	1.10961600	1.37374200
N	-0.29463300	0.61360400	2.84515400	C	-1.30009900	1.67349800	2.82806600
O	0.61918000	0.94382500	1.73744500	H	-2.03585200	1.43867300	3.60408100
C	1.95535600	0.89864400	2.23304200	H	-0.81898400	2.62471800	3.07226000
H	2.10150900	1.65494600	3.01235000	H	-1.80827600	1.77092500	1.85838800

**Table 2.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the differentially solvated, differentially-internal chelated dimers at  $-78\text{ }^{\circ}\text{C}$  with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP / 6-31G(d) optimized structures).



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.38871100	-2.60092400	-0.17750200
O	-0.72507000	1.72378600	-0.23537900	H	-2.72267000	-4.22304700	-0.41600100
C	-0.68465900	2.85673400	0.42756200	H	-3.87329000	-3.93504600	0.88759900
N	-1.97447900	3.44771300	0.81168700	O	-3.80051600	0.63636700	-1.20777500
O	-2.83223100	2.35343000	1.30959800	C	-5.20895200	0.73544700	-0.93948700
Li	-2.35585300	0.77087600	0.16810300	C	-5.75868500	-0.65499700	-1.24691400
O	-1.59256400	-0.89945400	0.48019400	C	-4.92849600	-1.05533900	-2.48080500
C	-1.33077300	-1.89204300	1.29754400	C	-3.57550200	-0.35313400	-2.24504500
N	-0.38851600	-1.54305200	2.34874400	H	-3.20716400	0.15556800	-3.14318900
O	0.74802200	-0.85159700	1.71671700	H	-2.80241300	-1.02851800	-1.86983400
C	1.13923900	0.24601500	2.54707800	H	-4.81609400	-2.13862700	-2.57989400
H	2.02725400	0.67334100	2.07295200	H	-5.40290900	-0.68273500	-3.39562000
H	0.35022400	1.00177200	2.60145500	H	-5.55501900	-1.33086900	-0.40934100
H	1.40034500	-0.09651100	3.55516300	H	-6.83645900	-0.65329400	-1.43676900
C	0.18200200	-2.63475300	3.13029800	H	-5.65734500	1.49889800	-1.59261900
H	0.63954900	-3.41851100	2.50877300	H	-5.32457400	1.05244700	0.09996200
H	0.93559600	-2.22729300	3.80931700	C	-2.83654900	2.39994300	2.73294800
H	-0.61481700	-3.07144400	3.73670900	H	-3.44129800	1.54936600	3.06223800
C	-1.89934300	-3.12538800	1.27385400	H	-1.82075300	2.30511300	3.13293200
H	-1.56856100	-3.89235900	1.96351300	H	-3.28040800	3.33743500	3.08564800
C	-3.02460300	-3.48869500	0.34755800	C	-2.70425300	3.99158700	-0.33615700

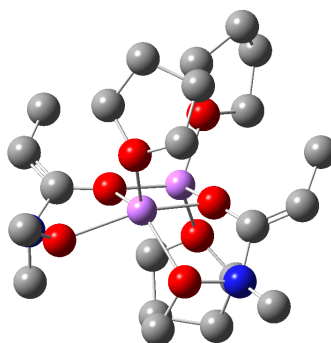
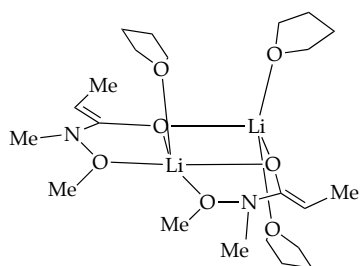
H	-3.64296500	4.43195900	0.01335500	H	1.85918300	-2.26599200	-2.17049800
H	-2.07849500	4.77857100	-0.76596200	C	3.46811300	-0.76870500	-2.18866800
H	-2.91772900	3.23773700	-1.10703100	C	2.89376900	0.53214200	-2.81859700
C	0.39316200	3.59586000	0.78498600	C	1.37694700	0.39198600	-2.62460400
H	0.21019900	4.49041400	1.37214400	H	0.84518300	1.32393600	-2.42670200
C	1.80280100	3.29945500	0.36183200	H	0.90984900	-0.12260700	-3.47797100
H	2.48755000	3.22115800	1.22001900	H	3.16157700	0.64470600	-3.87340000
H	1.85515600	2.35649600	-0.19327600	H	3.26183300	1.41339100	-2.28494800
H	2.21506100	4.08831300	-0.28703500	H	3.92991700	-1.42164900	-2.93531700
O	1.23990400	-0.42296100	-1.45043800	H	4.23035100	-0.53538700	-1.43974800
C	2.23999500	-1.44801400	-1.54269500	H	2.40856000	-1.82663200	-0.53289900



**15**  
 $G = -1515.384394$   
 $G_{\text{MP2}} = -1511.053713$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-1.48309200	-1.10393200	-0.47734800
Li	-2.54758800	0.40392100	-0.20020600	C	-1.55311800	-2.37841700	-0.78292100
O	-1.10507900	1.58237200	0.23634800	N	-0.75417700	-3.31915500	0.00612100
C	-1.14383700	2.71327300	-0.42660900	O	0.65776300	-2.96445900	-0.20972900
N	-2.47286900	3.17877100	-0.85203800	C	1.20375600	-3.92420600	-1.09689200
O	-3.20140000	2.00464400	-1.37142100	H	2.25055200	-3.63724500	-1.24940200
C	-3.20809200	2.08571300	-2.79200600	H	1.15904900	-4.93626100	-0.67234500
H	-3.72985500	1.19108500	-3.14606600	H	0.68048000	-3.92100800	-2.06243600
H	-3.73746900	2.98539400	-3.12582400	C	-0.95012700	-3.17475900	1.44559400
H	-2.18693900	2.09915900	-3.19012600	H	-0.31207800	-3.89976800	1.95985700
C	-3.27837600	3.64189400	0.27827300	H	-0.72802600	-2.16362000	1.81244500
H	-4.25875200	3.96549000	-0.08451500	H	-1.99647400	-3.41514000	1.66212800
H	-3.40918400	2.87630800	1.05804400	C	-2.30023600	-2.95680000	-1.75714000
H	-2.75653800	4.50018600	0.71017500	H	-2.23657200	-4.03571900	-1.85524200
C	-0.13532500	3.56131800	-0.74407400	C	-3.20311200	-2.20822700	-2.69542600
H	-0.39077300	4.43180300	-1.34101500	H	-3.06257300	-1.12690700	-2.59025400
C	1.28044000	3.41880900	-0.26524800	H	-3.00678000	-2.46902700	-3.74580800
H	1.38662100	2.54235400	0.38083400	H	-4.27032100	-2.42245900	-2.52216000
H	1.99460800	3.30405400	-1.09527400	O	-4.27881300	-0.10461700	0.68608300
H	1.60923000	4.30236400	0.30421500	C	-4.48515800	-1.46521800	1.15077600

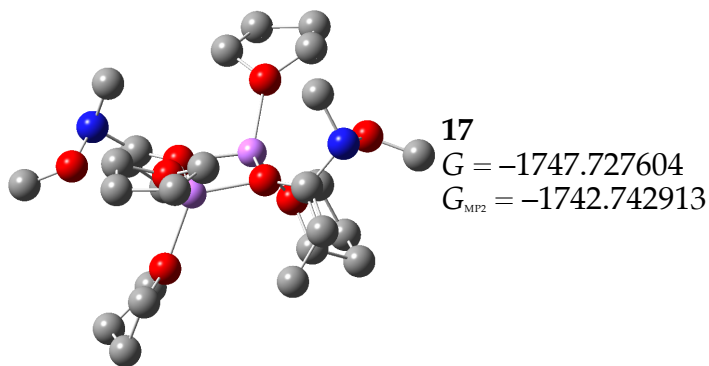
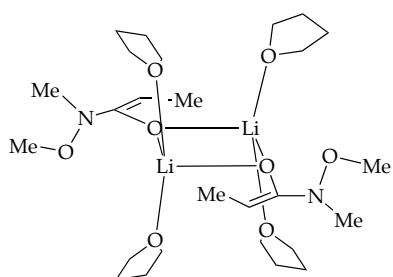
H	-4.01031600	-1.57496200	2.13153700	H	1.59206100	-1.37326500	-3.84994100
C	-6.00749300	-1.67588000	1.20018300	H	1.64020600	0.12860100	-4.79318300
C	-6.53300400	-0.59953800	0.23620700	H	3.88020500	-0.58979600	-3.39939500
C	-5.55117400	0.54139100	0.48923800	H	3.33128300	1.09378600	-3.29528400
H	-5.43519100	1.24017900	-0.34076300	H	3.25705100	0.53808700	-0.94765000
H	-5.82126500	1.10488000	1.39480800	O	0.97486800	-0.10698900	1.76836800
H	-7.57220000	-0.31563100	0.42902500	C	0.57352300	0.75034200	2.84968800
H	-6.45491800	-0.94063600	-0.80282300	H	0.02834700	0.15306600	3.59709500
H	-6.39169900	-1.49596300	2.21107000	C	1.89334100	1.28770100	3.42520500
H	-6.29195800	-2.69128800	0.90930800	C	2.92521100	0.17664800	3.07848400
H	-3.98980200	-2.13496800	0.44206100	C	2.11238900	-0.83546800	2.24279000
O	1.29735400	0.21817200	-1.50727900	H	2.63581100	-1.23464400	1.37296900
C	2.68969000	-0.12084700	-1.61306400	H	1.76989600	-1.67899300	2.85925400
H	2.82632200	-1.16006700	-1.28561000	H	3.34800600	-0.29559500	3.97063800
C	3.05031200	0.05378500	-3.09155300	H	3.75714900	0.58692800	2.49815900
C	1.72104400	-0.28666300	-3.78396500	H	1.82196600	1.47721500	4.50057900
C	0.69595000	0.31409100	-2.81982600	H	2.16266200	2.22905300	2.93719200
H	0.50273300	1.37369000	-3.02849800	H	-0.09407200	1.49893800	2.42246400
H	-0.25283600	-0.22689100	-2.78827400				



**16**  
 $G = -1515.386471$   
 $G_{MP2} = -1511.058795$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.16472900	3.15460400	-1.13749900
O	-1.10071000	0.66396900	-1.45168500	C	-0.88945100	0.78683800	-3.84190900
C	-0.47420700	0.95274100	-2.56370700	H	-0.18593400	1.03345100	-4.63151600
N	0.84922500	1.57769100	-2.42077400	C	-2.26186100	0.31293400	-4.22682900
O	1.50675000	0.93295500	-1.28048800	H	-2.24452000	-0.67691600	-4.71131900
C	2.70215300	0.31752000	-1.74275000	H	-2.90981700	0.23945800	-3.34685500
H	3.41080300	1.06709500	-2.11732300	H	-2.74525900	0.99411600	-4.94331300
H	3.12724200	-0.19950200	-0.87780000	Li	-2.53526000	0.54251400	-0.26444800
H	2.49198400	-0.40541400	-2.53879900	O	-1.54648000	-0.16028600	1.15022300
C	0.75131300	2.99055300	-2.05448800	C	-1.30878600	-0.25736400	2.42891700
H	1.75719300	3.39979200	-1.91674100	N	-0.33310400	0.70953000	2.90998700
H	0.26841100	3.51042800	-2.88672300	O	0.76923400	0.74118700	1.94801800

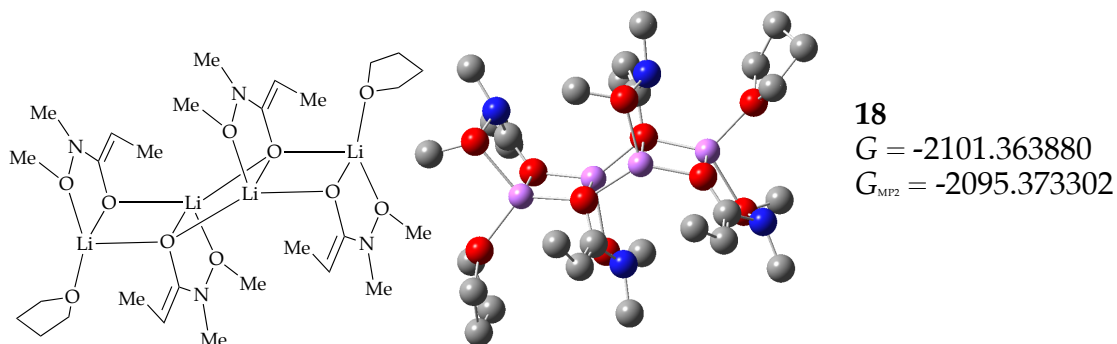
C	1.18769200	2.09189300	1.77841300	O	-4.14561000	-0.53785100	-0.85931100
H	1.96834800	2.06521100	1.01610900	C	-3.99299900	-1.89444300	-1.33823200
H	0.35485200	2.71692500	1.43713900	H	-3.10635300	-2.33021800	-0.86813400
H	1.59441100	2.50565100	2.71073700	C	-5.29162900	-2.62620700	-0.97188300
C	0.25854900	0.47037400	4.22239900	C	-6.30837000	-1.47629700	-0.88976100
H	0.68698900	-0.53738600	4.32586800	C	-5.45754000	-0.35849000	-0.28954400
H	1.03992100	1.21389500	4.39975100	H	-5.79506300	0.64952400	-0.54051400
H	-0.51682500	0.61200100	4.97909400	H	-5.39399700	-0.44893200	0.80380600
C	-1.92006000	-1.10313900	3.30382800	H	-7.18359700	-1.71522000	-0.27789200
H	-1.61625900	-1.13355700	4.34319700	H	-6.65492000	-1.19527100	-1.89135300
C	-3.07553700	-1.97837900	2.90549900	H	-5.19455500	-3.11459100	0.00446200
H	-3.33244300	-1.80935800	1.85488100	H	-5.55938700	-3.39046000	-1.70763500
H	-2.85410400	-3.05076400	3.02665200	H	-3.83279800	-1.85277500	-2.42135800
H	-3.97623800	-1.78234400	3.50888000	O	0.76635300	-1.89383700	-0.26003000
O	-3.46524000	2.28732800	0.15576900	C	0.68491200	-2.83836800	0.82648000
C	-3.38024700	2.81981900	1.50364800	H	0.41933200	-2.28631000	1.72989100
C	-3.37737800	4.34490900	1.35074500	C	-0.37442700	-3.84689300	0.39184100
C	-2.74941300	4.53434600	-0.03923000	C	-0.10724300	-3.95295500	-1.11881300
C	-3.33234200	3.35142700	-0.81214100	C	0.34197200	-2.52905600	-1.49271000
H	-2.69319300	2.98783400	-1.62054500	H	1.17950700	-2.52639700	-2.19902100
H	-4.32529300	3.59000200	-1.21880800	H	-0.46582500	-1.92095500	-1.91038300
H	-2.99208600	5.49760900	-0.49844200	H	-0.98369500	-4.27253900	-1.69115100
H	-1.65805100	4.44769400	0.01802800	H	0.69580900	-4.67390100	-1.31186800
H	-4.40121400	4.73770600	1.36064400	H	-1.36953300	-3.43366400	0.58768800
H	-2.81797100	4.84005700	2.15014200	H	-0.28831000	-4.80525200	0.91362700
H	-2.45988800	2.44395800	1.96266200	H	1.66532500	-3.31846800	0.96535500
H	-4.23573300	2.44466100	2.07437500				



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	1.62888500	2.74449000	-0.55669700
O	-1.00149200	1.62223300	-0.03928100	C	2.40329500	3.78472600	0.01127300
C	-0.66479800	2.88718700	-0.03817900	H	3.34014100	3.32013600	0.34043400
N	0.34999500	3.33043000	-1.00089500	H	2.62150700	4.57269200	-0.72246800

H	1.89635300	4.23445200	0.87528100	H	-4.88083200	1.04875500	4.24685400
C	0.14507600	2.79190800	-2.34139800	H	-4.83037000	2.05027600	2.04358000
H	0.95717700	3.14005200	-2.98657700	O	-3.92431000	1.33442700	-1.24053600
H	0.09369500	1.69506800	-2.36782600	C	-3.80926100	2.66694600	-1.76415200
H	-0.80034200	3.19627600	-2.71864200	H	-3.35061300	2.61831300	-2.76314700
C	-1.14282600	3.88047300	0.75820000	C	-5.25744600	3.19458300	-1.84870600
H	-0.75866400	4.88014800	0.58128200	C	-6.12518600	1.90382200	-1.83666900
C	-2.16566700	3.69303500	1.84290400	C	-5.08514600	0.77287200	-1.86798200
H	-3.11147700	4.21501900	1.62226800	H	-5.34930000	-0.13278300	-1.32257400
H	-2.39604400	2.63278700	1.98604800	H	-4.83625400	0.49535500	-2.90396300
H	-1.81733100	4.09675400	2.80580300	H	-6.81469200	1.84757300	-2.68467500
Li	-2.55267100	0.51577400	0.03808700	H	-6.72177500	1.84928700	-0.92035900
O	-1.55000800	-1.10244800	-0.07689300	H	-5.41015000	3.79100200	-2.75344400
C	-1.87669200	-2.36864500	-0.13446500	H	-5.49352300	3.83242100	-0.99174700
N	-2.88823000	-2.77403900	-1.11711600	H	-3.15078300	3.23062300	-1.10171400
O	-4.17104600	-2.21779600	-0.64721800	O	1.09429500	0.04965400	1.73763500
C	-4.93952900	-3.28872400	-0.13090700	C	0.74414800	1.03788000	2.73825500
H	-5.87984200	-2.84629200	0.21841000	H	-0.04806800	0.61618300	3.37081900
H	-5.15211400	-4.04220000	-0.90165700	C	2.02580000	1.28961700	3.53676000
H	-4.43151800	-3.77630700	0.71173200	C	2.74965700	-0.06075500	3.42514800
C	-2.68565200	-2.17173100	-2.43055900	C	2.40796800	-0.47740600	1.99284700
H	-3.49401500	-2.49541900	-3.09294800	H	3.11551700	-0.04317200	1.27318600
H	-2.64265500	-1.07446600	-2.40469900	H	2.37586100	-1.56109400	1.84586300
H	-1.73634100	-2.55011200	-2.82481800	H	2.33282800	-0.77938300	4.14088300
C	-1.39020900	-3.39386200	0.61490800	H	3.82849000	0.00510700	3.59733900
H	-1.76799900	-4.38697800	0.39292400	H	1.82233500	1.58934100	4.56941700
C	-0.36627100	-3.25004100	1.70548200	H	2.62006900	2.08102300	3.06492900
H	-0.12391300	-2.19743600	1.88153200	H	0.35887400	1.92115600	2.22685500
H	-0.71887100	-3.67951700	2.65577200	O	1.34027900	-0.76056400	-1.34688500
H	0.57346900	-3.77572600	1.46868500	C	1.29815500	-2.11343300	-1.82651900
O	-3.63614500	0.38802000	1.77694800	H	0.90628600	-2.11470100	-2.85511000
C	-4.92263300	0.96062900	2.07727900	C	2.76296400	-2.59274000	-1.79541100
H	-5.64163900	0.64425800	1.30985300	C	3.58598200	-1.27346200	-1.84459500
C	-5.30803700	0.41982600	3.45664100	C	2.50895900	-0.17850700	-1.94164900
C	-4.63619100	-0.96170300	3.45024100	H	2.72195500	0.74723600	-1.40760000
C	-3.32898100	-0.67787600	2.70844100	H	2.29143200	0.06537300	-2.99307300
H	-2.54842800	-0.32217800	3.39474900	H	4.27664100	-1.23730500	-2.69277400
H	-2.94351900	-1.52530700	2.14010900	H	4.17791300	-1.15297300	-0.93180200
H	-5.24456800	-1.67929200	2.88714000	H	2.98458700	-3.25760400	-2.63585700
H	-4.46960300	-1.36926800	4.45211500	H	2.96984200	-3.14660900	-0.87470200
H	-6.39191600	0.37949500	3.60290300	H	0.61432400	-2.67425200	-1.18762800

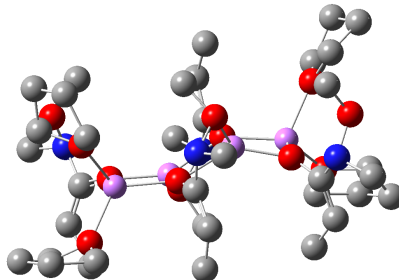
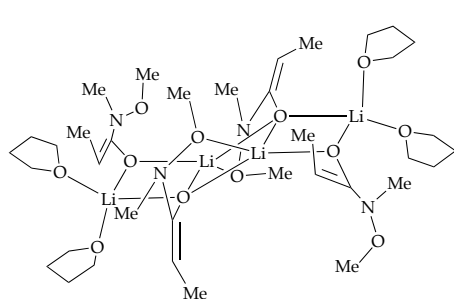
**Table 3.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the differentially solvated, differentially-internal chelated ladder tetramers at  $-78\text{ }^{\circ}\text{C}$  with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP / 6-31G(d) optimized structures).



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.10965600	-2.55996700	-0.89671300
Li	1.64830200	-0.74426400	-1.89924400	H	6.29290800	-1.53550300	0.55884300
O	3.29907700	-1.60703600	-2.05146000	H	6.19935900	-3.31239800	0.73058000
C	3.67799900	-2.85238500	-1.86331500	C	3.92712900	-4.59262400	-0.05663800
C	4.04791000	-3.74483300	-2.81613400	H	4.91758800	-4.96601300	-0.36080200
H	4.39650700	-4.72882400	-2.51990300	H	3.84423600	-4.64666600	1.03289200
C	3.96671200	-3.46064700	-4.28976700	H	3.16484400	-5.23675500	-0.50108500
H	3.57413500	-2.45462200	-4.46547400	O	1.93664000	0.35995900	-0.29076800
H	4.95258500	-3.52407800	-4.77492000	C	2.07798300	1.67156300	-0.46716200
H	3.31592800	-4.17414800	-4.81719300	C	2.57617200	2.53020300	0.46017600
N	3.63233200	-3.23086900	-0.46575300	H	2.67753200	3.58257900	0.22262500
O	4.42436300	-2.27706200	0.31315800	C	2.88662200	2.12279600	1.87550300
Li	3.70301100	-0.49897400	-0.53849000	H	2.71787000	1.05133300	2.02007100
O	5.40271100	0.49441400	-1.00680900	H	3.92958100	2.33682700	2.15533700
C	5.89706200	1.78462600	-0.58264600	H	2.25633000	2.65804400	2.60080700
C	6.24203800	2.57196700	-1.86969200	N	1.54930100	2.13715000	-1.72174600
C	5.80269600	1.62840600	-3.01016700	O	2.03757700	1.22276700	-2.76270500
C	5.87760800	0.25550500	-2.34967800	C	1.15594100	1.23718900	-3.88949500
H	6.91254000	-0.11853100	-2.30906600	H	0.11198600	1.21663500	-3.56336100
H	5.22182300	-0.50025900	-2.78340200	H	1.32665100	2.11590600	-4.52481100
H	6.43882000	1.70776400	-3.89733900	H	1.40557000	0.34075800	-4.46600100
H	4.76683900	1.82731900	-3.30240900	C	1.85436300	3.50791500	-2.10711300
H	7.31714800	2.77461200	-1.92164200	H	2.93325100	3.72699200	-2.12015800
H	5.72287200	3.53447800	-1.90689300	H	1.43376600	3.70599100	-3.09521000
H	5.09974200	2.24843200	0.00022800	H	1.35178200	4.16837300	-1.39786100
H	6.78059500	1.63815200	0.05242000	O	-0.16765200	-1.31096600	-1.57904500
C	5.84439600	-2.44687400	0.16023500	Li	-1.82049700	-0.28347600	-1.70568000



O	-1.61880500	0.90423500	-0.30707300	H	-0.50623800	-4.47027500	-3.81580000
C	-1.94028800	2.15346300	-0.53140800	N	-1.00878400	-2.51273700	0.19556200
C	-1.69687900	3.20210500	0.29697200	O	-0.23466000	-1.68497900	1.09854100
H	-1.96984700	4.20946200	0.00867800	C	1.00429100	-2.28284700	1.53535200
C	-1.11536700	3.02268100	1.67184400	H	1.55079400	-1.47070400	2.01904700
H	-1.14781800	1.96913200	1.97121600	H	0.81331600	-3.07684500	2.26644800
H	-0.06625200	3.34892800	1.73719000	H	1.58932900	-2.66537700	0.69288500
H	-1.67437100	3.59991100	2.42310700	C	-1.39707800	-3.75117800	0.84754500
N	-2.74852100	2.35046000	-1.73465600	H	-0.58115200	-4.48087400	0.96785300
O	-2.18726400	1.47818200	-2.79080100	H	-1.80338200	-3.50014200	1.83091200
C	-3.19746300	1.17209800	-3.75021600	H	-2.18381600	-4.21552100	0.24781200
H	-4.09948900	0.79849600	-3.25798500	C	-3.86692300	-2.53068400	-2.39568600
H	-3.44247100	2.03818300	-4.37733200	O	-3.54658800	-1.25730400	-1.78660200
H	-2.76927700	0.39363700	-4.38985400	C	-4.33407900	-1.06668400	-0.58319100
C	-2.78233500	3.71292100	-2.26160800	C	-5.54427700	-1.97761800	-0.76860200
H	-1.78134500	4.14507900	-2.40032900	C	-4.92256000	-3.18385200	-1.49165100
H	-3.32271200	3.72595100	-3.21066800	H	-4.44382700	-3.85161600	-0.76628100
H	-3.34720600	4.32691400	-1.55762300	H	-5.64877600	-3.77238100	-2.06035500
C	-0.42079500	-2.53592100	-1.11848600	H	-6.01899400	-2.24279200	0.18097000
C	-0.28059900	-3.69444000	-1.80667700	H	-6.29616700	-1.49284300	-1.40307000
H	-0.44754600	-4.63689900	-1.29525900	H	-3.72697400	-1.35559000	0.28249500
C	0.12024000	-3.76264900	-3.25412300	H	-4.56667100	-0.00252200	-0.51211700
H	0.03180000	-2.78057000	-3.73119200	H	-4.25934500	-2.33247900	-3.40119300
H	1.16235000	-4.08965300	-3.37423000	H	-2.94763900	-3.11861300	-2.47695000

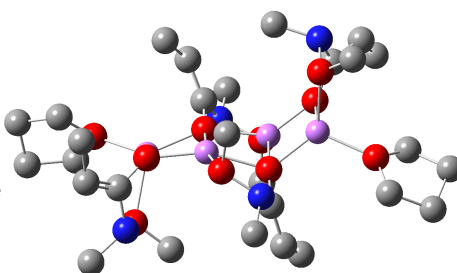
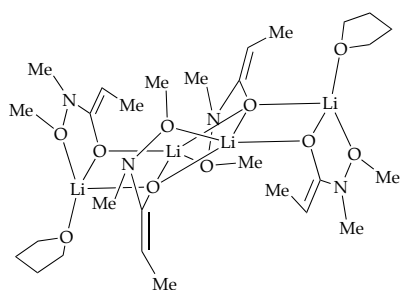


**19**  
 $G = -2566.057879$   
 $G_{\text{MP2}} = -2558.749048$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.61610900	-2.42210600	-3.19071300
Li	1.56098300	-1.92778800	-0.77203600	H	4.98472000	-3.25143400	-3.94691300
O	3.34445700	-2.45266400	-0.61394600	H	3.39429200	-3.99800000	-3.97440200
C	3.91745700	-3.61587400	-0.82972500	N	3.95466600	-4.47181100	0.33036200
C	4.36407100	-4.07742500	-2.03133700	O	4.48060700	-3.74161500	1.46364400
H	4.86513900	-5.03712500	-2.08442200	C	3.48922400	-3.69644200	2.47900100
C	4.07655000	-3.40327300	-3.34436400	H	3.22933900	-4.70549300	2.83065100

H	3.93952200	-3.13664100	3.30702100	H	5.94165000	1.78393600	0.86551200
H	2.58140200	-3.19521900	2.13008300	H	4.21831600	1.89132900	1.33469700
C	4.70816700	-5.71616100	0.26294200	O	-0.33943600	-1.88891300	0.05353500
H	5.76704600	-5.56907800	-0.00211700	Li	-2.20299300	-1.27928500	-0.33755400
H	4.65209600	-6.19992100	1.24184700	O	-1.68643700	0.49467500	-0.60566100
H	4.24148200	-6.37289200	-0.47514100	C	-2.22204200	1.47790400	-1.29283600
Li	3.81714100	-0.66290000	-0.56651900	C	-2.48638000	1.46356500	-2.62952700
O	5.12142300	-0.04180000	-2.03615300	H	-2.98348200	2.31004700	-3.08869600
C	6.21283300	-0.86125900	-2.48415100	C	-2.02056600	0.37645000	-3.55749500
C	7.47469400	-0.04757000	-2.15732900	H	-1.35626300	-0.31946400	-3.03576700
C	6.97978700	1.42571300	-2.19628200	H	-2.84810500	-0.21503200	-3.98283200
C	5.45819100	1.29763000	-2.42288900	H	-1.46723200	0.78629400	-4.41601500
H	5.20450400	1.43622200	-3.48343000	N	-2.44100400	2.68004900	-0.52583200
H	4.84308300	1.97608400	-1.82935300	O	-3.19361100	2.36141200	0.67189200
H	7.45161900	2.00383000	-2.99680600	C	-2.44767900	2.78663900	1.80219500
H	7.19741800	1.93541900	-1.25258300	H	-1.48692300	2.26664000	1.86449200
H	8.27988000	-0.24263400	-2.87219900	H	-2.27080500	3.87227100	1.78146900
H	7.84805600	-0.30341300	-1.16070000	H	-3.06732200	2.54847300	2.67433600
H	6.13166800	-1.82620700	-1.98014700	C	-3.13611000	3.79395800	-1.15675300
H	6.11685700	-1.02152800	-3.56768800	H	-4.13638300	3.52520100	-1.53061200
O	1.94159100	-0.00345300	-0.68815400	H	-3.23868700	4.59392300	-0.41819500
C	1.86194400	1.30983100	-0.85312100	H	-2.52890000	4.16431000	-1.98620300
C	1.83655900	1.97207900	-2.03470900	O	-3.43466500	-1.60837700	1.24332000
H	1.68072000	3.04456300	-2.04405800	C	-3.99385100	-2.89219700	1.59800800
C	1.94849800	1.28779500	-3.36788400	C	-4.76530800	-2.67283600	2.90726000
H	2.24780400	0.24242100	-3.24895300	C	-5.10122500	-1.17326600	2.84792800
H	0.99168000	1.30101000	-3.90945000	C	-3.84422000	-0.60328100	2.19377400
H	2.68518300	1.77937500	-4.01979900	H	-3.04474300	-0.46212900	2.93544000
N	1.86082500	2.02451800	0.41488000	H	-3.98402400	0.32848600	1.64384400
O	0.89292400	1.35602400	1.28683500	H	-5.30227100	-0.73526100	3.83051300
C	1.56599800	0.85255800	2.43961200	H	-5.97651000	-0.99799900	2.21040300
H	2.33180200	0.12467300	2.15831500	H	-4.12207100	-2.88102300	3.77012200
H	2.01847400	1.67374800	3.01013400	H	-5.64814300	-3.31514300	2.98315600
H	0.79200400	0.37320200	3.04598100	H	-4.65637800	-3.20831300	0.78270400
C	1.47174100	3.43364900	0.40233300	H	-3.17506300	-3.61223700	1.68725900
H	0.48133400	3.59486700	-0.04313700	O	-3.54750900	-2.09451200	-1.63662800
H	1.46965400	3.79510100	1.43412000	C	-4.76265700	-1.31365200	-1.79008700
H	2.22713700	3.99320500	-0.15556700	C	-5.56401000	-1.99503000	-2.90786000
O	4.90779300	-0.00800800	1.04742300	C	-5.03212400	-3.43735500	-2.87355200
C	5.14678500	1.33736400	1.48331900	C	-3.55785700	-3.20654500	-2.54828800
C	5.60410400	1.21320300	2.95147200	H	-2.99515300	-2.94276200	-3.45498600
C	6.08552200	-0.26104200	3.06808800	H	-3.05735600	-4.04421600	-2.05692800
C	5.94859300	-0.80464100	1.63651300	H	-5.17757700	-3.97703800	-3.81448700
H	5.64074200	-1.84820400	1.56278900	H	-5.51501700	-4.00961700	-2.07183800
H	6.88166700	-0.65398600	1.07019900	H	-5.34003600	-1.53370900	-3.87644300
H	5.44212300	-0.82345800	3.75178000	H	-6.64396800	-1.92679700	-2.74523500
H	7.11224700	-0.34289500	3.43757800	H	-5.29172300	-1.33844200	-0.83046100
H	4.77436600	1.40753100	3.63799900	H	-4.48151600	-0.28033200	-2.01386200
H	6.39650300	1.93171400	3.18298200	C	-0.30600200	-3.14143100	0.47886700

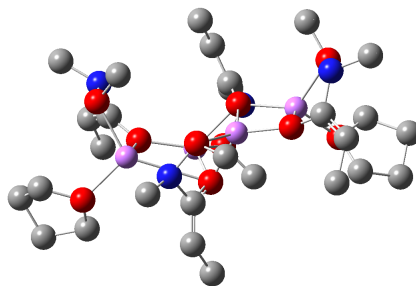
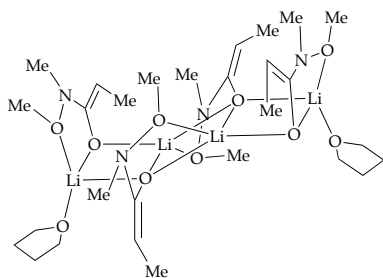
C	-0.33203500	-3.55311200	1.77188000	C	0.11428700	-3.52075600	-2.86621500
H	-0.22263000	-4.60661500	2.00086800	H	0.94487100	-3.28098400	-3.53612700
C	-0.48995100	-2.61462500	2.93520200	H	-0.34489200	-4.46498300	-3.18412500
H	0.42801700	-2.54209700	3.53943500	H	-0.63206200	-2.72023600	-2.88442200
H	-0.73966200	-1.60744900	2.58927100	C	0.01154100	-5.48282500	-0.30917800
H	-1.28461600	-2.94076300	3.62273000	H	-0.78724400	-5.89447300	0.31342800
N	-0.31210200	-4.09042200	-0.61507600	H	0.03651400	-6.04098400	-1.24846100
O	0.69689900	-3.65016400	-1.57355100	H	0.97828300	-5.58738100	0.20123500



**20**  
 $G = -2101.381220$   
 $G_{MP2} = -2095.377705$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-7.66017300	0.11658700	-0.15205300
Li	-1.54040600	-1.85095700	1.18009800	C	-6.25164400	0.55621200	-0.55437800
O	-3.34110900	-2.17363400	1.49406100	H	-6.19996900	1.63763800	-0.73643300
C	-4.20483700	-3.12622300	1.23720800	H	-5.86392500	0.02734700	-1.42977400
C	-4.97493800	-3.77664600	2.14948200	H	-8.43948700	0.68450800	-0.66938400
H	-5.69077800	-4.52312900	1.82509700	H	-7.80363800	-0.94687000	-0.37578600
C	-4.81104300	-3.58487800	3.63200600	H	-7.81583200	1.40405800	1.59619900
H	-4.09011500	-2.78805800	3.83710300	H	-8.39564700	-0.24398600	1.90047500
H	-5.75825300	-3.31392700	4.12219200	H	-6.13539600	-1.13784600	1.94795200
H	-4.45533300	-4.49869700	4.13360900	H	-5.80662500	0.49566800	2.58553600
N	-4.25204100	-3.49425600	-0.16629700	O	-1.90834100	0.05173500	0.49442000
O	-4.25192400	-2.25495000	-0.95460100	C	-2.03844000	1.37601700	0.52528000
C	-3.33753100	-2.41494700	-2.03971700	C	-2.36438300	2.12576400	1.60507200
H	-3.66020400	-3.22132400	-2.71051000	H	-2.38620000	3.20585300	1.51733000
H	-3.36013600	-1.46754600	-2.58746300	C	-2.74103900	1.55167400	2.94188800
H	-2.32652500	-2.62721800	-1.67807300	H	-2.74625500	0.45767200	2.92037500
C	-5.38956400	-4.28107700	-0.62555700	H	-2.04450800	1.86642400	3.73263800
H	-6.36027500	-3.83400400	-0.36249900	H	-3.73987300	1.88535700	3.26128500
H	-5.32550900	-4.39397100	-1.71099800	N	-1.87809400	1.97077400	-0.78438800
H	-5.31881300	-5.27573800	-0.17930400	O	-0.63063500	1.44633400	-1.34957400
Li	-3.68685200	-0.70212400	0.41186400	C	-0.87587400	1.00076100	-2.67999000
O	-5.40772100	0.23419000	0.57128000	H	-1.59945300	0.17921800	-2.69188700
C	-6.21744600	-0.06456400	1.74151800	H	-1.24095700	1.82183300	-3.30885800
C	-7.64356500	0.34548800	1.36767800	H	0.09110000	0.65915000	-3.06111500

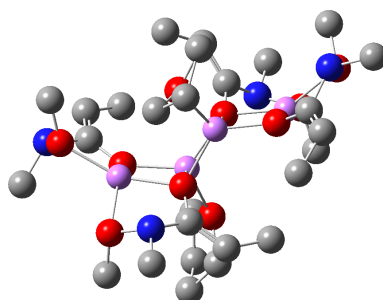
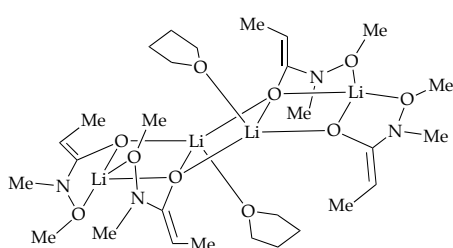
C	-1.78142600	3.42495600	-0.86728900	C	5.71409800	-1.67859400	-0.72674900
H	-0.98664300	3.83914300	-0.23143100	C	4.40715300	-0.97520900	-0.37306500
H	-1.58883700	3.69949600	-1.90760700	H	3.86779400	-0.65120100	-1.27272600
H	-2.74502800	3.84988500	-0.57583200	H	4.50648700	-0.12020800	0.29917300
O	0.23856500	-1.94414900	0.28831900	H	6.23982600	-1.19648200	-1.55651600
Li	1.90597800	-1.36324300	1.07671200	H	6.38569800	-1.69629800	0.14015100
O	1.61019700	0.46624100	0.79203300	H	4.83662600	-3.12869500	-2.08792500
C	2.30284500	1.13453400	1.68491200	H	6.00217600	-3.85940500	-0.97289600
C	3.07826400	2.22847500	1.50251000	H	4.43272900	-3.80421100	0.85861600
H	3.61916800	2.60550800	2.36542000	H	3.23744800	-3.86478200	-0.46477500
C	3.17529700	2.97845900	0.20475500	C	0.32910000	-3.21497100	-0.07719600
H	2.52406800	2.52669400	-0.54990600	C	0.48886800	-3.67300400	-1.34422900
H	2.87831000	4.03163900	0.31844300	H	0.47195000	-4.73975700	-1.53434400
H	4.20139600	2.98951500	-0.19428400	C	0.70665600	-2.76693600	-2.52490700
N	2.23524800	0.64075200	3.06680000	H	-0.19734300	-2.64338000	-3.14228300
O	2.36744300	-0.83307300	2.99119400	H	1.01722400	-1.76829200	-2.19937600
C	3.56663800	-1.20339600	3.66120800	H	1.48512800	-3.15855900	-3.19421000
H	4.43999400	-0.72736100	3.20144300	N	0.34577300	-4.10351100	1.05910800
H	3.51972600	-0.92752500	4.72097200	O	-0.75650800	-3.71330900	1.92719700
H	3.64451900	-2.29126000	3.56563400	C	-0.29320600	-3.59193200	3.27204800
C	0.91903400	0.85838800	3.66933100	H	-1.18368700	-3.34960200	3.85892100
H	0.10081600	0.41307100	3.08746800	H	0.12714600	-4.54001200	3.62995200
H	0.91608200	0.44649000	4.68317800	H	0.45609200	-2.79732500	3.36343300
H	0.76338800	1.93958700	3.72274700	C	0.19629000	-5.53484400	0.81248600
O	3.62413000	-1.98315600	0.31142800	H	1.08008300	-5.88924000	0.27602200
C	4.08376600	-3.30636900	-0.05437600	H	0.15359300	-6.04698300	1.77665500
C	5.22302800	-3.09652200	-1.06264600	H	-0.70773700	-5.77480400	0.23581500



**21**  
 $G = -2101.373672$   
 $G_{\text{MP2}} = -2095.375961$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	1.14780900	0.24642200	-1.51172700
Li	1.51103400	-1.61236500	-1.25986200	C	1.79453300	1.38065900	-1.49182900
O	3.26817900	-1.74396300	-0.66496100	C	2.03551700	2.22330400	-2.52699700
C	4.09417500	-2.56401600	-0.05582600	H	2.55272100	3.16019600	-2.35170200
C	4.78615500	-3.58347900	-0.63016300	C	1.62050200	1.91549000	-3.93817000
H	5.47173000	-4.17544900	-0.03494400	H	1.13808200	0.93532500	-3.98831800
C	4.57222700	-4.01907200	-2.05350600	H	0.90821600	2.65857200	-4.32619600
H	3.81994700	-3.39257400	-2.54110300	H	2.47528300	1.91243300	-4.63119400
H	5.49676300	-3.96506600	-2.64892800	N	2.35423800	1.66113000	-0.15755800
H	4.22544300	-5.06175300	-2.11703000	O	1.26948300	1.55451400	0.82587800
N	4.18623500	-2.33161900	1.37428200	C	0.37504700	2.68687300	0.82131200
O	4.29800300	-0.88101600	1.59210700	H	0.81926300	3.53845000	1.34816000
C	3.42609000	-0.51510300	2.66637100	H	0.10812300	2.96687600	-0.20255100
H	3.72176700	-1.01579900	3.59599000	H	-0.52059400	2.34962700	1.34464000
H	3.53889500	0.56600000	2.78735500	C	3.10565100	2.89838900	0.06032800
H	2.38876700	-0.76228600	2.42736200	H	2.56396300	3.80599300	-0.23454100
C	5.29121900	-2.94781600	2.09791800	H	3.35846200	2.95672400	1.12306500
H	6.27635800	-2.73102200	1.65786300	H	4.02760500	2.82736900	-0.51964500
H	5.27316600	-2.59650500	3.13282100	O	-0.14804600	-1.96208600	-0.12499600
H	5.13114300	-4.02834800	2.10744100	Li	-1.99116500	-1.44971200	-0.35354000
Li	3.67993700	-0.01419600	-0.15812600	O	-1.80939500	0.36967100	0.06763200
O	5.33351000	0.65219700	-1.06342800	C	-2.92150800	0.81813600	0.59081300
C	5.40876700	0.19177000	-2.44699500	C	-3.56975000	1.96106900	0.23622600
C	6.87547400	-0.18314900	-2.68801600	H	-4.50448800	2.22794900	0.71475400
C	7.36872100	-0.52605300	-1.27344400	C	-3.01940100	2.93046700	-0.77328500
C	6.62599400	0.50665800	-0.43022200	H	-2.14373400	2.50760900	-1.27412000
H	7.13876100	1.47910000	-0.43704400	H	-3.76220800	3.17631500	-1.54653400
H	6.45217100	0.19776700	0.60346200	H	-2.72037500	3.89020800	-0.32204400
H	8.45550600	-0.45733500	-1.16329900	N	-3.42656700	-0.00599700	1.67747700
H	7.04427300	-1.53496200	-0.99405600	O	-3.33881400	-1.40592600	1.24445900
H	7.43377800	0.66982100	-3.09239700	C	-2.87525300	-2.19482400	2.34147700
H	6.97429200	-1.01636600	-3.38974000	H	-1.93230700	-1.80106200	2.72700600
H	4.74101300	-0.67025500	-2.53547200	H	-3.62043000	-2.22962800	3.14637400
H	5.04842400	0.99670100	-3.09342000	H	-2.72555700	-3.20309700	1.94445200

C	-4.80274200	0.21390100	2.10724800	C	0.05755000	-3.27260200	-0.07509300
H	-5.52647600	0.17488700	1.27939400	C	0.39826500	-3.99728900	1.01602300
H	-5.06456500	-0.54122000	2.85273400	H	0.60540600	-5.05581700	0.90775500
H	-4.85729400	1.19299800	2.58903600	C	0.58866900	-3.41049600	2.38509200
O	-3.15531800	-1.75218100	-1.92591800	H	0.29153900	-2.35798900	2.40351700
C	-3.66311700	-0.58794500	-2.63666800	H	0.00854300	-3.94370500	3.15287400
C	-4.88221700	-1.08390700	-3.41877100	H	1.64405100	-3.45663600	2.68750200
C	-5.38699000	-2.23862900	-2.53870200	N	-0.17183300	-3.90188900	-1.36284300
C	-4.07644000	-2.85525500	-2.04988000	O	0.67453500	-3.18454100	-2.32494700
H	-3.67232700	-3.57688900	-2.77205900	C	-0.11121500	-2.80544400	-3.45497000
H	-4.15785300	-3.34168400	-1.07327100	H	0.56662000	-2.25005600	-4.11014100
H	-6.01356200	-2.95617000	-3.07724800	H	-0.48004800	-3.69252000	-3.98588100
H	-5.96055000	-1.84826500	-1.69011500	H	-0.95279000	-2.17833500	-3.15026600
H	-4.58685300	-1.45901600	-4.40610500	C	0.16711700	-5.31432400	-1.50379200
H	-5.62658100	-0.29557800	-3.56506000	H	-0.50948000	-5.89378200	-0.87006600
H	-3.92532200	0.17448600	-1.89614400	H	-0.00196100	-5.60707100	-2.54342800
H	-2.85988900	-0.20382200	-3.27174700	H	1.20807500	-5.53621400	-1.23073600



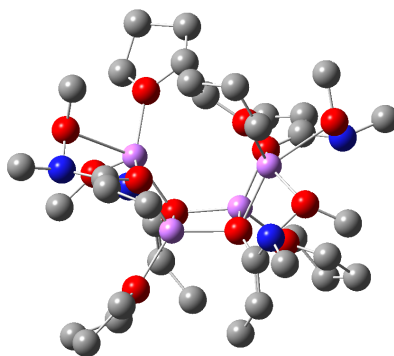
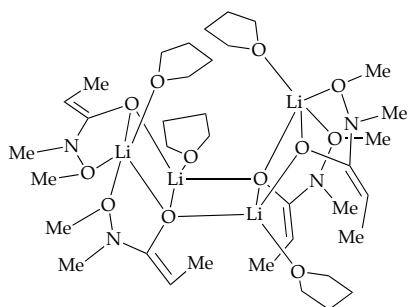
**22**

$G = -2101.378036$

$G_{MP2} = -2095.385319$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	3.09646500	-0.97570700	-0.24339600
Li	2.31137200	1.35792000	0.49850600	O	1.65013400	-0.47137900	0.95775300
O	3.80499500	0.74992500	-0.54653200	C	1.58488300	-1.31623100	1.97934100
C	4.40341700	0.82137700	-1.71671600	C	1.08091800	-1.07705900	3.21478300
C	4.64455800	1.89283000	-2.50738300	H	1.13899500	-1.86410400	3.95968500
H	5.13290700	1.69404900	-3.45665400	C	0.36738600	0.18036000	3.62504500
C	4.34551200	3.32166100	-2.15855000	H	0.78702200	0.59078100	4.55479300
H	3.63116900	3.39296500	-1.33397400	H	0.43862800	0.94812600	2.85047400
H	5.25073400	3.88169200	-1.86977800	H	-0.70056500	0.00302300	3.80763600
H	3.90914900	3.85641800	-3.01303800	N	2.07581500	-2.62498400	1.61918400
N	4.94316300	-0.43933800	-2.24870500	O	3.43098700	-2.50269300	1.08677300
O	3.95027900	-1.49297400	-1.97994800	C	4.42415900	-2.19480400	2.07916700
C	3.30864000	-1.82534000	-3.20837300	H	4.11718500	-1.34047200	2.69250000
H	4.03650300	-2.21864400	-3.92625100	H	4.62721300	-3.06060600	2.71862300
H	2.57188700	-2.59642500	-2.96384600	H	5.32553300	-1.94572800	1.51499000
H	2.80534200	-0.95135400	-3.63576500	C	1.99816200	-3.73241500	2.55724200

H	0.94084000	-3.92433500	2.75375400	H	0.09783300	1.69715700	-4.12899800
H	2.43449000	-4.61207400	2.07651700	C	0.49647300	5.45708800	-1.09597100
H	2.50321000	-3.55801500	3.51998500	H	-0.41202600	5.48710500	-1.71545800
C	6.14975300	-0.87493400	-1.54835100	H	0.46765700	6.28018300	-0.37730700
H	6.00640600	-0.98252100	-0.46153300	H	1.37418100	5.58865800	-1.73311900
H	6.48553100	-1.82921300	-1.96404600	C	0.03877500	4.51068800	1.90222700
H	6.91543300	-0.11498900	-1.72627100	H	-0.81917900	4.42914500	2.57731300
O	0.60885700	1.90575500	-0.29951700	H	0.84324400	3.83459200	2.20652800
Li	-1.13737600	2.22368500	0.50777900	H	0.40124100	5.54600700	1.90808800
O	-1.64350700	0.47322200	0.76178600	O	3.07386100	2.48223900	2.04009200
C	-2.92683100	0.29282200	0.95952300	C	3.39113900	1.93975100	3.34172600
C	-3.50400100	-0.65487300	1.74277400	C	4.86890800	2.25439800	3.56794100
H	-4.58040400	-0.67361100	1.86354900	C	5.01005900	3.60793600	2.85467800
C	-2.72903500	-1.72906400	2.45243100	C	4.10540600	3.42194600	1.63365600
H	-1.65879300	-1.64888100	2.24153000	H	4.64363200	2.97947400	0.79061100
H	-2.85355300	-1.67231600	3.54491600	H	3.61447300	4.34144200	1.30266500
H	-3.05961000	-2.73885900	2.16119500	H	6.04032200	3.84504200	2.57286300
N	-3.75855300	1.18323300	0.15946200	H	4.63909400	4.41614500	3.49661900
O	-3.16203000	2.52542500	0.24199200	H	5.49910600	1.50033600	3.08168100
C	-3.30628200	3.18030100	-1.02053000	H	5.13244100	2.29097900	4.62955900
H	-2.78610900	2.62857200	-1.81126900	H	2.76111100	2.43339800	4.09447500
H	-4.36259000	3.29920800	-1.28894400	H	3.14856800	0.87464400	3.33237400
H	-2.85557100	4.16680000	-0.88829500	O	-0.36096500	-1.33199100	-1.48300900
C	-5.15580200	1.32379400	0.56049300	C	-1.59956100	-1.12384900	-2.21556700
H	-5.27347600	1.57249600	1.62481300	C	-2.36014400	-2.46650600	-2.18722400
H	-5.62448700	2.10129600	-0.04761900	C	-1.60489100	-3.28585500	-1.12417000
H	-5.66717900	0.38232900	0.34775300	C	-0.18495700	-2.74518300	-1.26412300
O	-0.45523600	4.15638800	0.60738100	H	0.32310800	-3.19088500	-2.13398100
N	0.65263300	4.20761500	-0.36099500	H	0.44814200	-2.86561300	-0.38146800
C	0.61422600	2.96367000	-1.10358400	H	-1.66649400	-4.36591300	-1.29195600
C	0.63011700	2.95630200	-2.45756500	H	-1.98969300	-3.06404500	-0.12369400
H	0.59771900	3.89917000	-2.99181000	H	-2.30461100	-2.96292800	-3.16284900
C	0.80999300	1.71991100	-3.29192500	H	-3.41615300	-2.32963000	-1.93935900
H	1.81988000	1.67089400	-3.72563200	H	-2.13845500	-0.32213300	-1.70650100
H	0.66585800	0.81299400	-2.69912300	H	-1.35471200	-0.80490100	-3.23498200

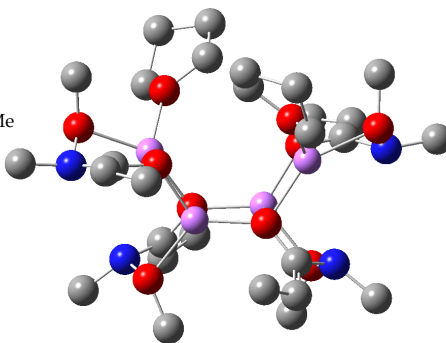
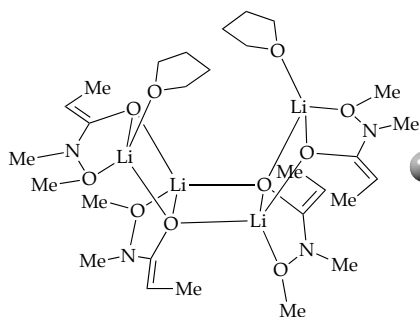


**23**  
 $G = -2566.058157$   
 $G_{\text{MP2}} = -2558.768773$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.39470800	0.97105900	3.82727300
O	0.81873600	-1.71186700	0.28026000	H	-3.85991800	0.20994700	4.46025100
C	1.97019900	-1.87466100	0.88608800	H	-2.50706400	1.35791400	4.33290200
C	2.22094600	-1.78765600	2.22147800	H	-4.10622500	1.80113100	3.68905200
H	3.21542200	-2.01060900	2.59268100	O	-3.17973500	-1.69618800	-1.18376700
C	1.20392800	-1.35461400	3.24008100	C	-4.27286600	-2.07829900	-1.79796100
H	0.22568600	-1.18707600	2.77889300	C	-4.40083300	-2.41451900	-3.11281300
H	1.07676200	-2.10458300	4.03598900	H	-5.35752900	-2.77222400	-3.47808700
H	1.49089500	-0.42310900	3.75354500	C	-3.30070900	-2.27760300	-4.12938000
N	3.06570800	-2.10498900	-0.03792200	H	-2.36009600	-1.96408200	-3.66680100
O	2.68482100	-3.10120800	-1.01535100	H	-3.11147200	-3.22564700	-4.65630600
C	2.52649300	-4.41565000	-0.46384100	H	-3.54395400	-1.54583300	-4.91677200
H	1.96414900	-4.97344200	-1.21392000	N	-5.44118900	-2.06616700	-0.93978600
H	3.49685100	-4.89735900	-0.28902700	O	-5.15470300	-2.74888300	0.30144200
H	1.95892800	-4.37978100	0.47302700	C	-4.97180200	-4.16108200	0.14994800
Li	0.65020800	-2.09230100	-1.61276200	H	-4.48811700	-4.48710700	1.07217500
O	-0.31788400	-0.19410700	-1.95208300	H	-5.92972900	-4.68351500	0.02999100
Li	-2.22933600	-0.04696200	-1.37277100	H	-4.32329200	-4.38377600	-0.70502800
Li	-3.03701700	-1.54902200	0.71614100	C	-6.73463900	-2.48309100	-1.45663300
N	-2.96450400	0.32603800	2.59899500	H	-7.45886000	-2.42233300	-0.63931400
C	-2.29191800	1.07507400	1.55891700	H	-7.02821000	-1.78080000	-2.24068300
O	-1.88407600	0.30585600	0.56559400	H	-6.75497800	-3.50027500	-1.88020800
C	-2.12143400	2.41536000	1.72151000	O	-2.51583000	-3.03376700	2.01938100
H	-2.60477800	2.89163900	2.56787600	C	-3.03970400	-3.02981500	3.36526700
C	-1.30520800	3.32010900	0.84363100	C	-2.48993900	-4.29937500	4.01403800
H	-0.64775300	2.75679100	0.17914500	C	-1.10329200	-4.40605800	3.36082400
H	-1.93199100	3.97320700	0.21694000	C	-1.37491500	-3.92357400	1.93214200
H	-0.67299700	3.99232800	1.44229000	H	-1.65468300	-4.76240200	1.28237000
O	-4.06516100	-0.42950500	2.02858800	H	-0.54656200	-3.37369300	1.47675900
C	-5.16997300	0.36867300	1.56837300	H	-0.68877000	-5.41891600	3.38398200
H	-5.70825800	-0.27024500	0.86662600	H	-0.39614100	-3.73853600	3.86228400
H	-5.81895900	0.65586900	2.40426900	H	-3.10949400	-5.16641700	3.75187500
H	-4.80949500	1.26500500	1.05375700	H	-2.45125200	-4.22799400	5.10568600



H -2.68679500 -2.12699400 3.87697200 H 1.39733200 0.00046700 -5.69913000  
H -4.12966600 -2.99244200 3.29937400 O -0.12277500 -3.88139300 -2.28339700  
O -3.41978400 1.37080100 -2.24866100 C 0.05292900 -4.36151300 -3.63212300  
C -4.02754200 1.23405600 -3.55710400 C -0.63603700 -5.72477600 -3.66279400  
C -5.09563900 2.34288100 -3.65996700 C -1.82958000 -5.49582600 -2.72163400  
C -5.26833300 2.80335900 -2.20096700 C -1.24604300 -4.55187600 -1.66094400  
C -3.85912900 2.60103300 -1.65302800 H -0.85962400 -5.10740000 -0.79791700  
H -3.79128100 2.48527900 -0.56980300 H -1.95197700 -3.78913800 -1.32252400  
H -3.19546900 3.42221500 -1.96136200 H -2.21451800 -6.42249100 -2.28356500  
H -5.97433100 2.15488100 -1.66944200 H -2.65124500 -5.00534100 -3.25174900  
H -5.61488700 3.83809700 -2.11453800 H 0.02943300 -6.49996900 -3.26239300  
H -6.02576000 1.97835700 -4.10622600 H -0.93281200 -6.02124500 -4.67392500  
H -4.73373300 3.17330600 -4.27687700 H -0.41458400 -3.65444700 -4.32689900  
H -3.24727600 1.33082000 -4.32006000 H 1.12553200 -4.39665500 -3.83598400  
H -4.45503100 0.23004300 -3.60319700 C 4.40201400 -2.38286500 0.46500100  
C 0.02317800 0.20361700 -3.16444000 H 5.05382200 -2.56895200 -0.39318300  
C 0.05393800 1.46948000 -3.65813200 H 4.75805900 -1.49342000 0.99048500  
H 0.41872600 1.62134700 -4.66886900 H 4.46258100 -3.23862500 1.15624500  
C -0.39899500 2.69860700 -2.92682400 O 1.40598200 1.41461200 0.38446800  
H -0.77825400 2.45106400 -1.93471900 C 1.82065700 1.91291900 1.66556100  
H 0.42074100 3.42260300 -2.79890100 C 2.73028900 3.09013200 1.32184200  
H -1.19606500 3.23144700 -3.46727800 C 3.49758000 2.55226500 0.09619900  
N 0.36336700 -0.90612700 -4.02940400 C 2.52624000 1.51973100 -0.52589400  
O 1.47424500 -1.64351100 -3.44624600 H 2.98608900 0.53170900 -0.63549900  
C 2.73858500 -0.96289700 -3.50710300 H 2.11827600 1.83193900 -1.49035500  
H 3.37218700 -1.48665400 -2.79083300 H 4.42595200 2.06296300 0.41047600  
H 3.17273100 -1.03012200 -4.51186200 H 3.76541100 3.34497400 -0.60875700  
H 2.62906100 0.08751500 -3.21951600 H 3.38954000 3.37507900 2.14792000  
C 0.58777400 -0.70402400 -5.44953600 H 2.12310200 3.96036200 1.04906800  
H 0.81758600 -1.67640800 -5.89512400 H 0.91695300 2.17718900 2.21844900  
H -0.34179500 -0.32817700 -5.88323400 H 2.36391500 1.12762700 2.20794000



**24**  
 $G = -2101.366869$   
 $G_{\text{MP2}} = -2095.368141$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.56043900	1.75750200	3.66819600
Li	-2.03480800	1.72675200	0.00371400	H	-2.16810100	0.71523600	3.23088200
O	-3.05827600	1.90215500	-1.56802500	C	-4.84129900	-0.25696800	2.20981500
C	-4.27734800	2.39892700	-1.65426900	H	-5.58159500	0.54711100	2.18520400
C	-4.61976900	3.70660400	-1.78654500	H	-5.29681500	-1.16681400	1.81246500
H	-5.66329000	3.97502800	-1.90854600	H	-4.54430700	-0.44445700	3.25463200
C	-3.63707900	4.83811600	-1.69322100	O	-2.49928300	-1.34873200	-2.93477700
H	-2.62134900	4.45823900	-1.54565900	C	-2.84257600	-2.74142800	-2.83270300
H	-3.63325500	5.46200500	-2.60137200	C	-2.43875000	-3.33173700	-4.18106500
H	-3.86264100	5.51816500	-0.85720700	C	-1.13160100	-2.57230500	-4.47510700
N	-5.30427600	1.39383200	-1.51337500	C	-1.35719300	-1.19392600	-3.82350800
O	-4.97715100	0.22779800	-2.30955200	H	-1.63164800	-0.42648400	-4.55627900
C	-5.04730800	0.46107500	-3.72622100	H	-0.49772700	-0.85322500	-3.23746900
H	-4.53319000	-0.38635500	-4.18230300	H	-0.91900600	-2.49336700	-5.54554300
H	-6.08796200	0.49484700	-4.06867800	H	-0.28519500	-3.07937800	-4.00232100
H	-4.53840100	1.39486100	-3.99064200	H	-3.20223500	-3.10554800	-4.93508800
C	-6.70596400	1.73667600	-1.66721000	H	-2.30518100	-4.41723000	-4.14425400
H	-7.29165100	0.82018000	-1.55627400	H	-2.28469800	-3.20445500	-2.00704700
H	-6.97228800	2.42250200	-0.85951900	H	-3.91292200	-2.80049700	-2.61511800
H	-6.95975900	2.21705200	-2.62671700	O	-0.14515900	2.04451800	0.08306800
Li	-3.04362400	-0.01657200	-1.54453200	Li	1.00709800	1.75088600	-1.54080300
O	-1.88987200	-0.31766400	0.07744200	O	1.02311300	-0.16782700	-1.57279100
C	-2.65166200	-0.76784200	1.06744000	C	2.24258100	-0.66322300	-1.66148500
C	-2.51901800	-1.94613000	1.72680600	C	2.58609700	-1.96998900	-1.79974700
H	-3.18710100	-2.15952700	2.55548000	H	3.62982300	-2.23690800	-1.92326200
C	-1.54679100	-3.02298800	1.33244000	C	1.60446400	-3.10280300	-1.71129800
H	-1.03387600	-2.76505300	0.40049000	H	0.58860000	-2.72460600	-1.56036700
H	-0.77274300	-3.19462300	2.09640100	H	1.59995200	-3.72182100	-2.62278100
H	-2.04903200	-3.99020700	1.18352100	H	1.83171400	-3.78713700	-0.87925600
N	-3.75636700	0.11144200	1.32304200	N	3.26870900	0.34203000	-1.51613900
O	-3.27266500	1.45041000	1.61532000	O	2.94076800	1.51137300	-2.30705000
C	-2.75145400	1.59693000	2.94653100	C	3.01087900	1.28443300	-3.72474800
H	-2.10166400	2.47480100	2.91800600	H	2.49681100	2.13393900	-4.17699200

H	4.05151400	1.25212900	-4.06738400	H	1.87537700	4.53947700	-2.59899400
H	2.50186500	0.35189800	-3.99334500	C	0.61605000	2.48988400	1.07571000
C	4.67070000	0.00102600	-1.67125800	N	1.72039600	1.60922300	1.32813400
H	5.25562500	0.91748200	-1.55604100	O	1.23627200	0.26899800	1.61383300
H	4.93741400	-0.68825900	-0.86665000	C	0.71307400	0.11670600	2.94362800
H	4.92511800	-0.47476000	-2.63289100	H	0.06328400	-0.76099600	2.91035900
O	0.46207400	3.08880100	-2.92511600	H	1.52097000	-0.04701200	3.66580000
C	0.80518700	4.48113100	-2.81753900	H	0.12934600	0.99722200	3.23081600
C	0.40222500	5.07658000	-4.16390700	C	2.80447600	1.97342800	2.21770900
C	-0.90456600	4.31805300	-4.46182500	H	3.54461100	1.16929200	2.19032300
C	-0.67911000	2.93717200	-3.81555000	H	3.26061000	2.88493600	1.82490900
H	-0.40373200	2.17277400	-4.55116400	H	2.50640400	2.15631300	3.26304000
H	-1.53894000	2.59381300	-3.23161500	C	0.48301300	3.66507000	1.74051200
H	-1.11645200	4.24330000	-5.53270100	H	1.15054400	3.87456600	2.57061800
H	-1.75137100	4.82309600	-3.98757900	C	-0.48890400	4.74379400	1.35055700
H	1.16628500	4.85348300	-4.91827300	H	-1.00316000	4.48898400	0.41850200
H	0.26842300	6.16189500	-4.12297100	H	-1.26179100	4.91364300	2.11607300
H	0.24672100	4.94101700	-1.99052700	H	0.01377600	5.71114700	1.20386600

### **Part 3: Full References**

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