Evans Enolates: Solution Structures of Lithiated Oxazolidinone-Derived Enolates

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Part 2: Uncharacterized/oligomerized substrates

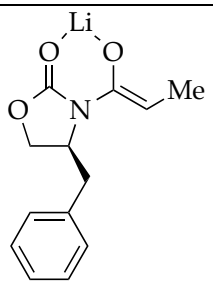
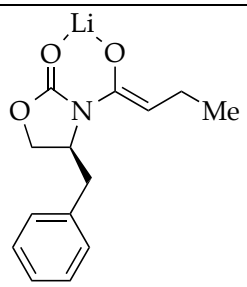
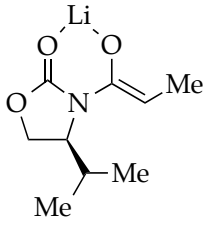
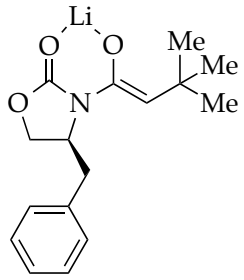
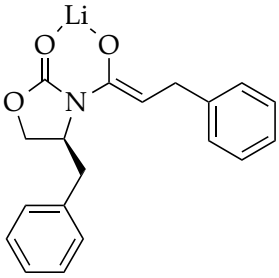
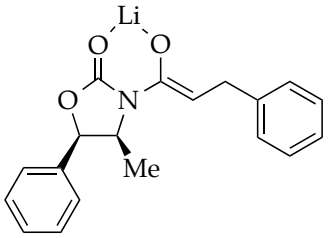
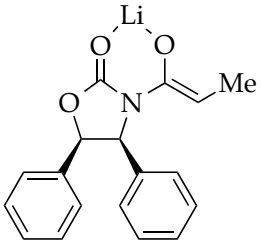
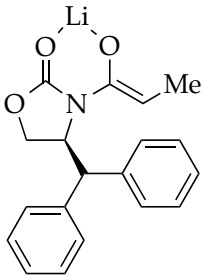
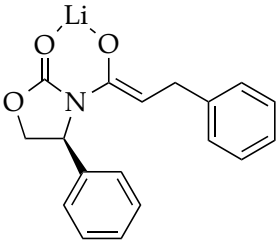
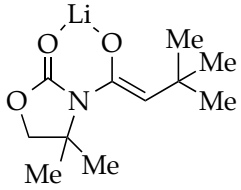
Part 3: Solvation Studies of 5 and 6

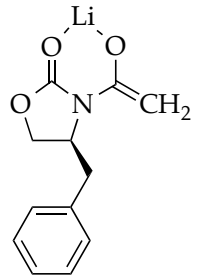
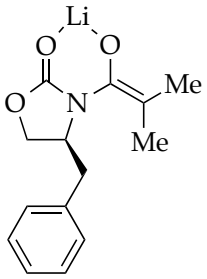
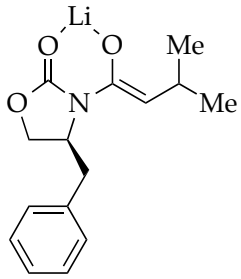
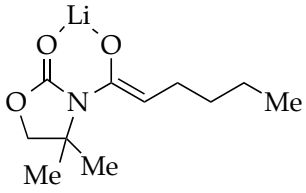
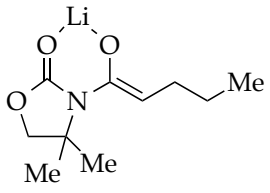
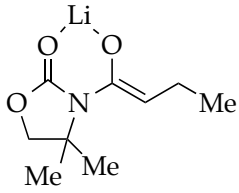
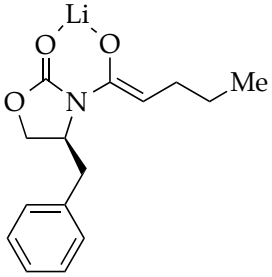
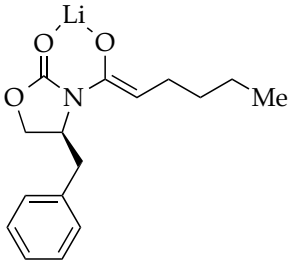
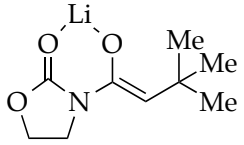
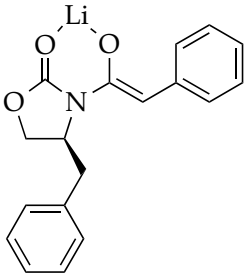
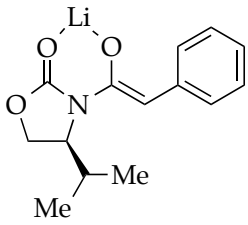
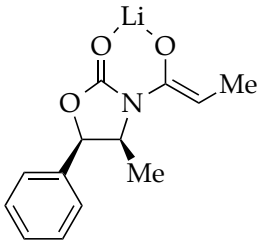
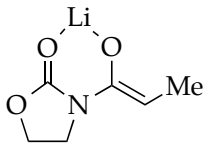
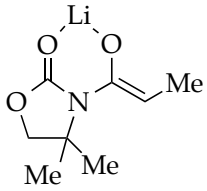
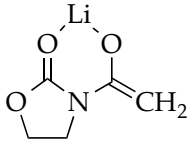
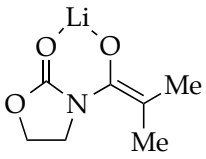
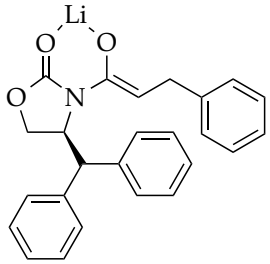
Part 4: Aggregation Studies of 5 and 6

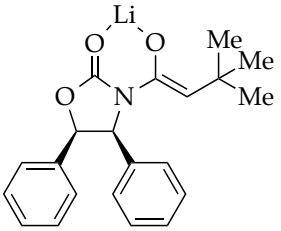
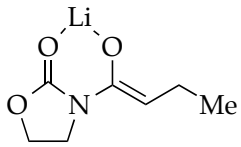
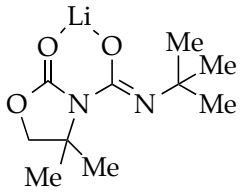
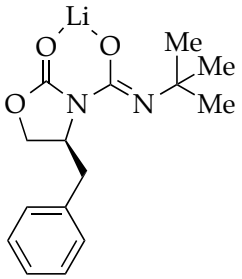
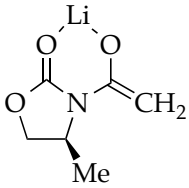
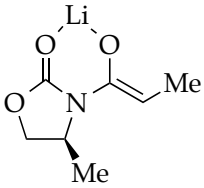
Part 5: Dimer Computations

Part 7: 6 Ground State Computations

Chart 1. Substrates

Dimer/ Tetramer mix	 **5**	 **6**		
Dimer in neat THF, oligomer at low THF	 **10**			
Dimers except under unusual conditions (low DMEA or TMCDA in toluene)	 **7**			
Dimers	 **8**	 **12**	 **15**	 **16**
	 **17**	 **18**		

Sharp undetermined aggregate that ages to oligomer	 **24**			
Sharp but undetermined aggregates	 **22**	 **23**	 **25**	 **26**
	 **27**	 **28**	 **29**	 **33**
Oligomers	 **9**	 **11**	 **13**	 **14**
	 **19**	 **30**	 **35**	 **40**

	 **41**	 **42**	 **43**	 **44**
Computations Only	 **31**	 **32**		

Part 1: Dimer Characterization

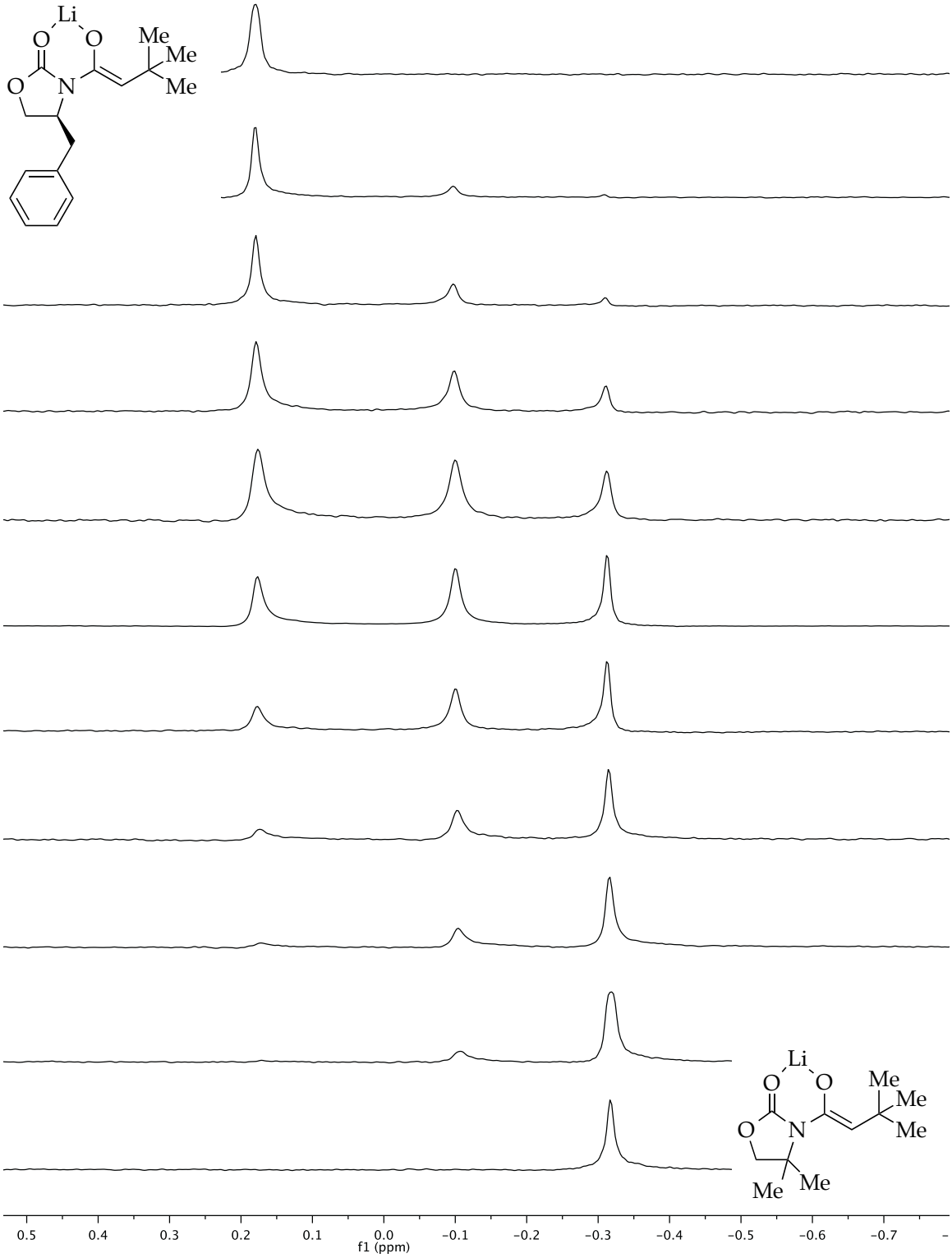


Figure 1. ^{6}Li NMR spectra of the method of continuous variation of **7**/**18** dimers (0.10 M total oxazolidinone, 0.105 M [^{6}Li]LDA) in neat THF at –80 °C.

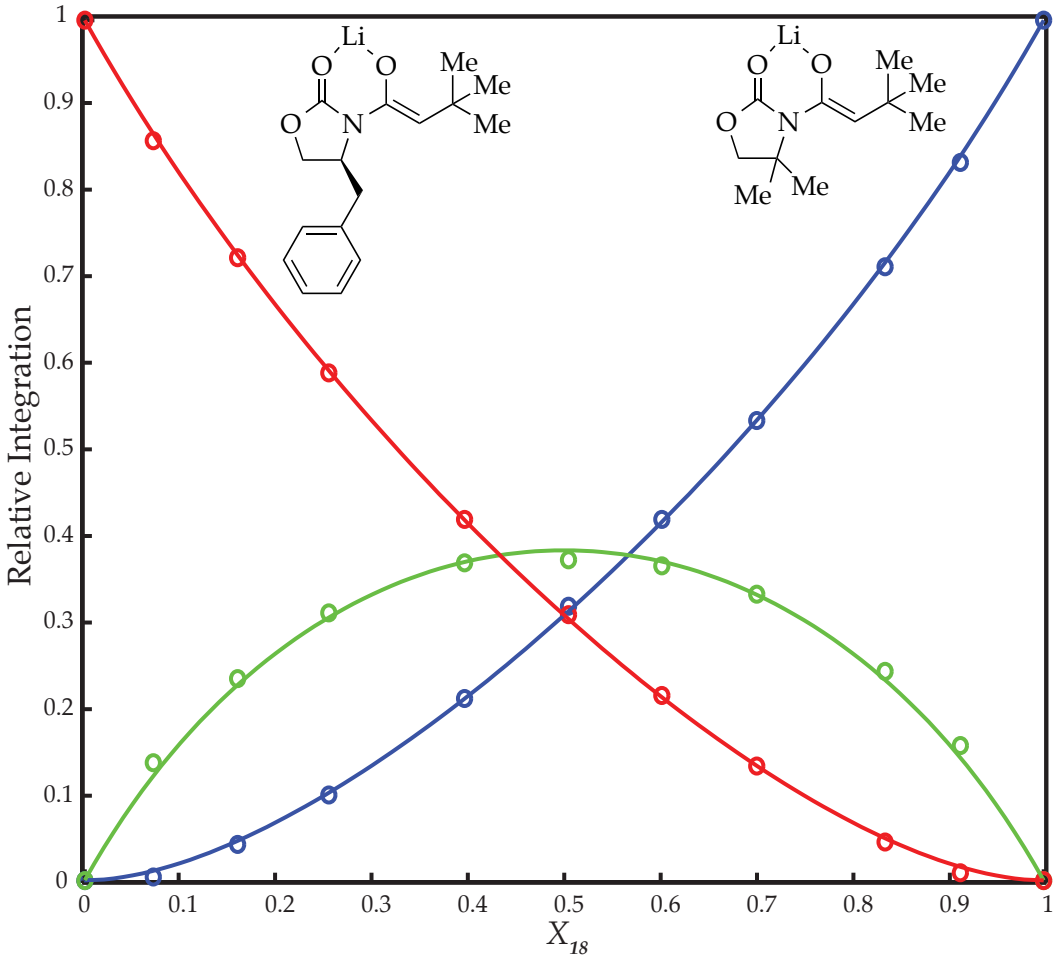


Figure 2. Job plot of **7** and **18** dimers (0.10 M total oxazolidinone, 0.105 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations are plotted as a function of the mole fraction of **18**.

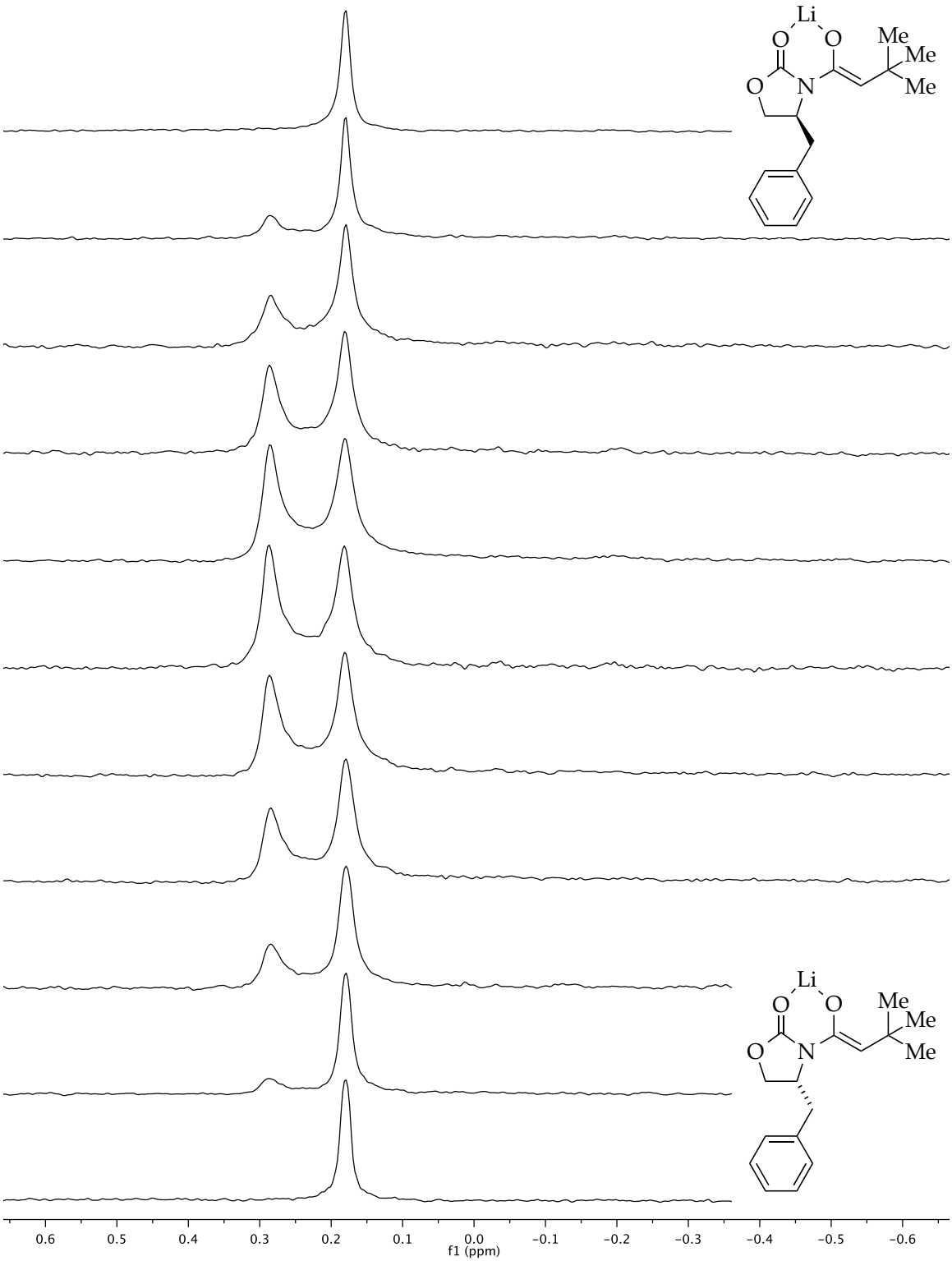


Figure 3. ^{6}Li NMR spectra of the method of continuous variation of **(S)-7**/**(R)-7** dimers (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

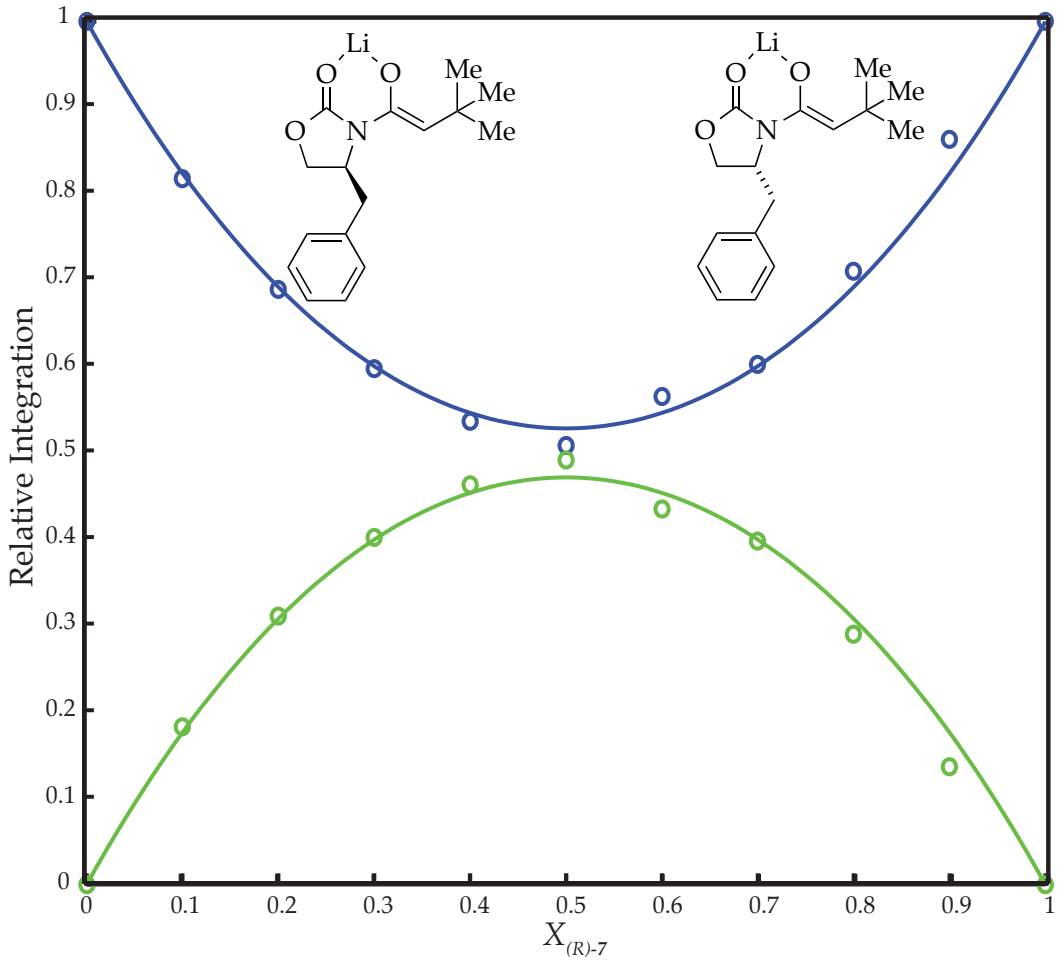


Figure 4. Job plot of **(*S*)-7**/**(*R*)-7** dimers (0.10 M total substrate, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **(*R*)-7**.

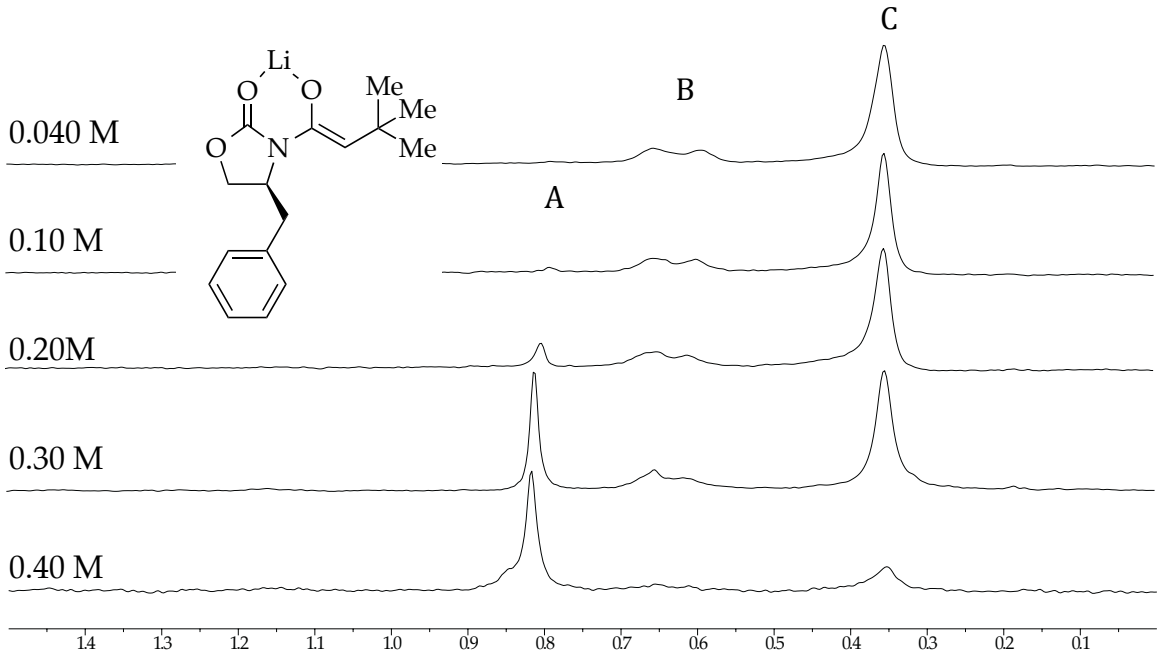


Figure 5. ^{6}Li NMR spectra of **7** at varying enolate concentrations (as labeled) in neat THF at –100 °C. **A** is an unknown higher aggregate; **B** is a pair of 1:1 peaks that are both dimers, **C** is a dimer. Mixed aggregate appears far downfield (>2.0 ppm).

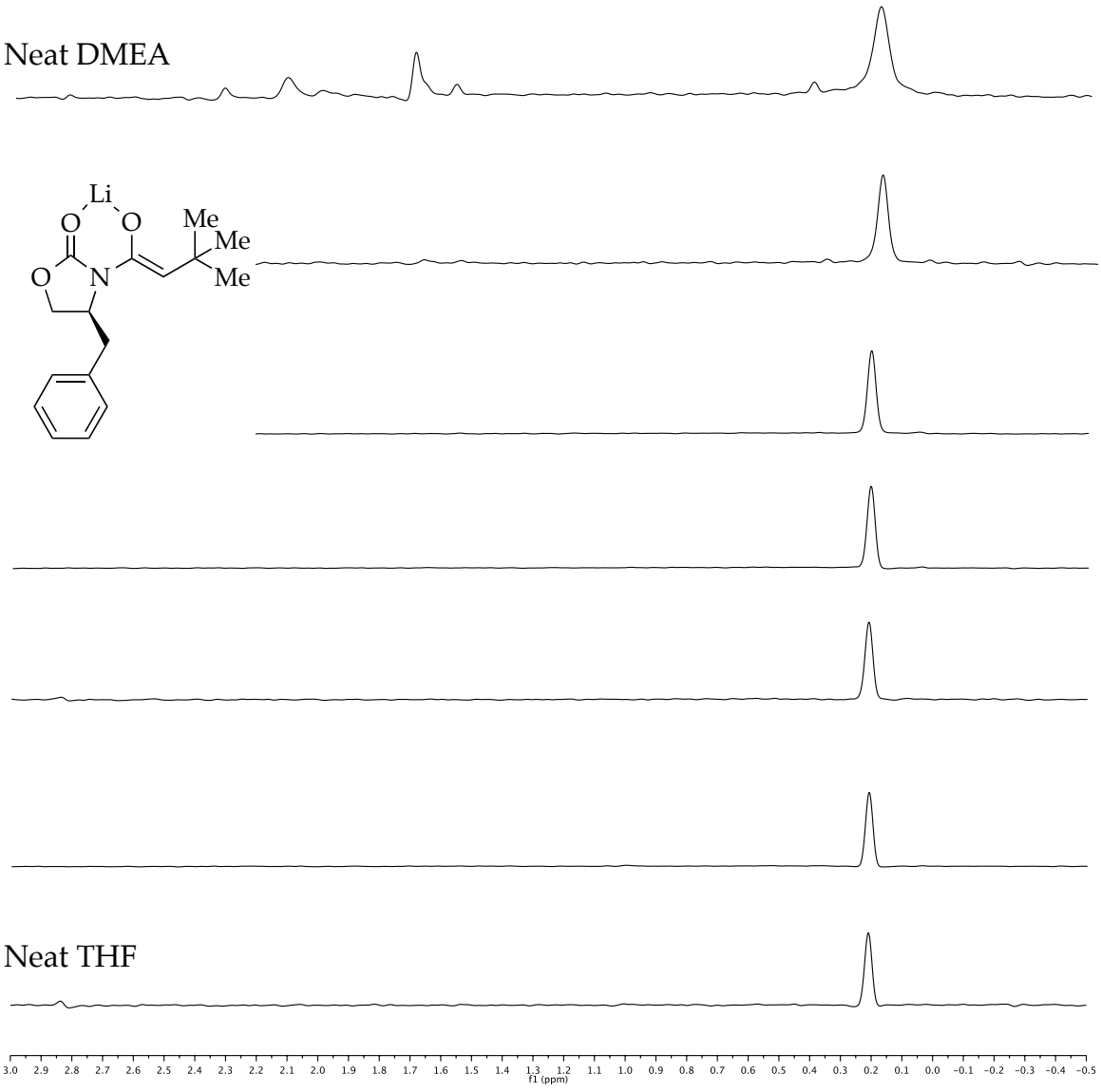


Figure 6. ^{6}Li NMR spectra of a solvent swap between DMEA and THF with **7** at 0.10 M and –80 °C.

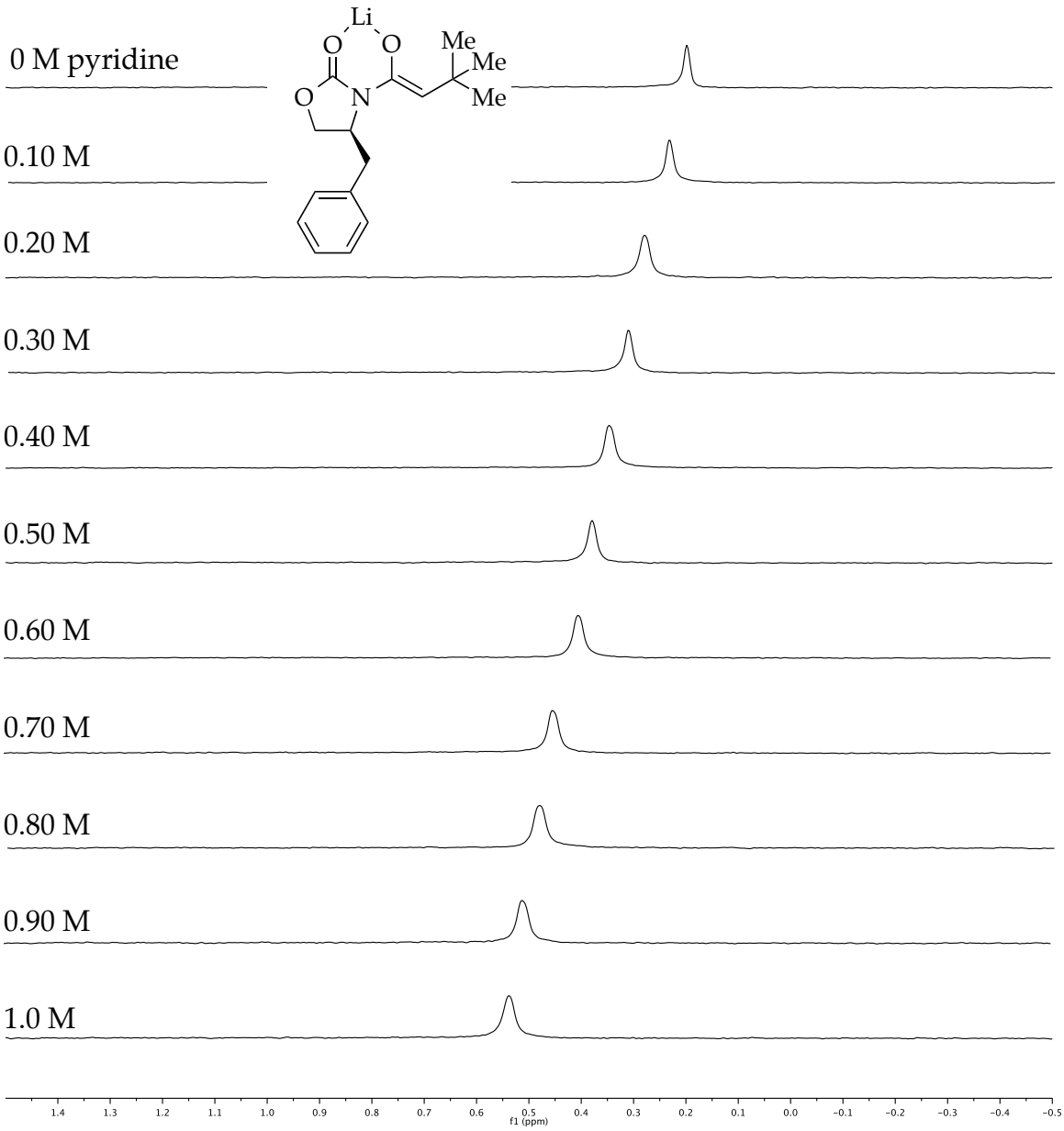


Figure 7. ^{6}Li NMR spectra of the solvation of **7** with pyridine in neat THF at 0.10 M and –80 °C.

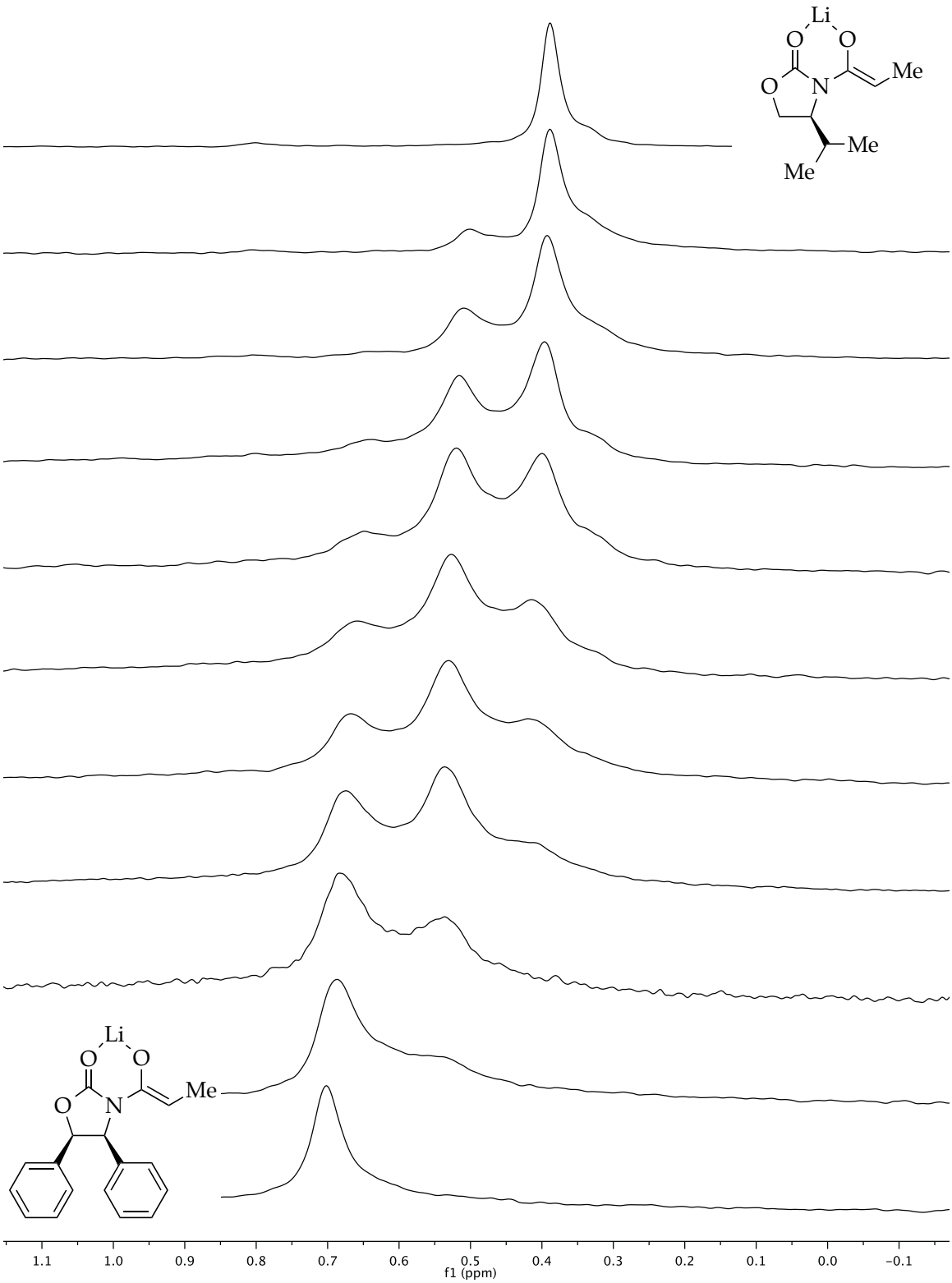


Figure 8. ^{6}Li NMR spectra of the method of continuous variation of **10** and **15** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

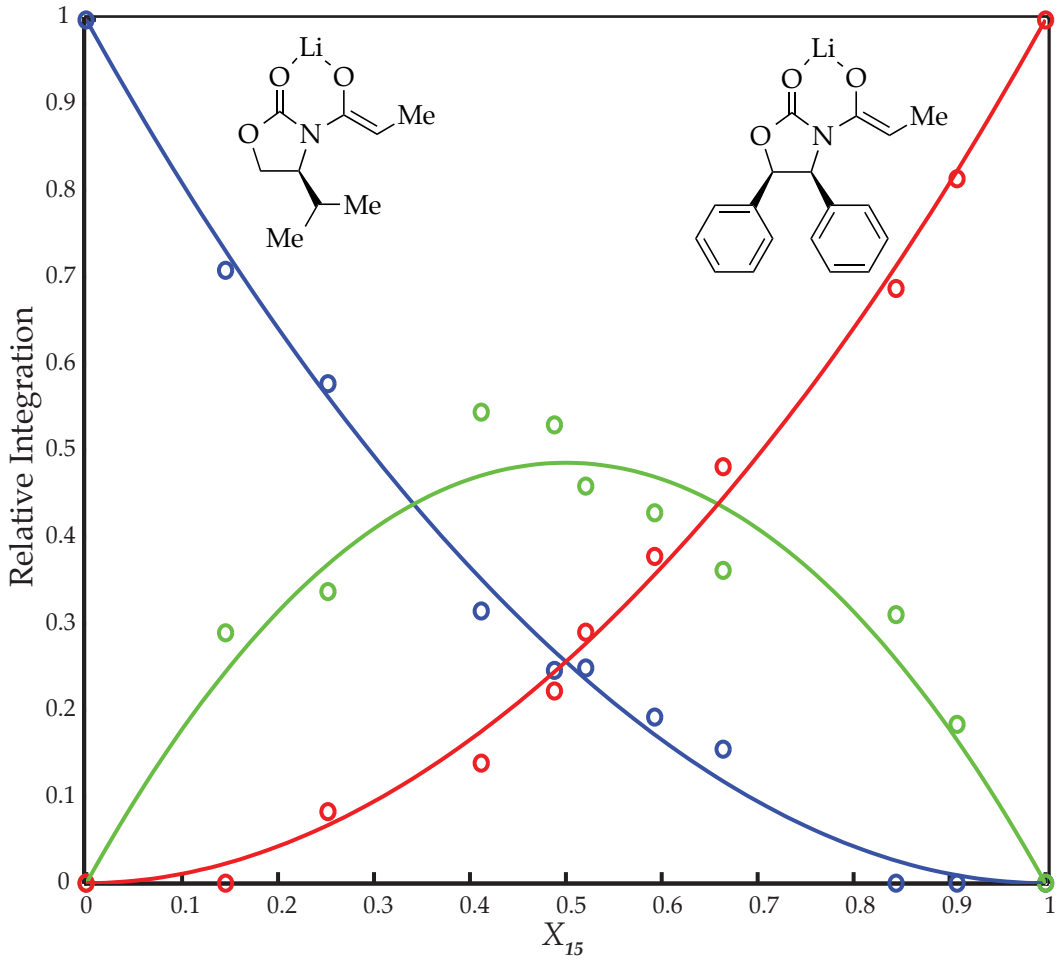


Figure 9. Job plot of **10** and **15** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **15**.

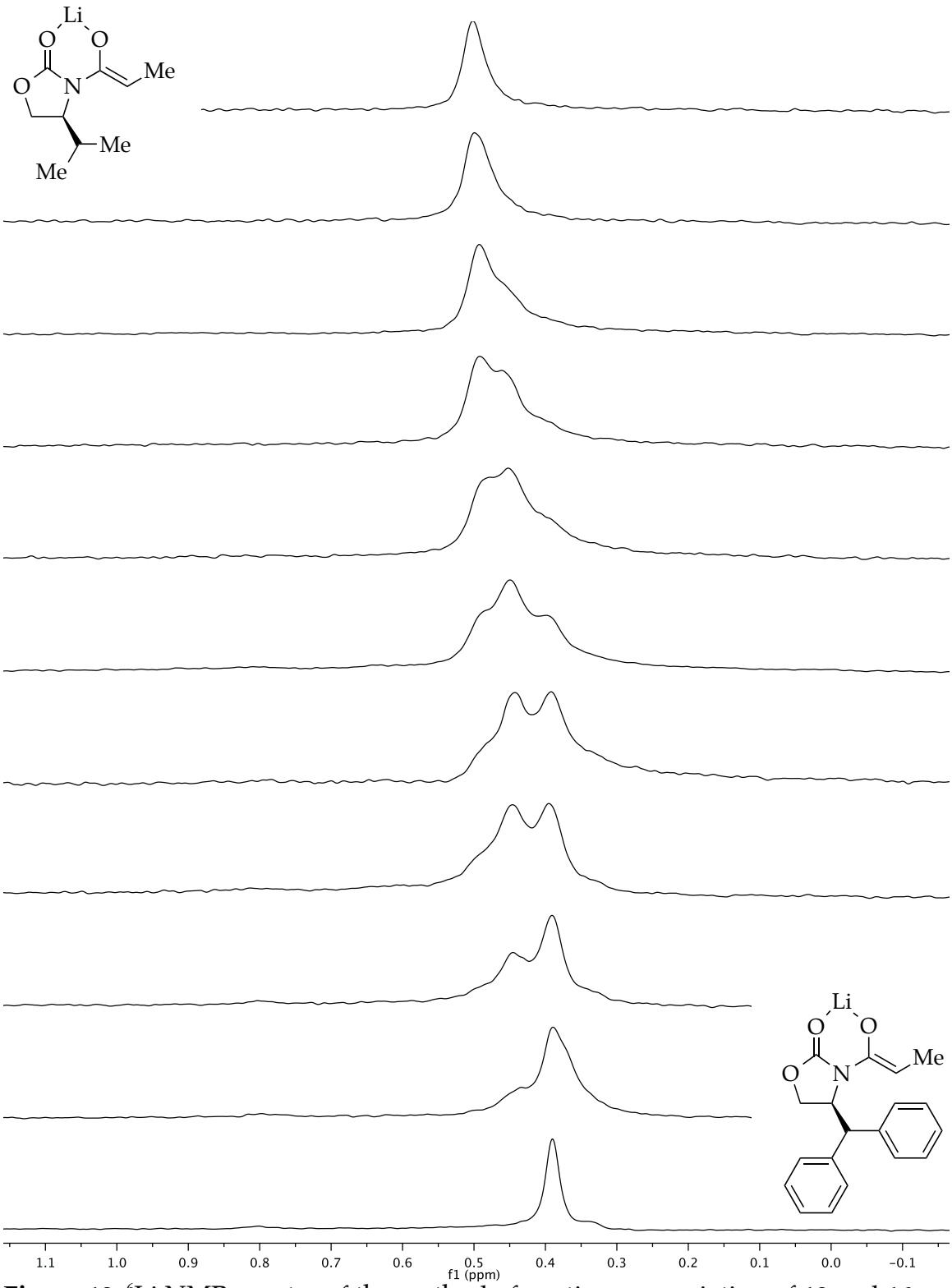


Figure 10. ^{6}Li NMR spectra of the method of continuous variation of **10** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

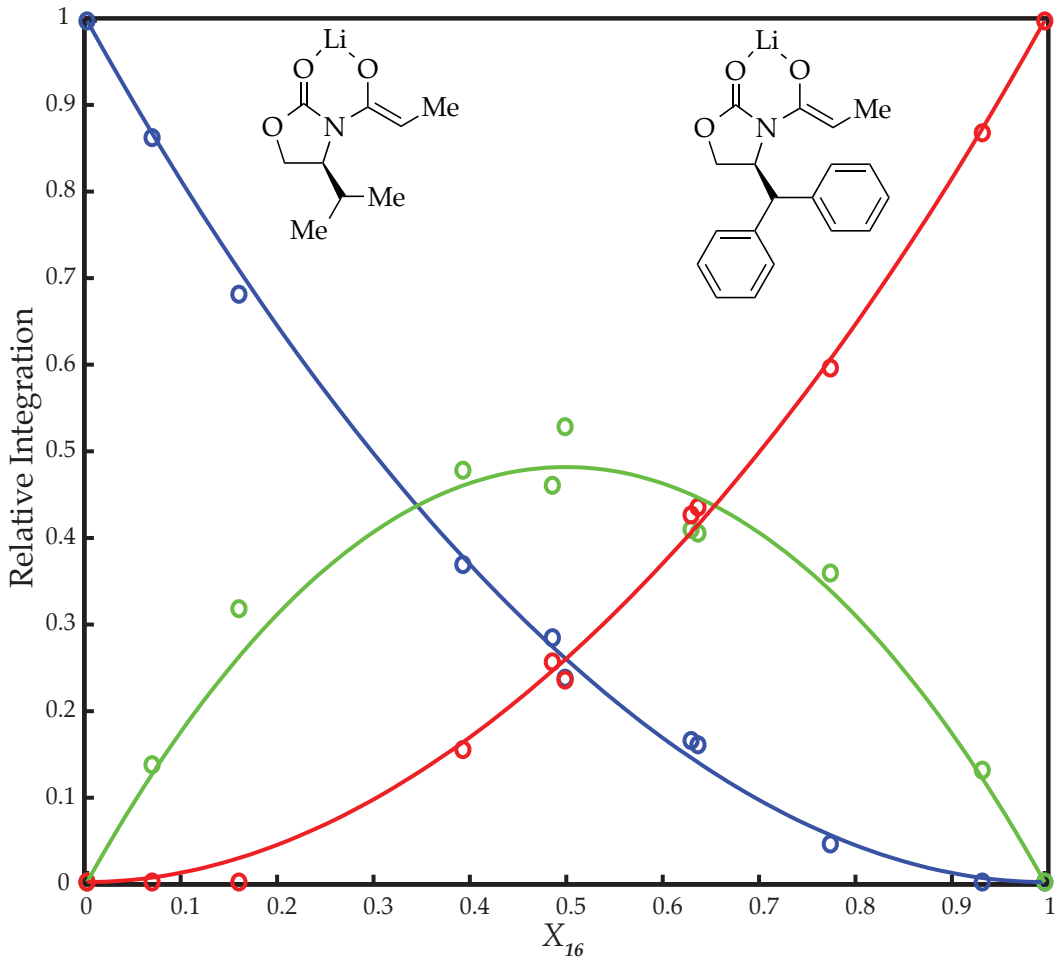


Figure 11. Job plot of **10** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **16**.

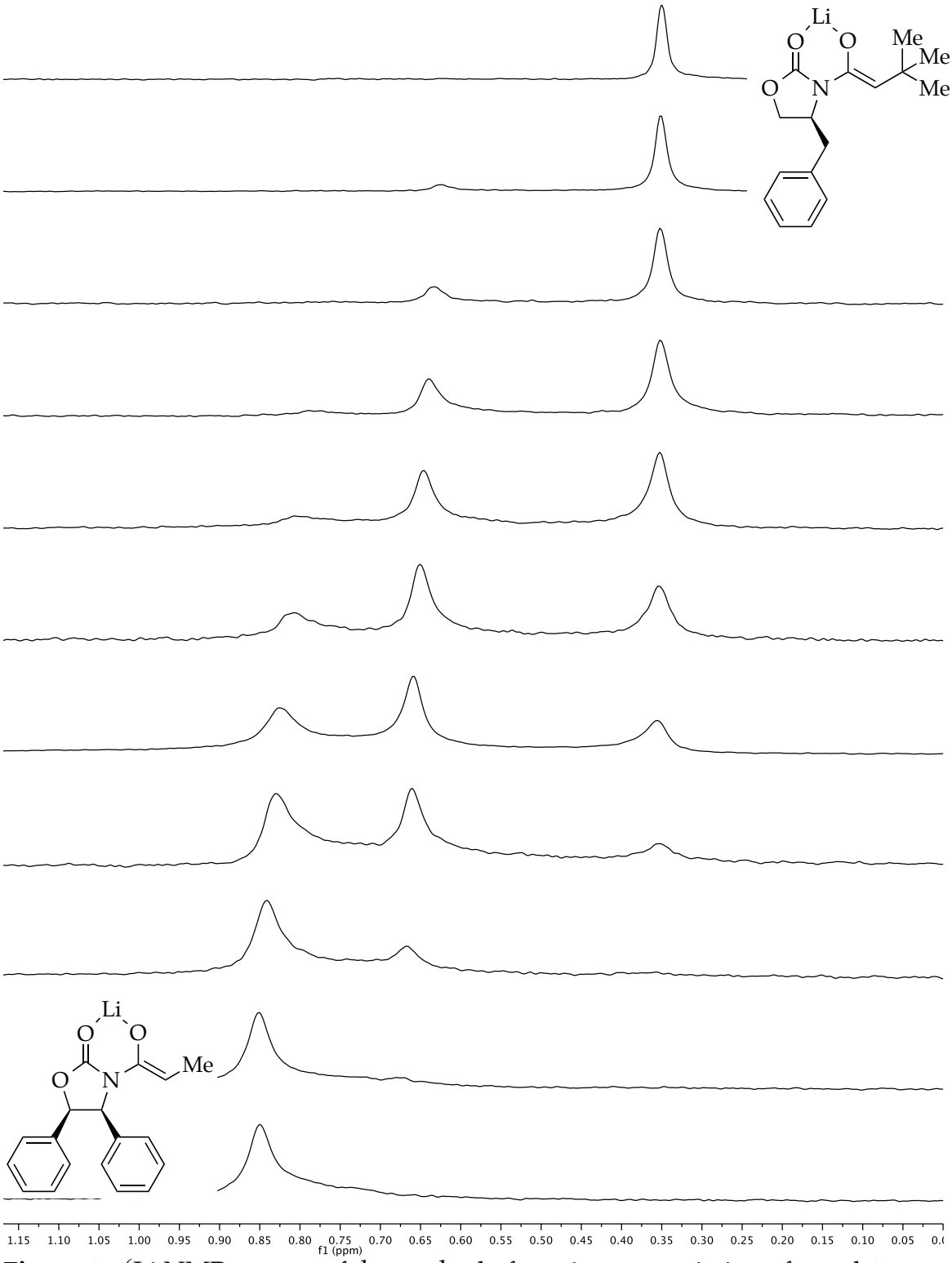


Figure 12. ^{6}Li NMR spectra of the method of continuous variation of **7** and **15** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

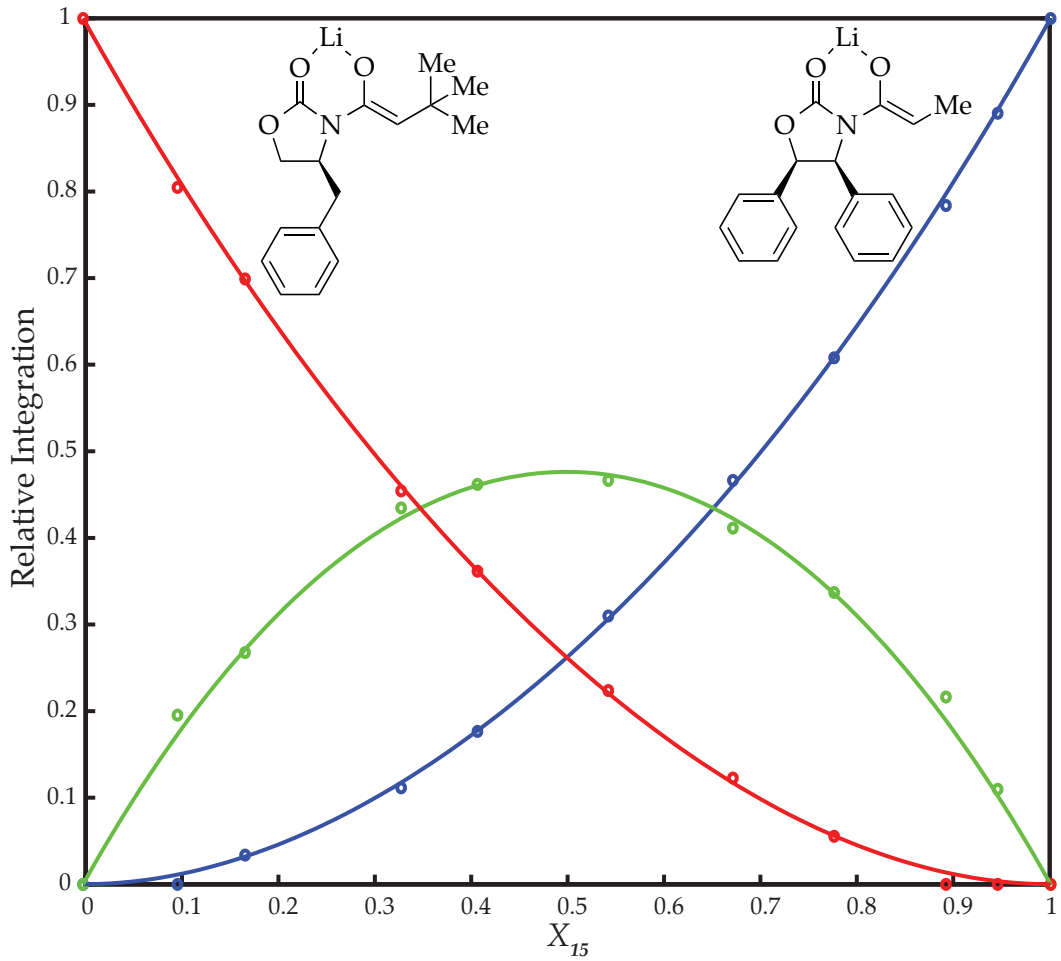


Figure 13. Job plot of **7** and **15** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **15**.

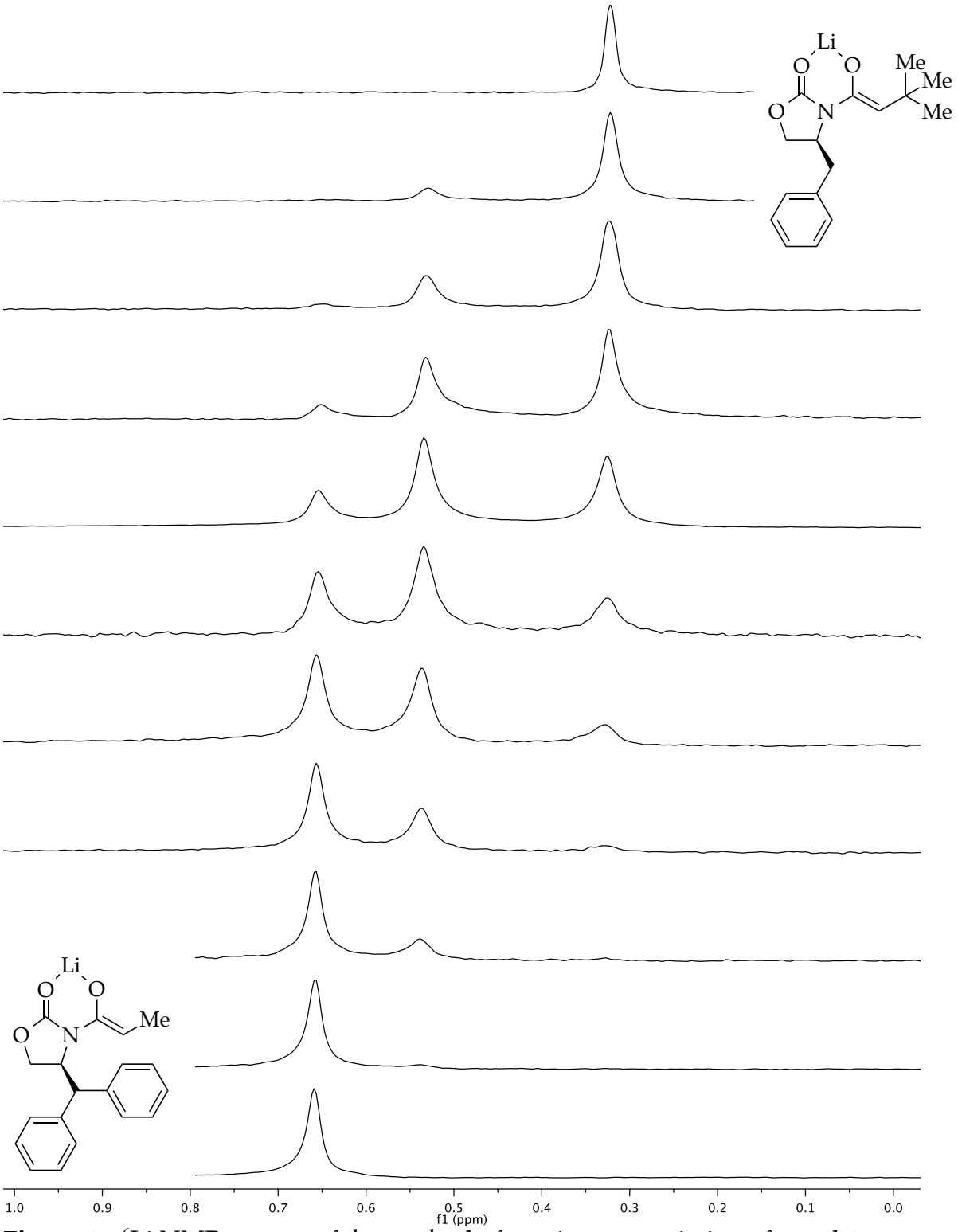


Figure 14. ^{6}Li NMR spectra of the method of continuous variation of **7** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

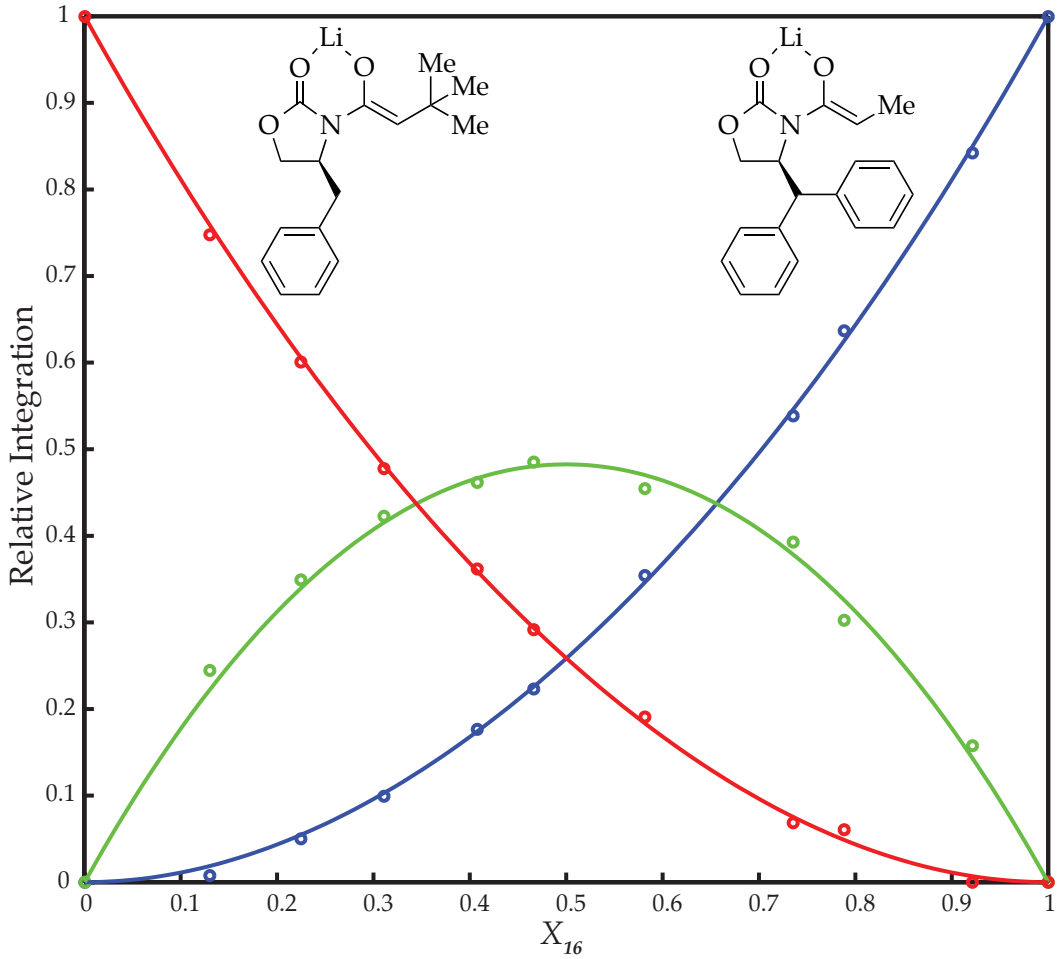


Figure 15. Job plot of **7** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **16**.

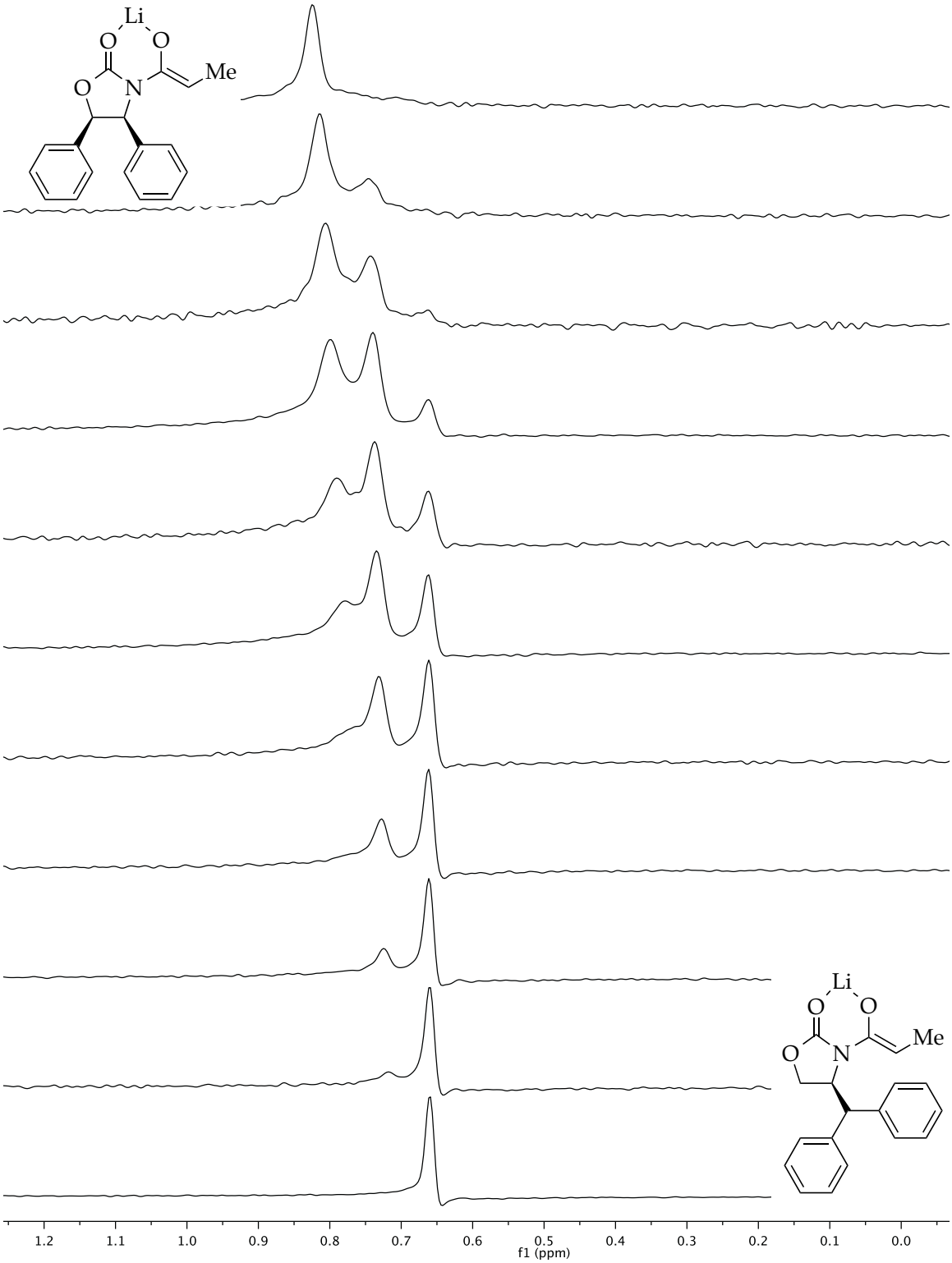


Figure 16. ^{6}Li NMR spectra of the method of continuous variation of **15** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

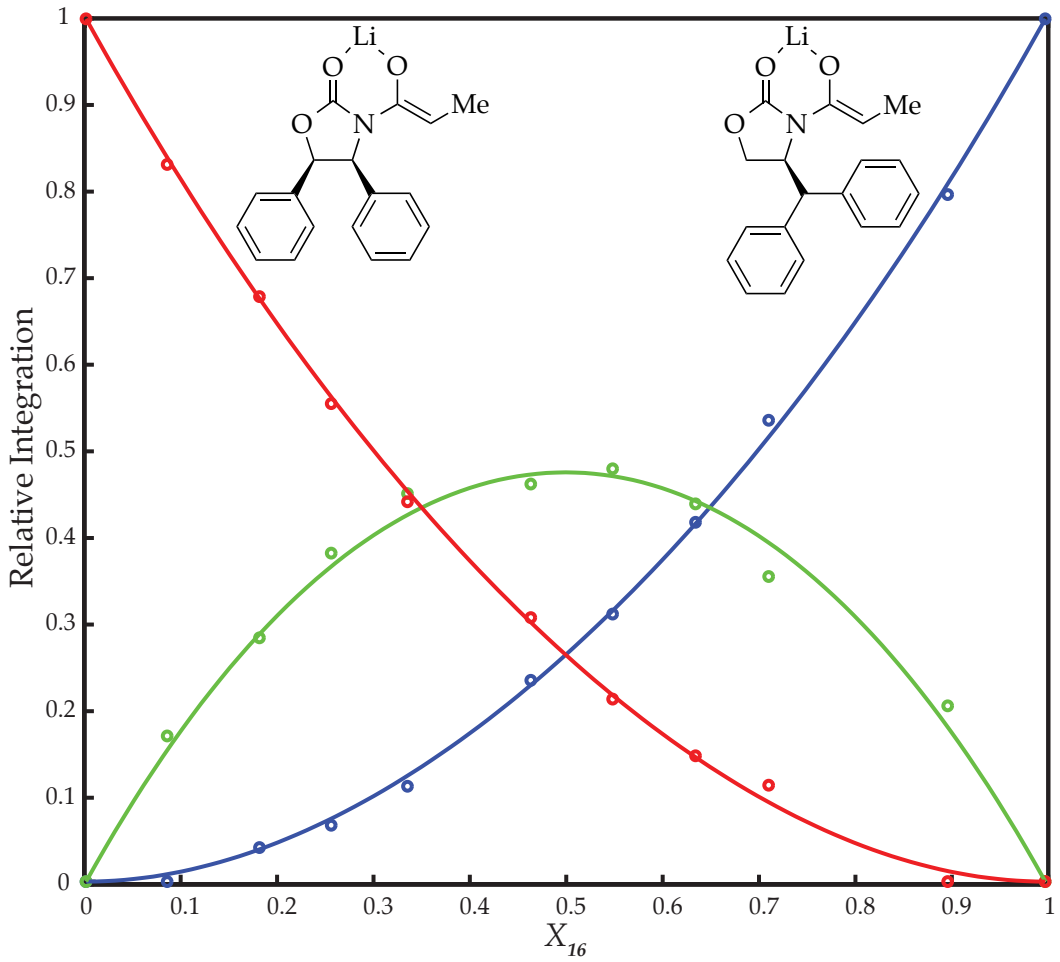


Figure 17. Job plot of **15** and **16** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C. The relative integrations of the homoaggregates and the heteroaggregate are plotted as a function of the mole fraction of **16**.

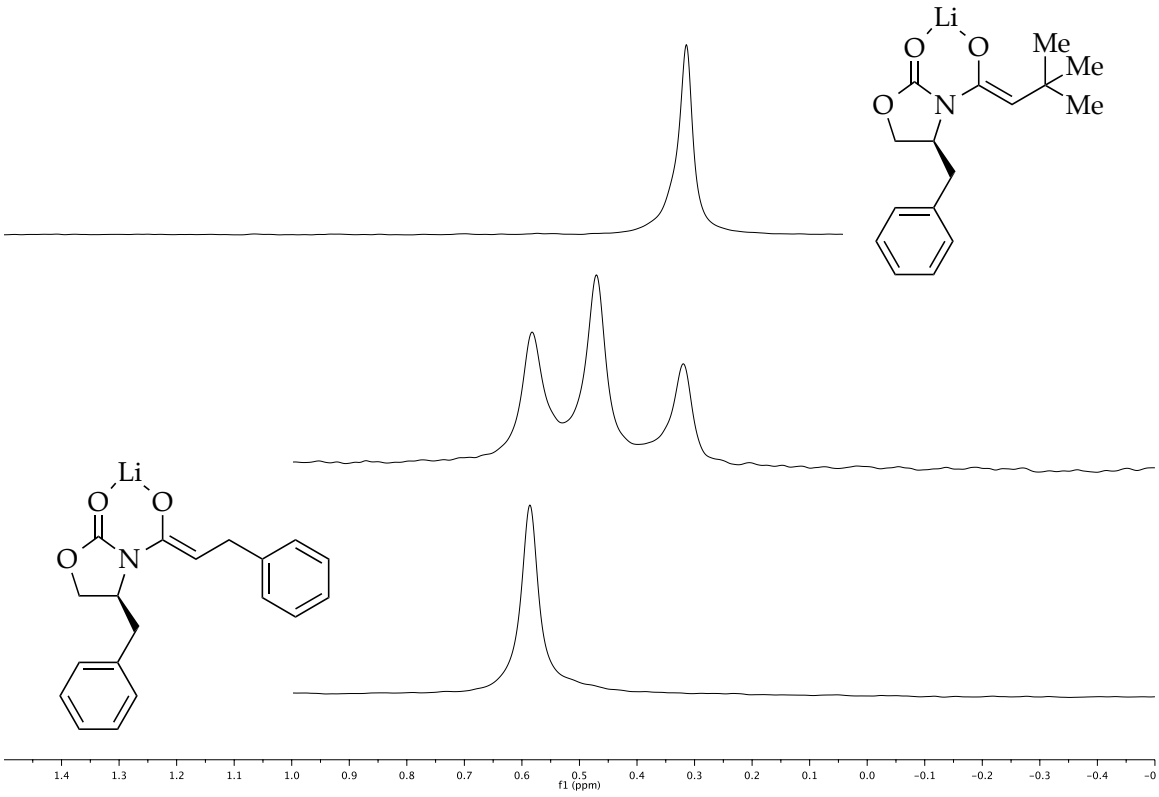


Figure 18. ^{6}Li NMR spectra of the method of continuous variation of **7** and **8** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

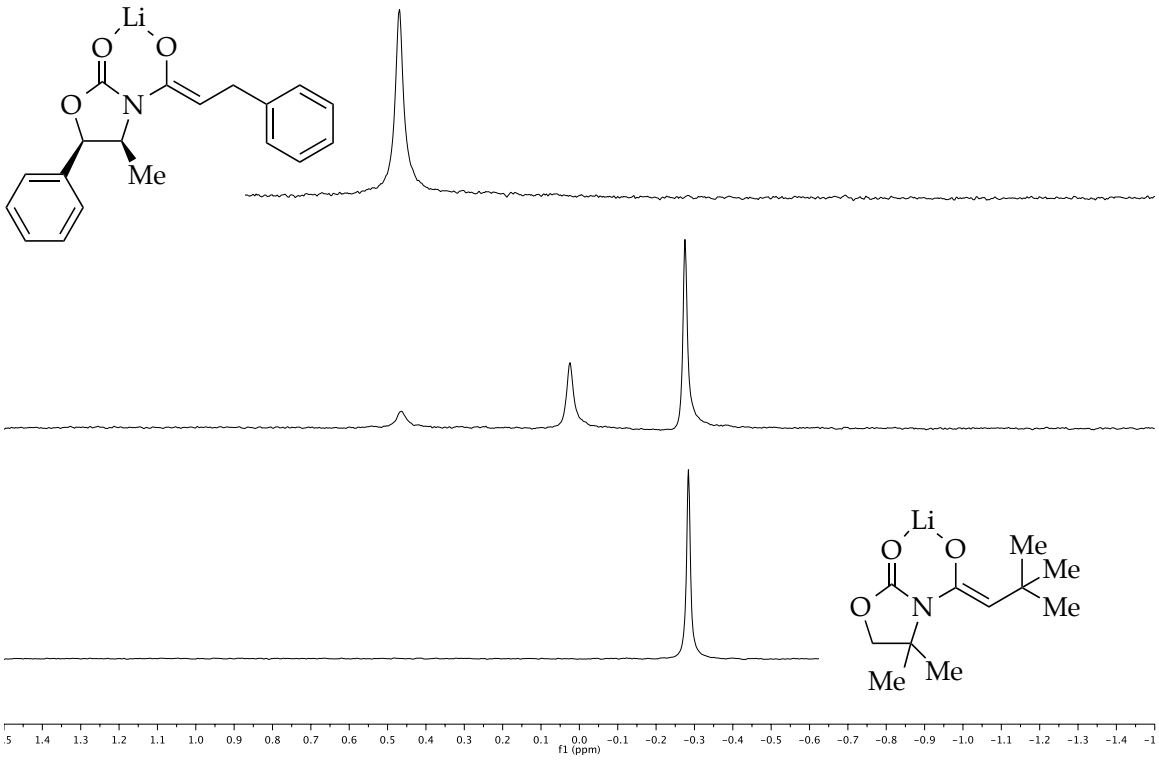


Figure 19. ^{6}Li NMR spectra of the method of continuous variation of **12** and **18** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

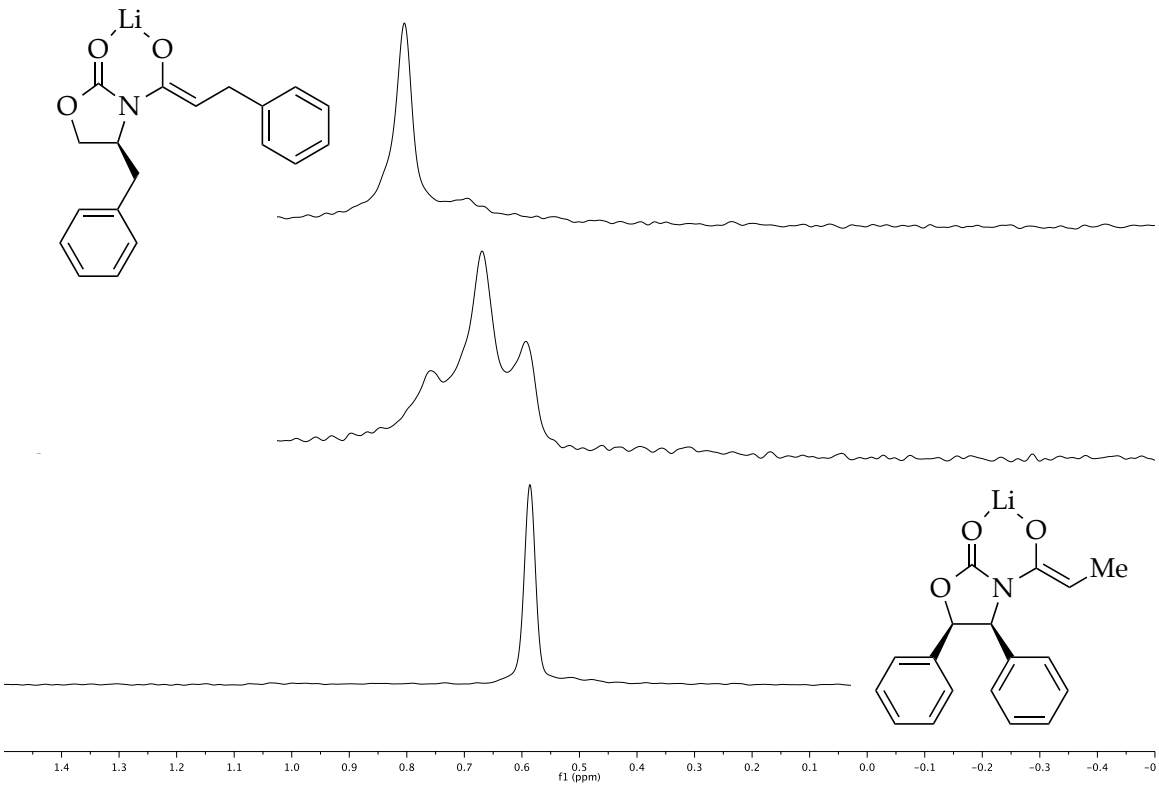


Figure 20. ^{6}Li NMR spectra of the method of continuous variation of **8** and **15** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

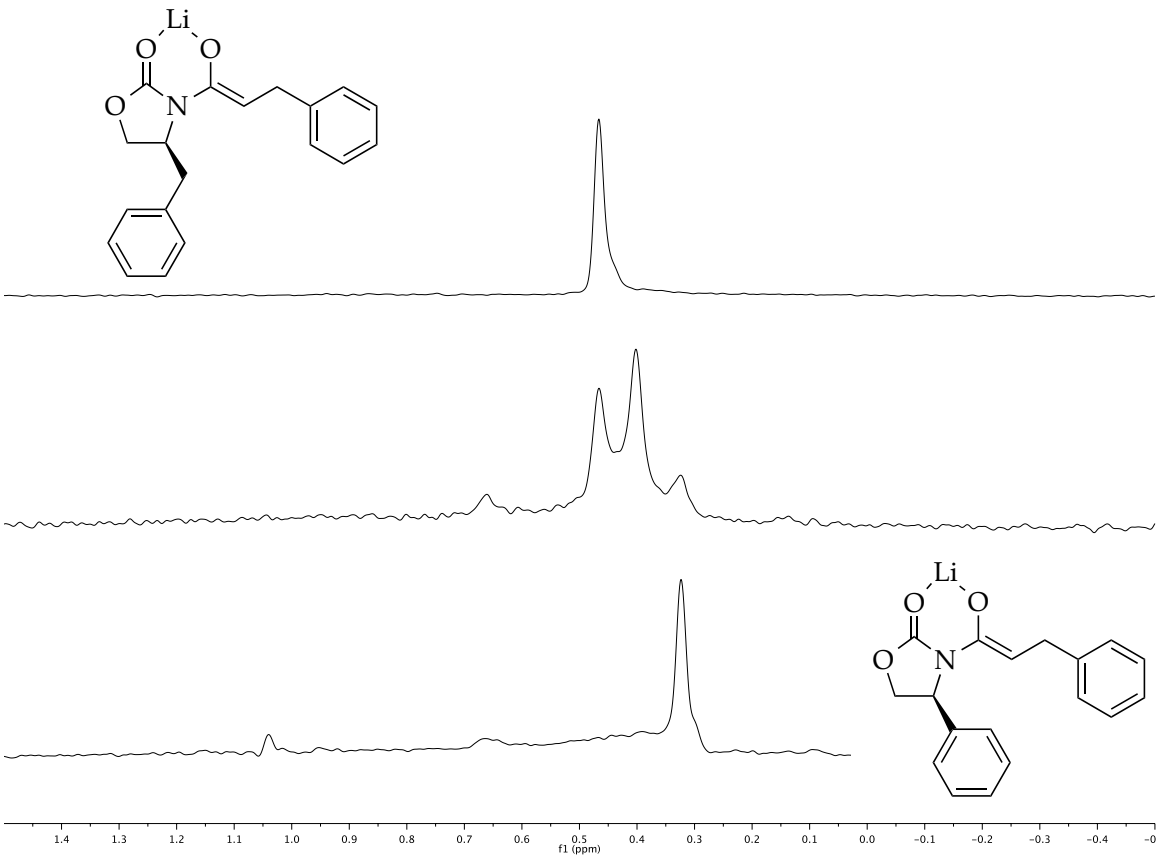


Figure 21. ^{6}Li NMR spectra of the method of continuous variation of **8** and **17** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

Part 2: Uncharacterized/oligomerized substrates

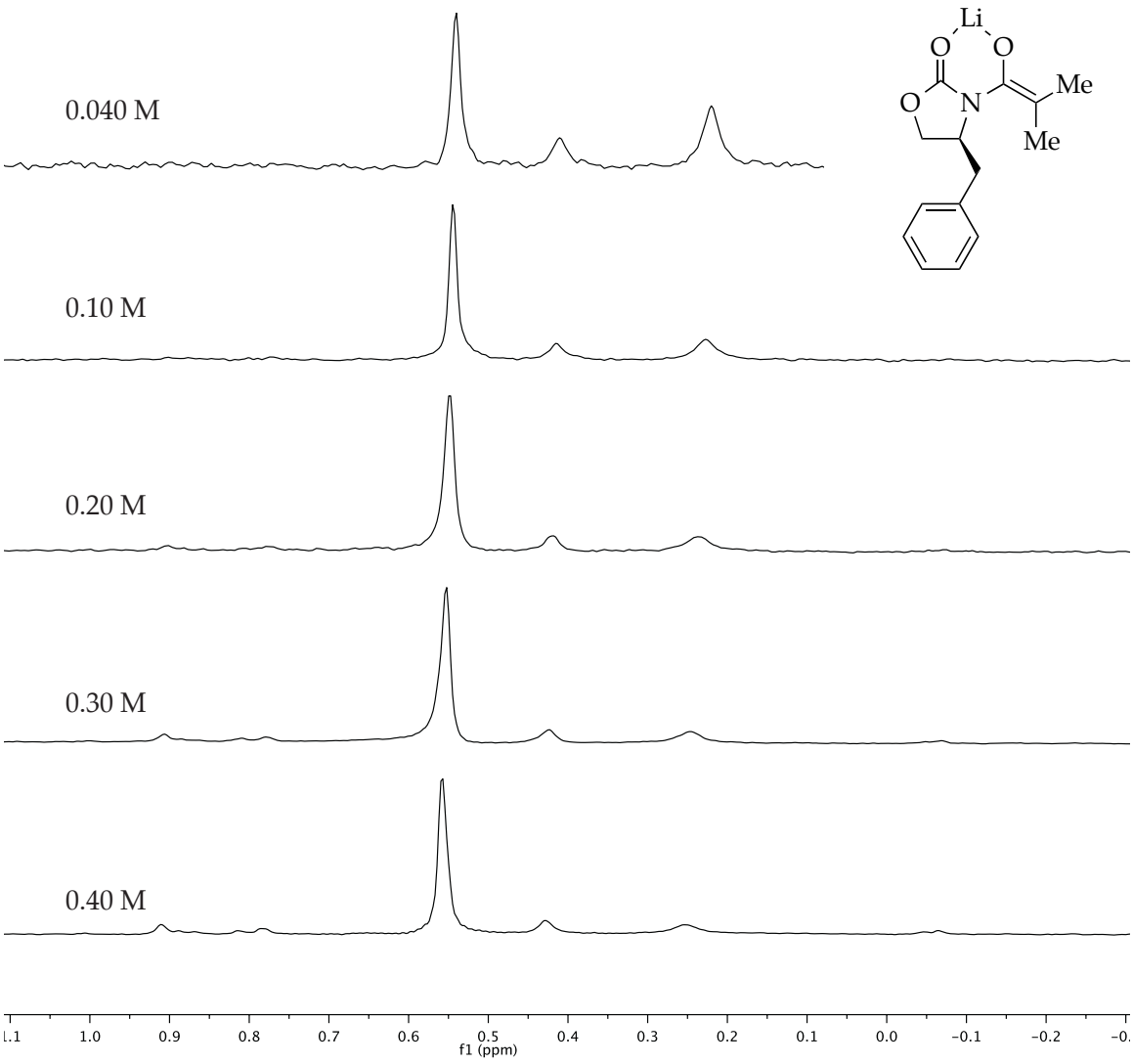


Figure 22. ^{6}Li NMR spectra of changing concentration of **22** in neat THF at –80 °C.

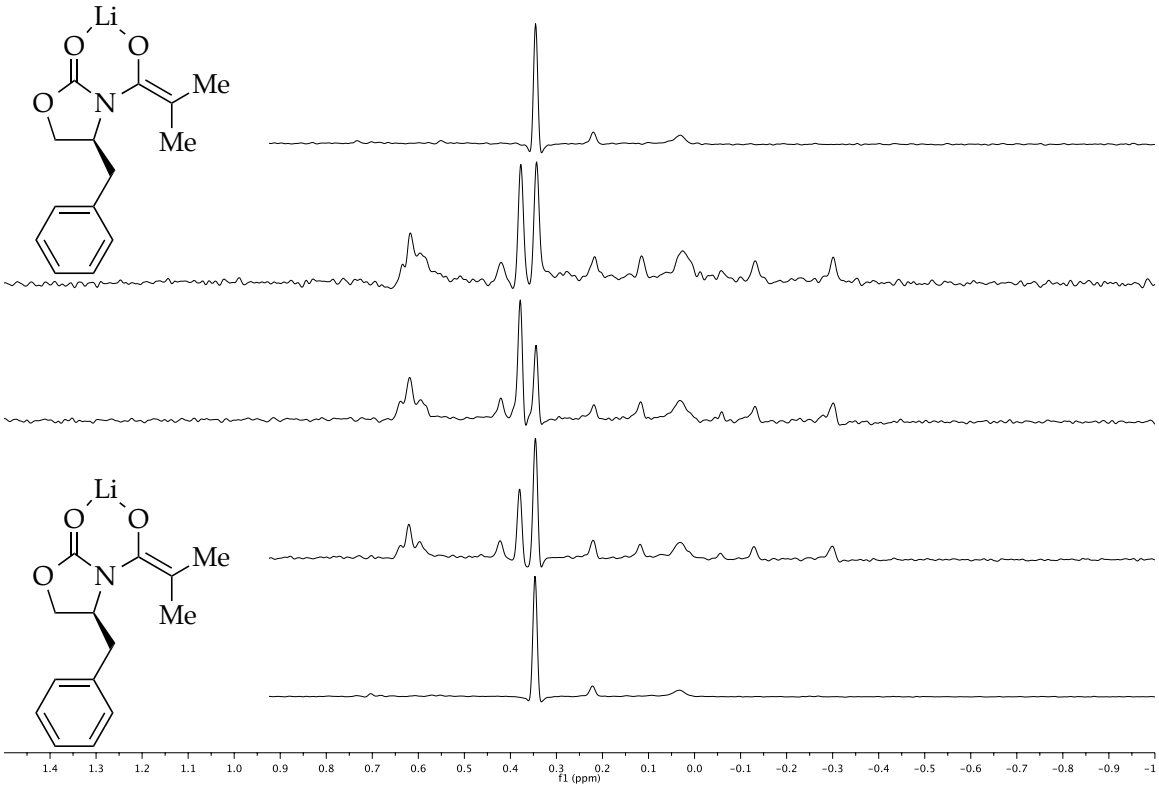


Figure 23. ^{6}Li NMR spectra of the method of continuous variation of **(*S*)-22** and **(*R*)-22** (0.10 M total oxazolidinone, 0.11 M [^{6}Li]LDA) in neat THF at –80 °C.

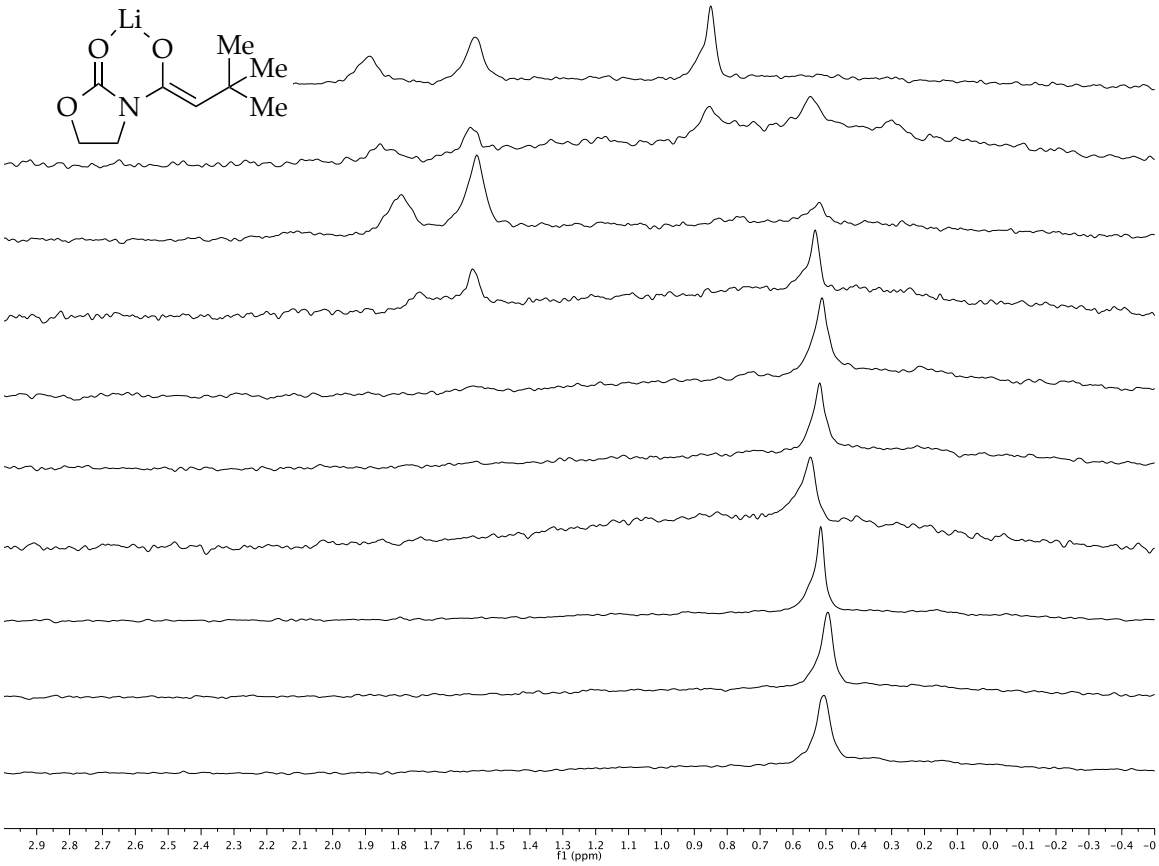


Figure 24. ^{6}Li NMR spectra of changing THF equivalents (0 to 15) with toluene cosolvent of **33** (0.10 M oxazolidinone, 0.11 M [^{6}Li]LDA) at –80 °C.

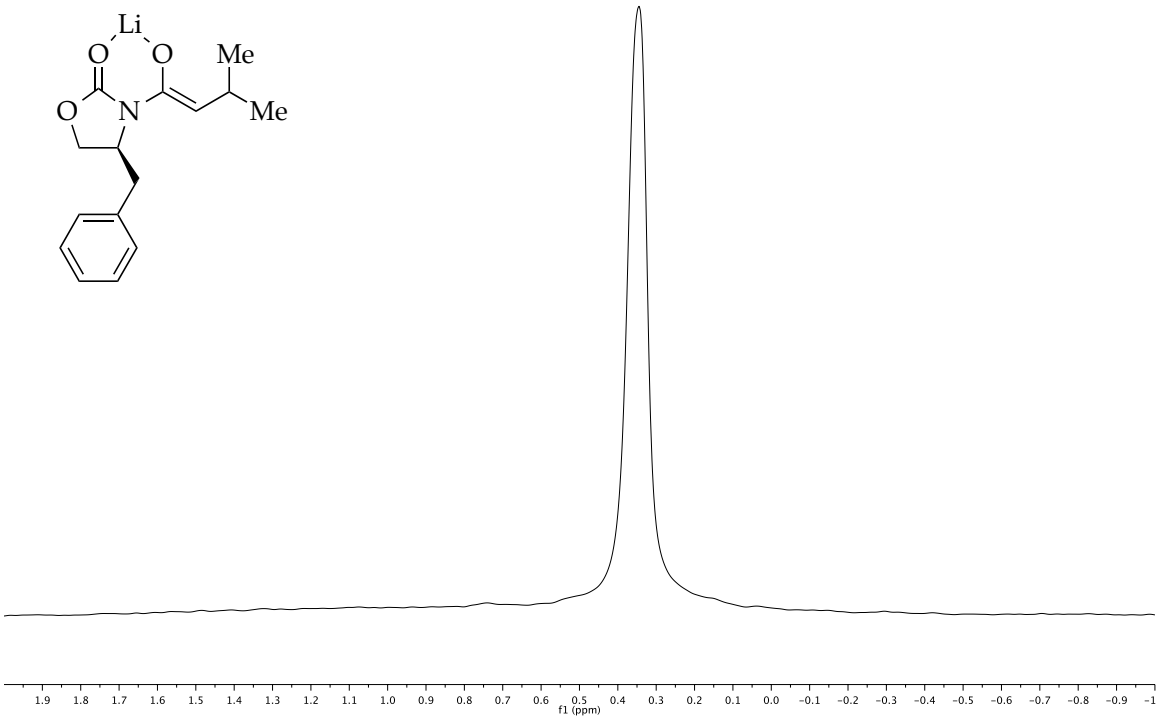


Figure 25. ^{6}Li NMR spectrum of **23** (0.10 M oxazolidinone, 0.11 M [^{6}Li]LDA) in THF at –80 °C.

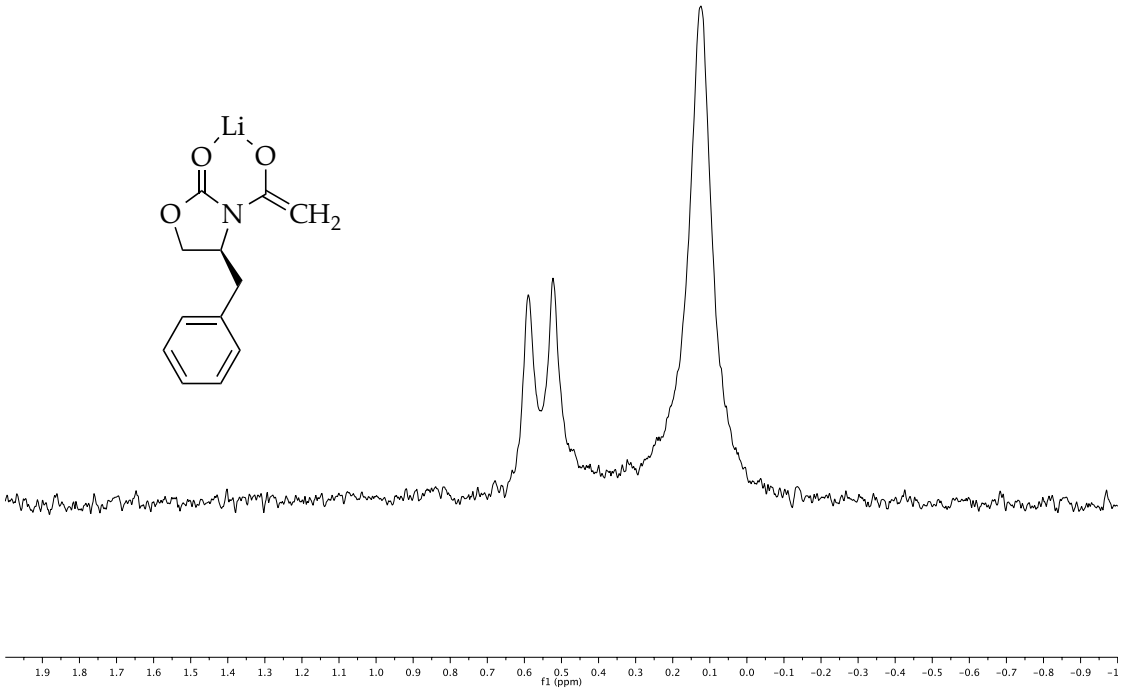


Figure 26. ^{6}Li NMR spectrum of **24** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C, unaged.

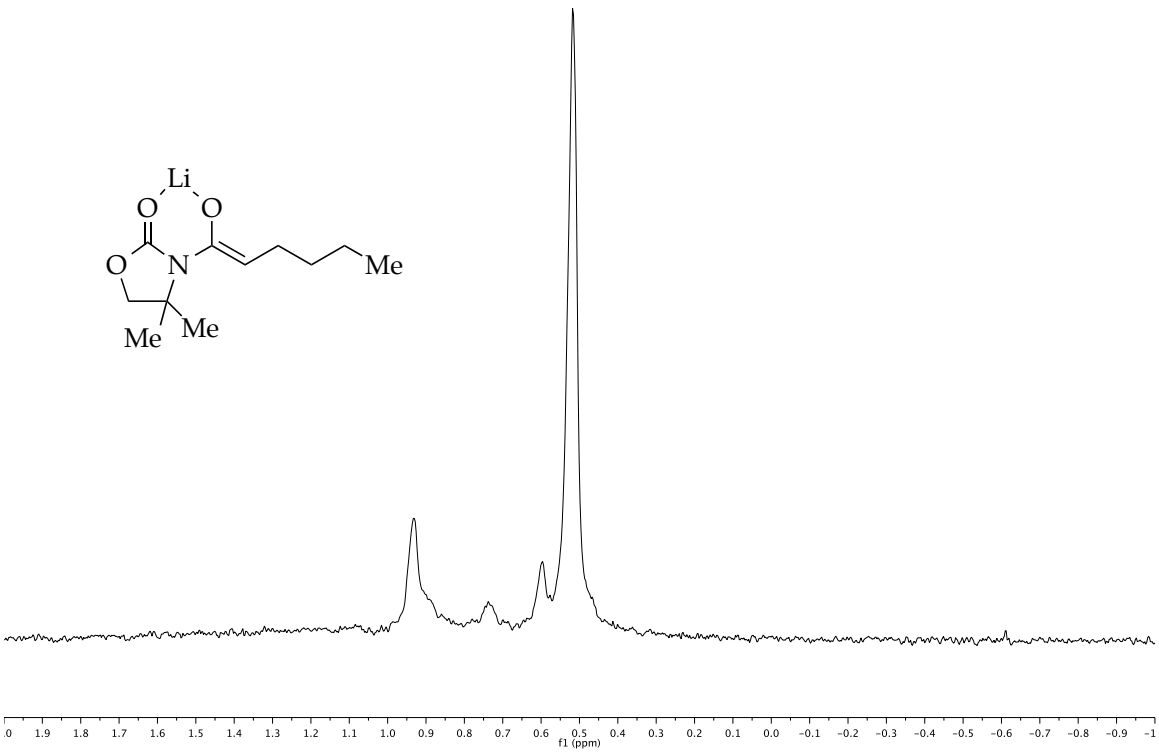


Figure 27. ^{6}Li NMR spectrum of **25** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C.

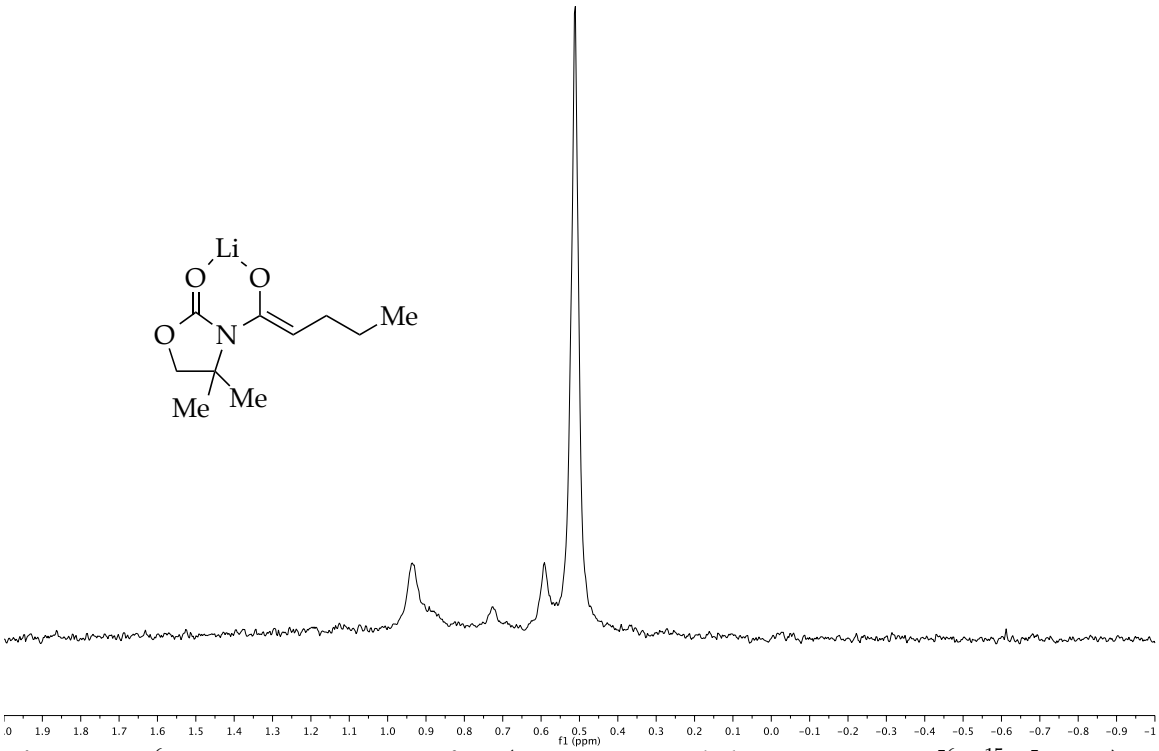


Figure 28. ^{6}Li NMR spectrum of **26** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C.

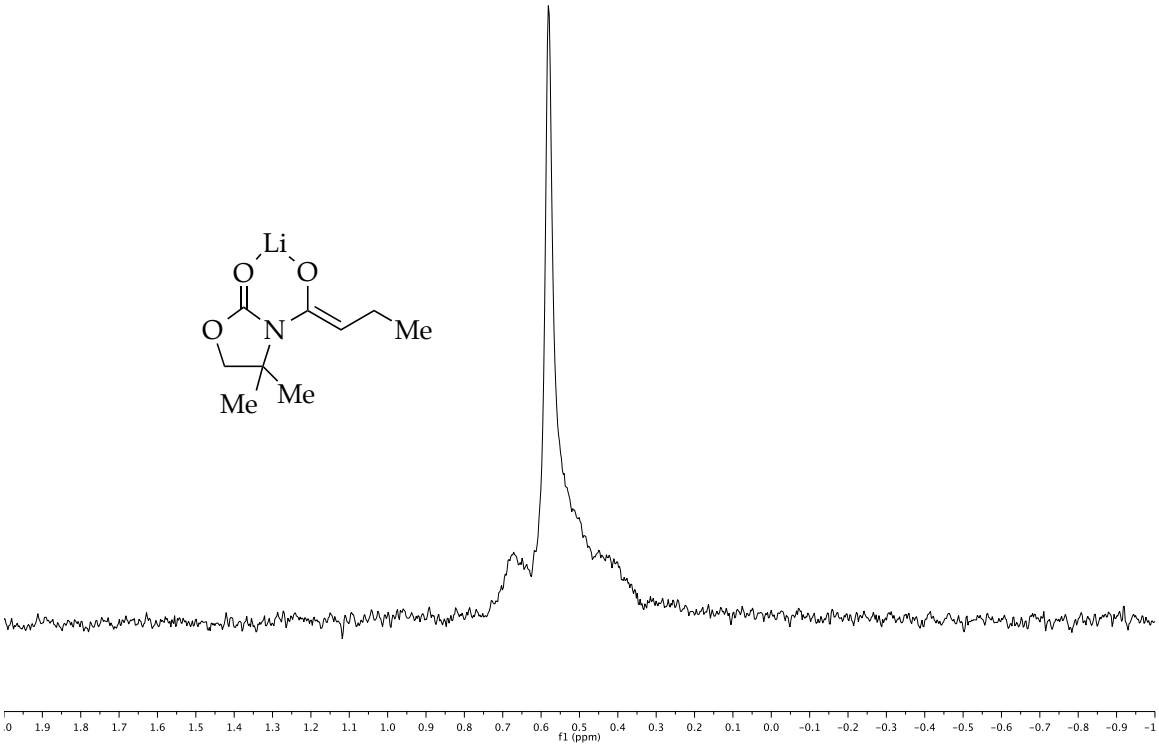


Figure 29. ^{6}Li NMR spectrum of **27** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C.

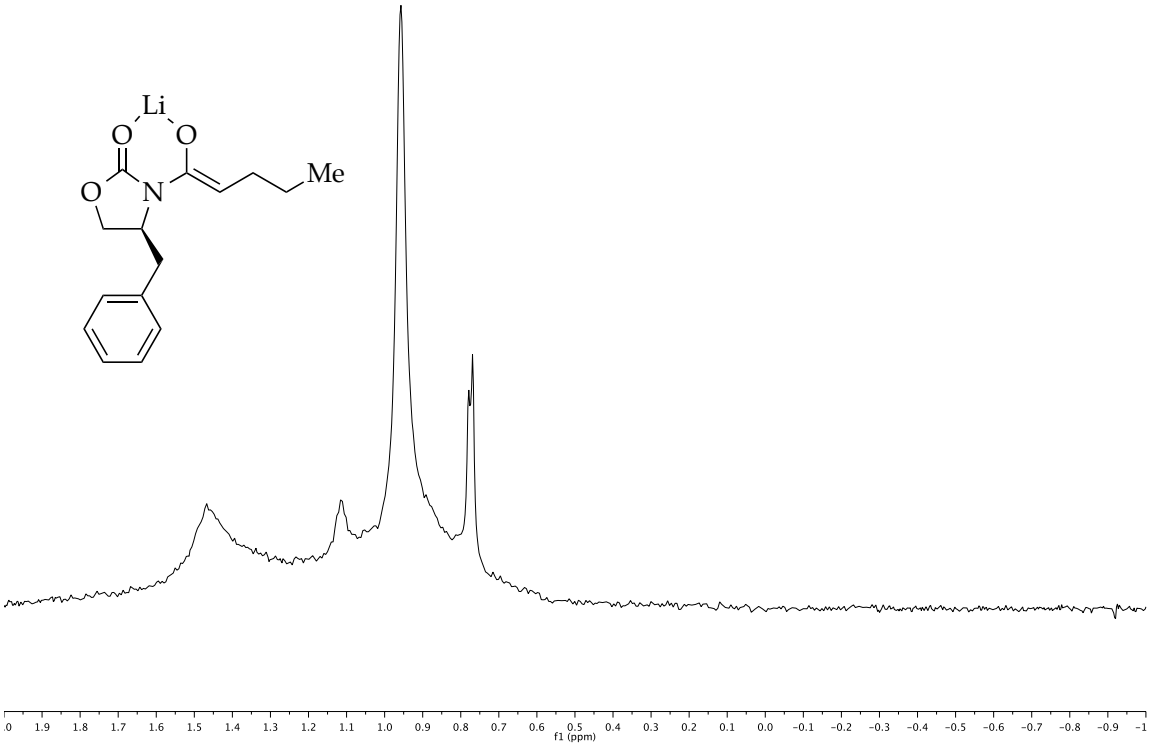


Figure 30. ^{6}Li NMR spectrum of **28** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C.

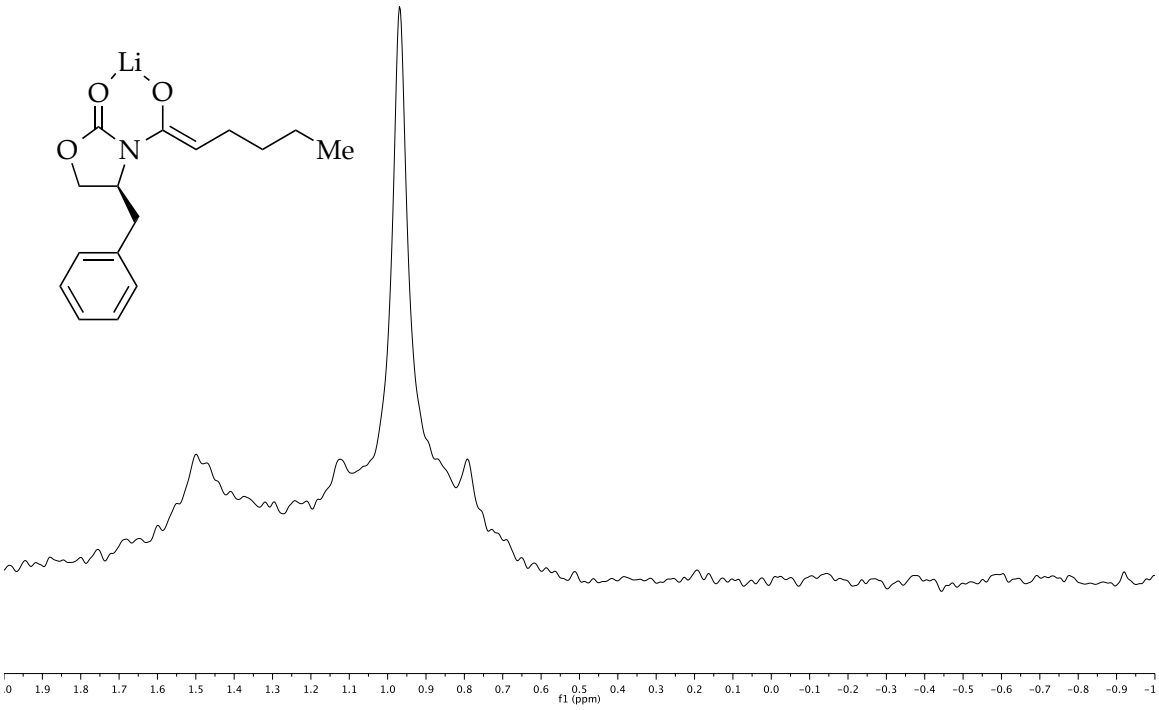


Figure 31. ^{6}Li NMR spectrum of **29** (0.10 M oxazolidinone, 0.11 M [^{6}Li^{15}N]LDA) in THF at –80 °C.

Part 3: Solvation Studies of 5 and 6

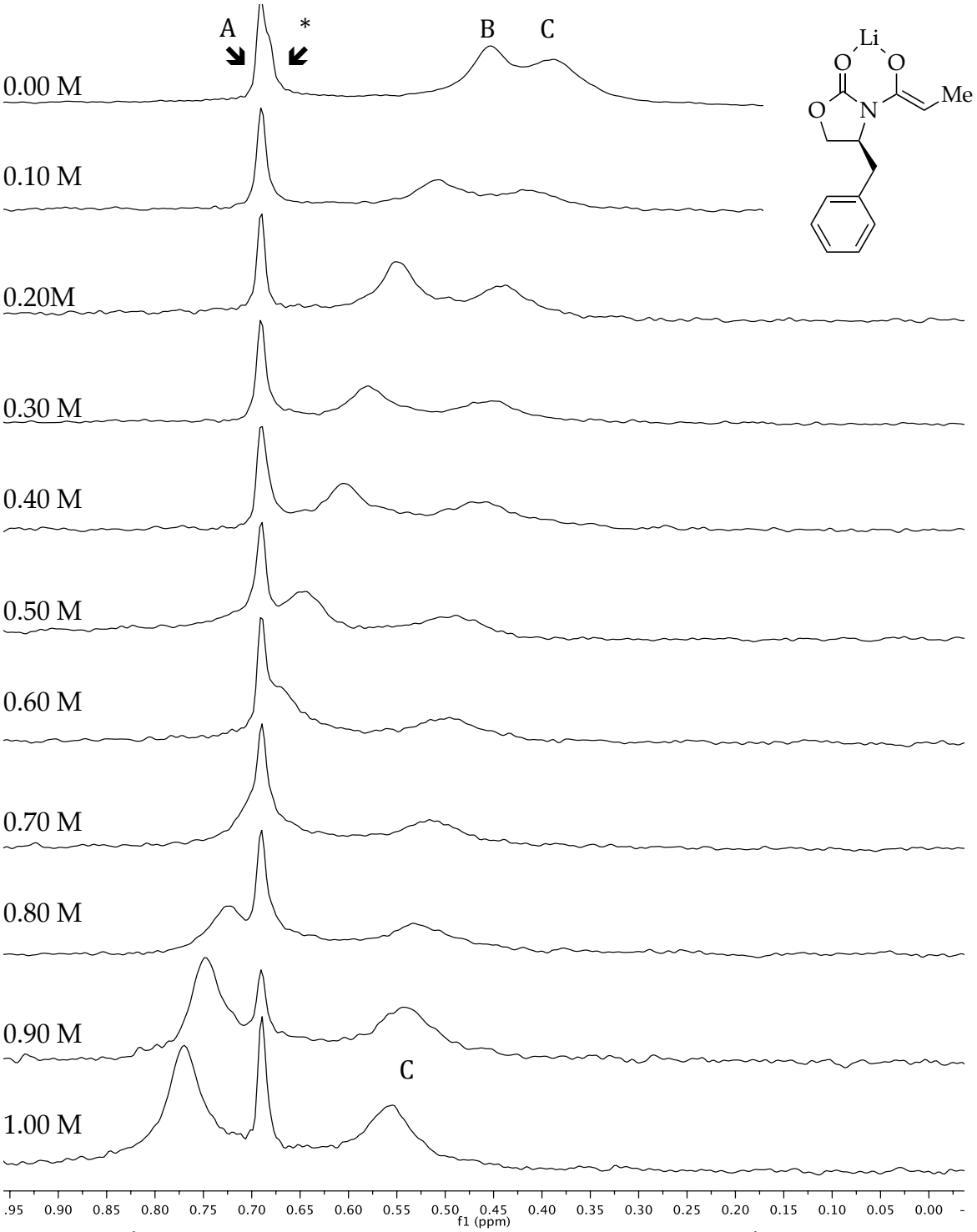


Figure 32. ^{6}Li NMR spectra of **5** (0.10 M oxazolidinone, 0.10 M [^{6}Li]LDA) with varying pyridine concentrations (as labeled) in THF at –80 °C. **A** is the unsolvated tetramer; **B** and **C** are the trisolvated dimers. The mixed aggregate is denoted by *.

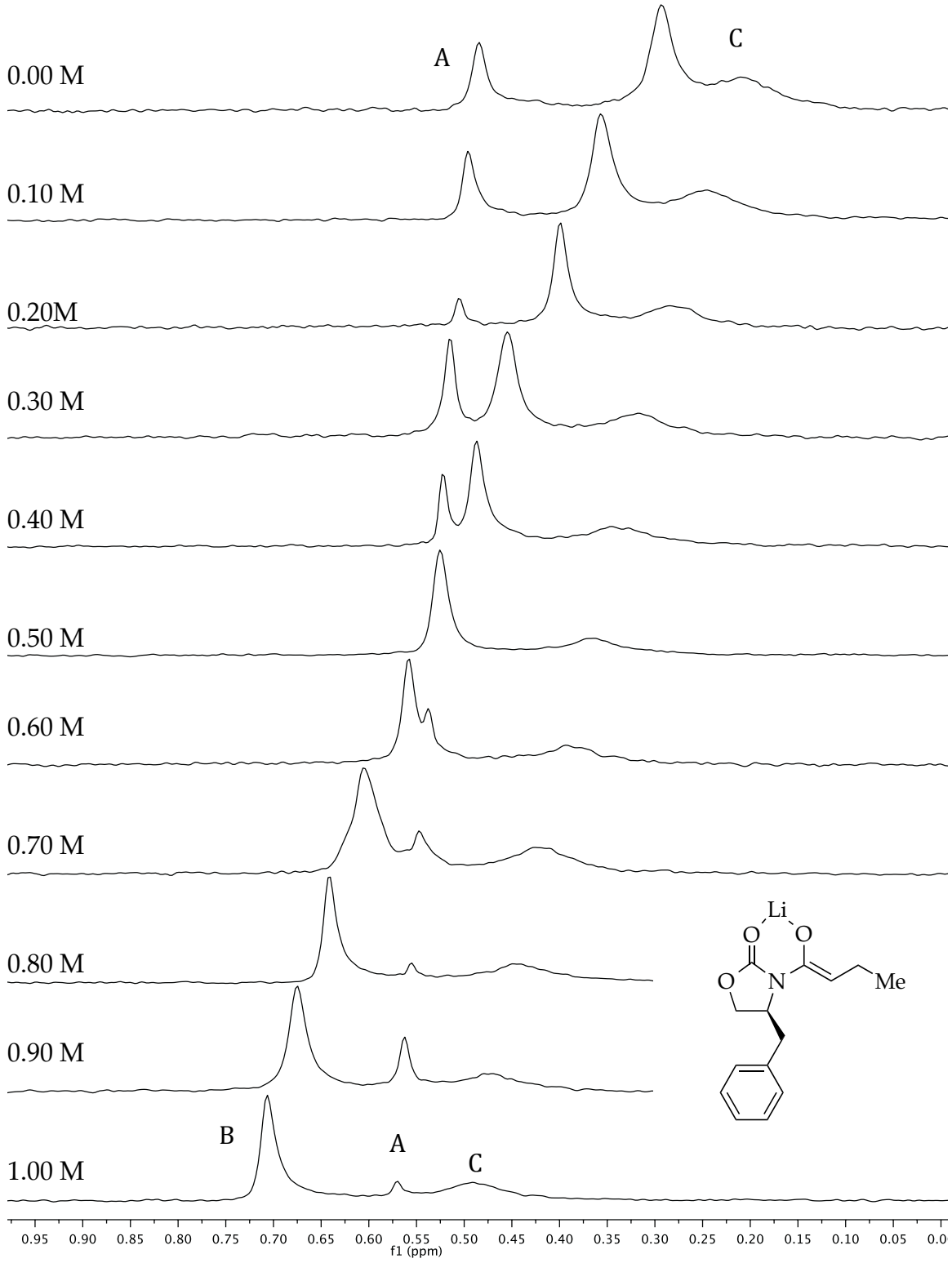


Figure 33. ^{6}Li NMR spectra of **6** (0.10 M oxazolidinone, 0.10 M [^{6}Li]LDA) with varying pyridine concentrations (as labeled) in THF at –80 °C. **A** is the unsolvated tetramer; **B** and **C** are the trisolvated dimers.

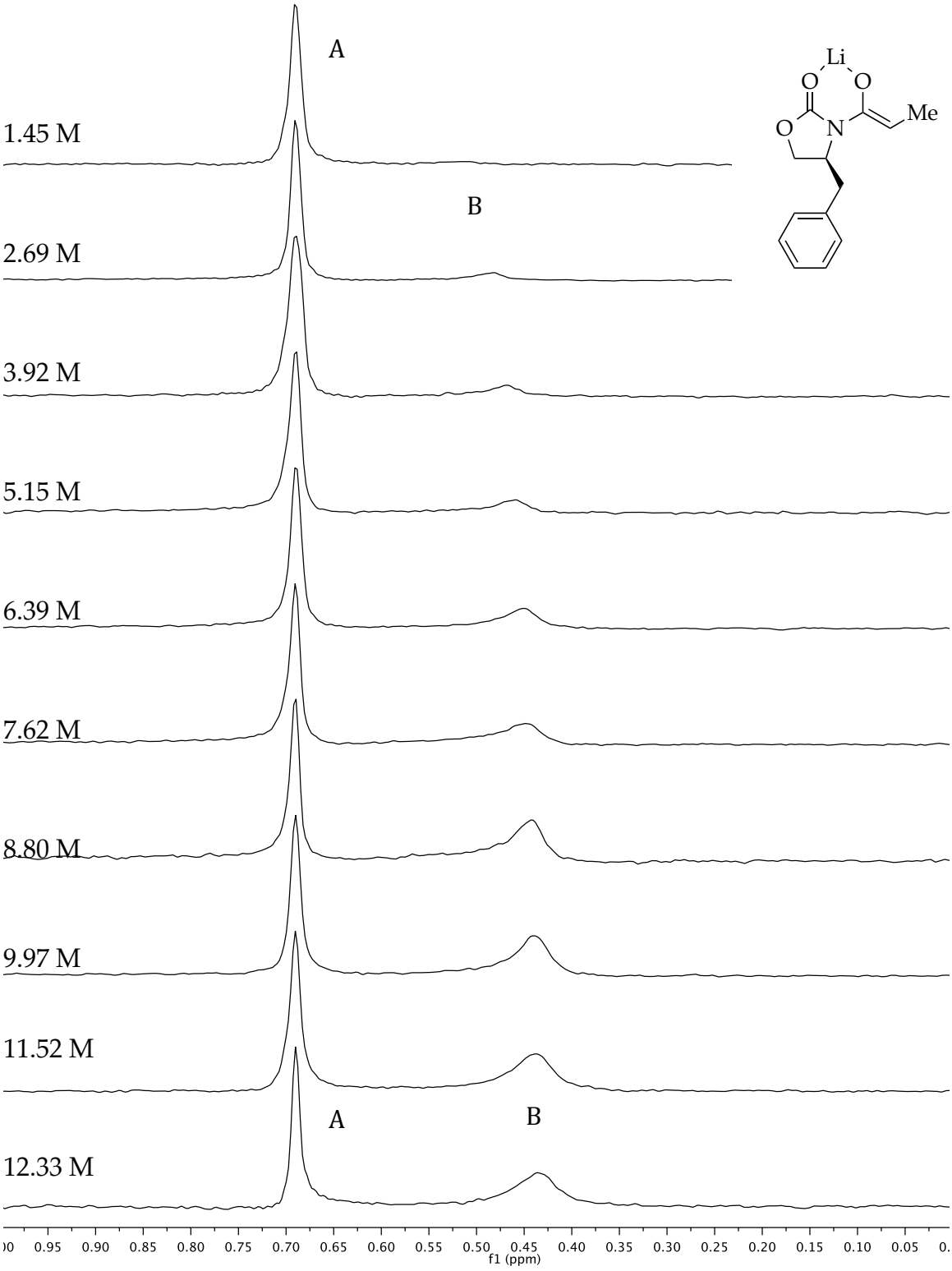


Figure 34. ^{6}Li NMR spectra of **5** (0.10 M oxazolidinone, 0.10 M [^{6}Li]LDA) with varying THF concentrations (as labeled) in toluene at –60 °C. **A** is the unsolvated tetramer; **B** is the coalesced trisolvated dimers.

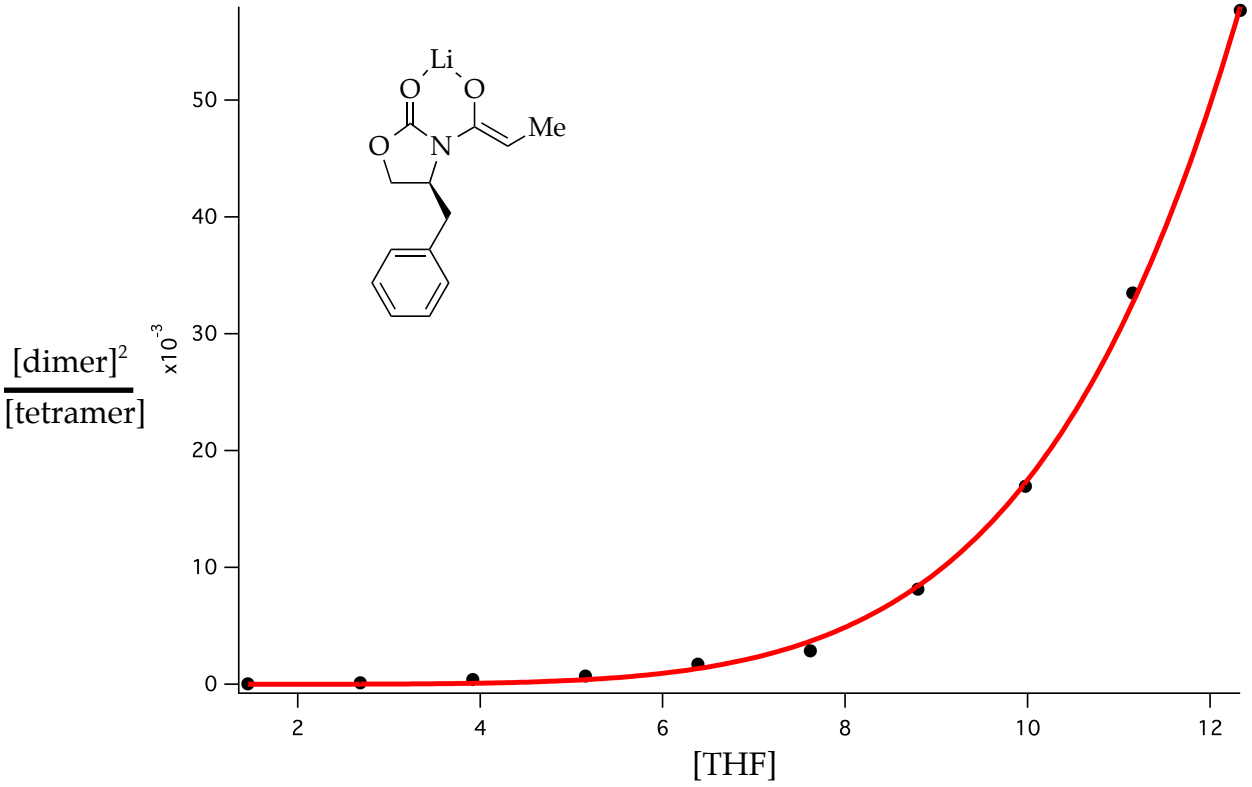


Figure 35. Fit of aggregate concentration vs. changing THF concentration for **5** to determine the dimer solvation at –60 °C. The best fit, in red, gives a solvation of the dimer peak of 2.86 ± 0.04. The fitting equation was $Y=(X^{2n})/k$.

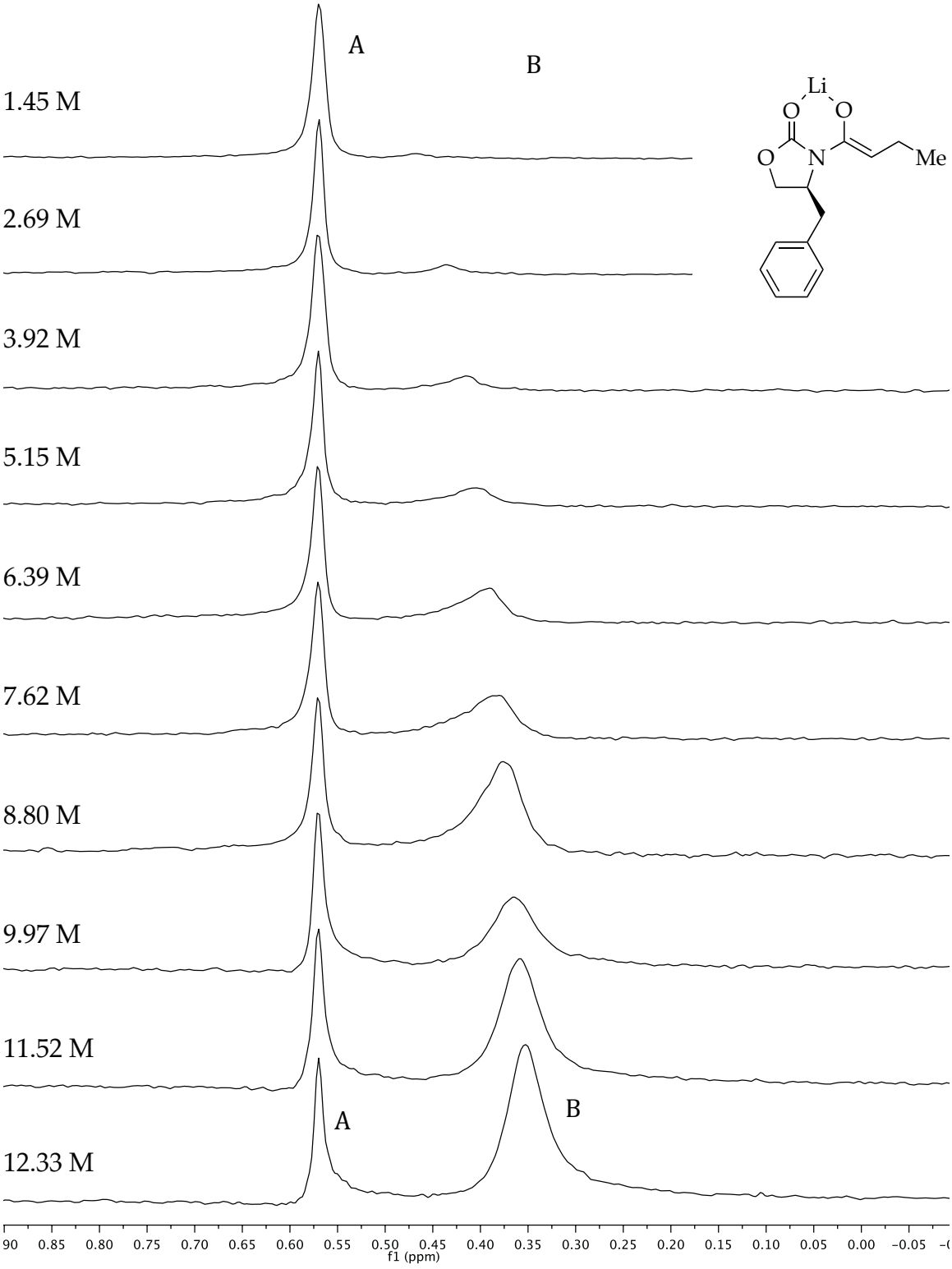


Figure 36. ^{6}Li NMR spectra of **6** (0.10 M oxazolidinone, 0.10 M [^{6}Li]LDA) with varying THF concentrations (as labeled) in toluene at –60 °C. **A** is the unsolvated tetramer; **B** is the coalesced trisolvated dimers.

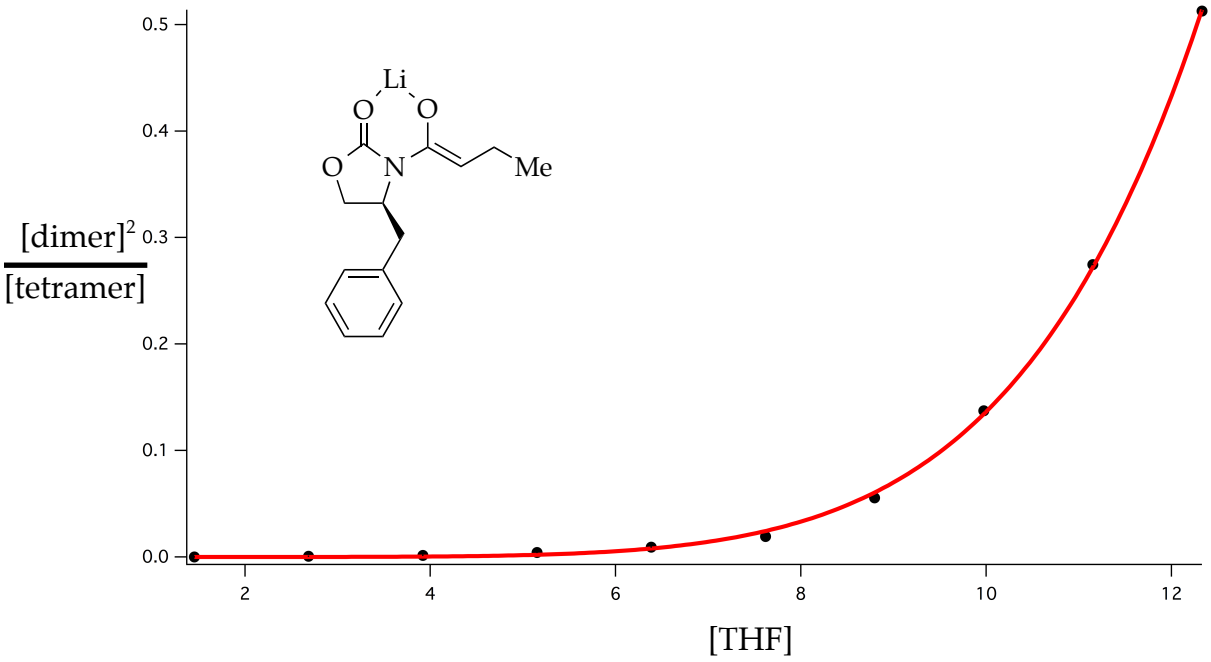


Figure 37. Fit of aggregate concentration vs. changing THF for **6** to determine dimer solvation at –40 °C. The best fit, in red, gives a solvation of the dimer peak of 3.17 ± 0.03. The fitting equation was $Y=(X^{2n})/k$.

Part 4: Aggregation Studies of 5 and 6

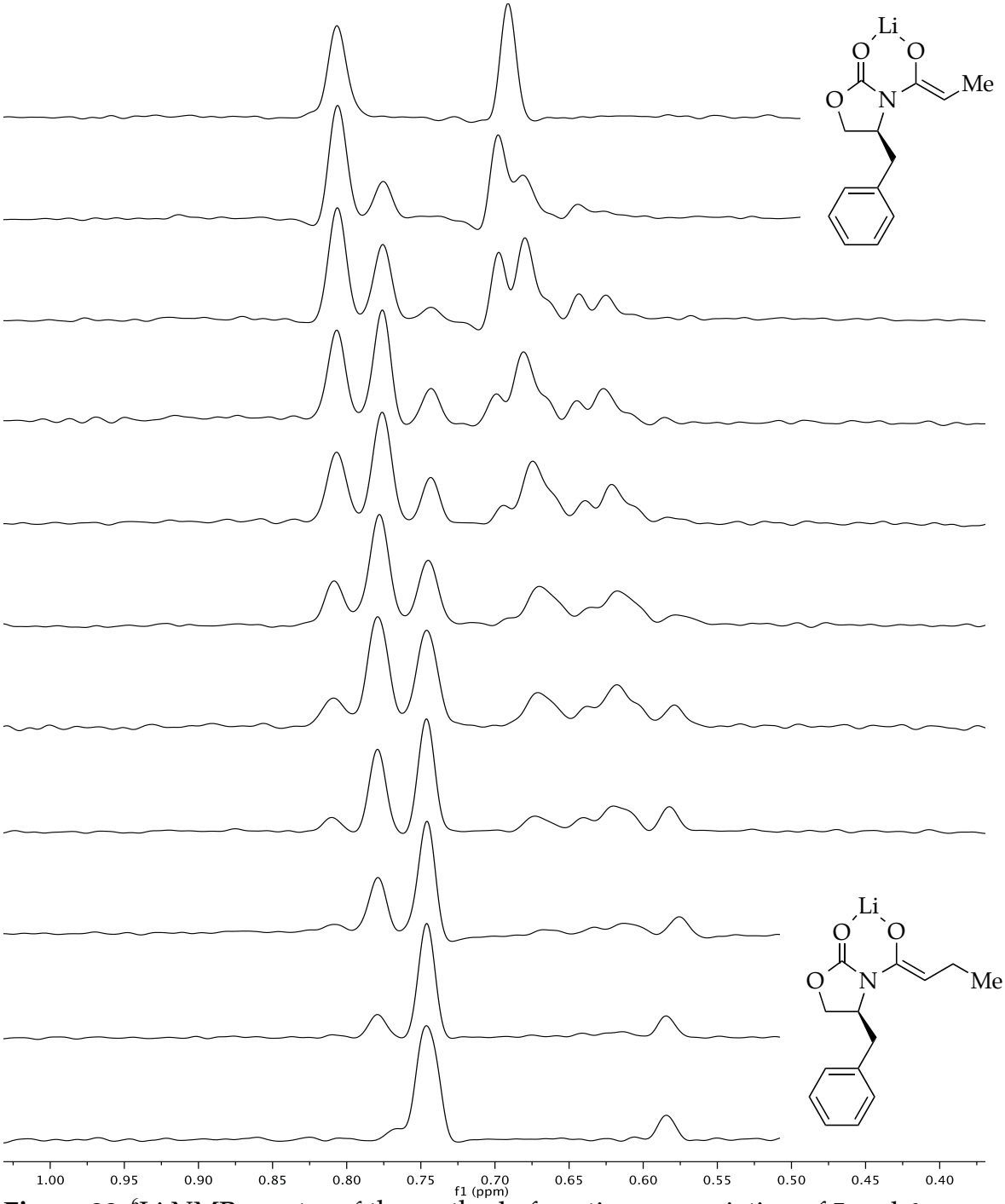


Figure 38. ^{6}Li NMR spectra of the method of continuous variation of **5** and **6**, dimer peaks downfield, (0.10 M total oxazolidinone, 0.10 M [^{6}Li]LDA) with 1.0 M pyridine in THF at –80 °C.

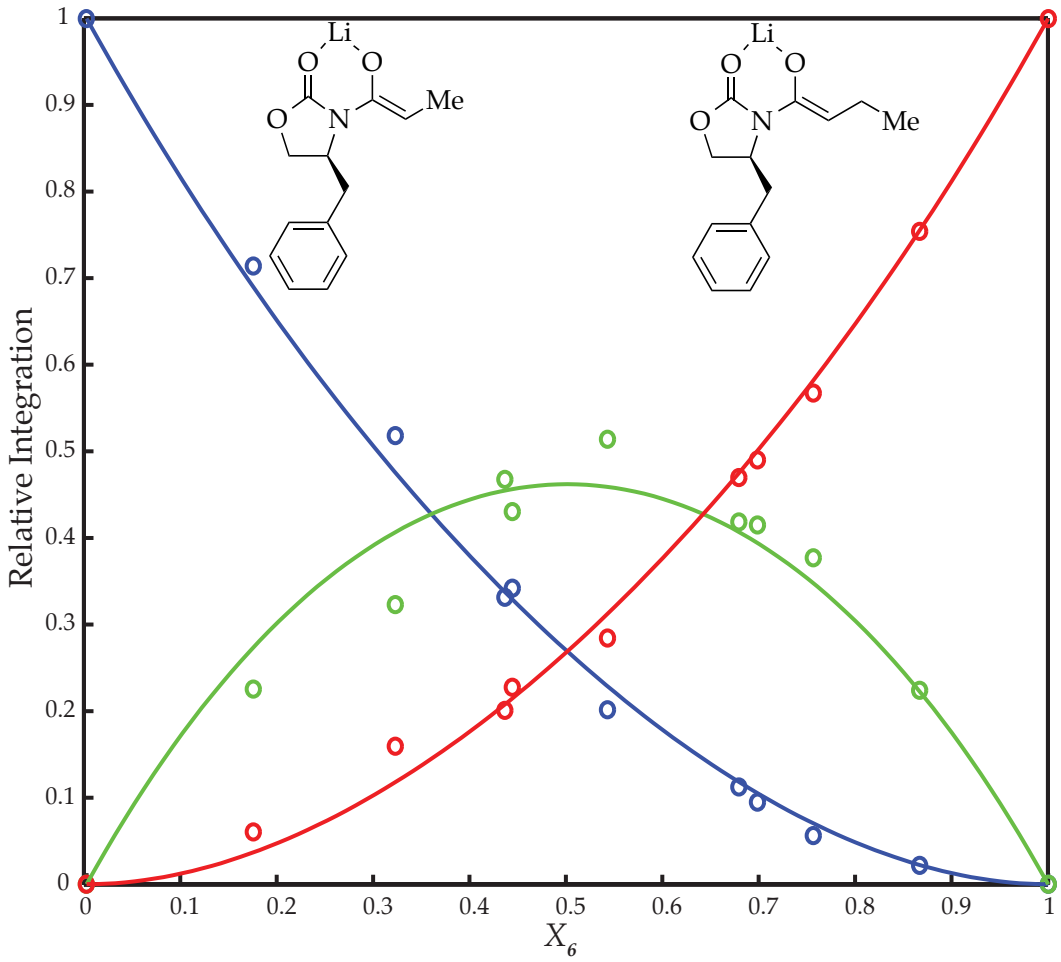


Figure 39. Job plot of **5** and **6** dimers (0.10 M total oxazolidinone, 0.10 M [^{6}Li]LDA) with 1.0 M pyridine in THF at –80 °C. The relative integrations are plotted as a function of the mole fraction of **6**.

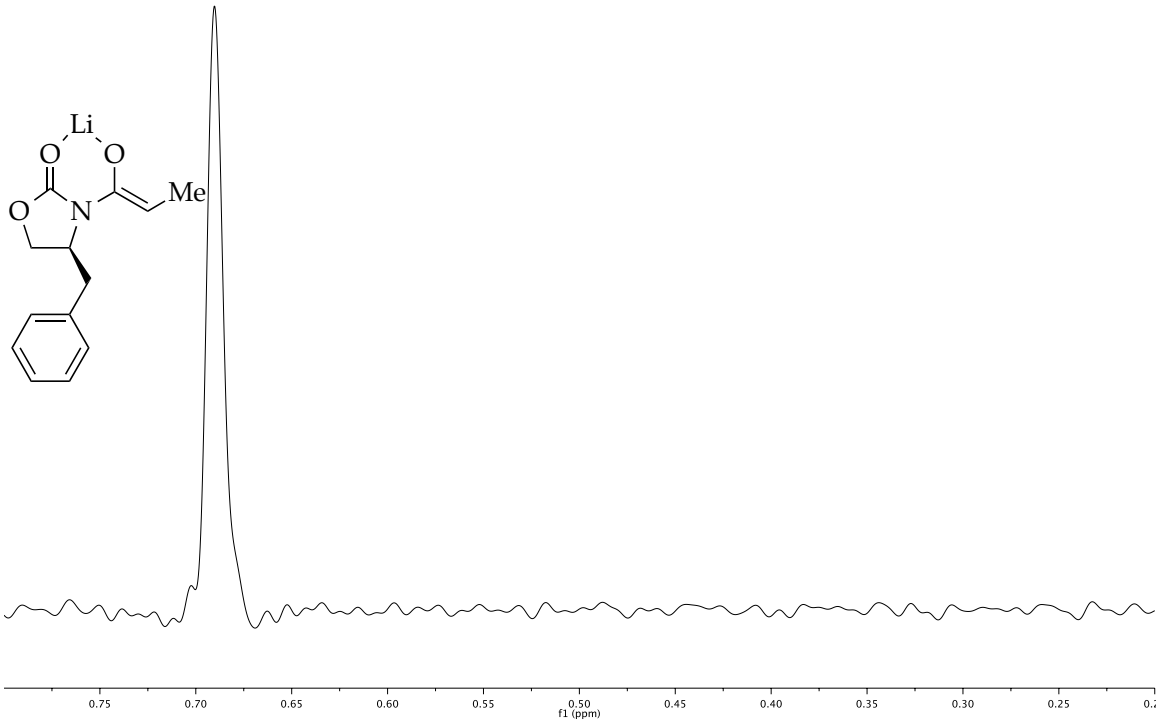


Figure 40. ^{6}Li NMR spectrum of **5** tetramer (0.10 M **5**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

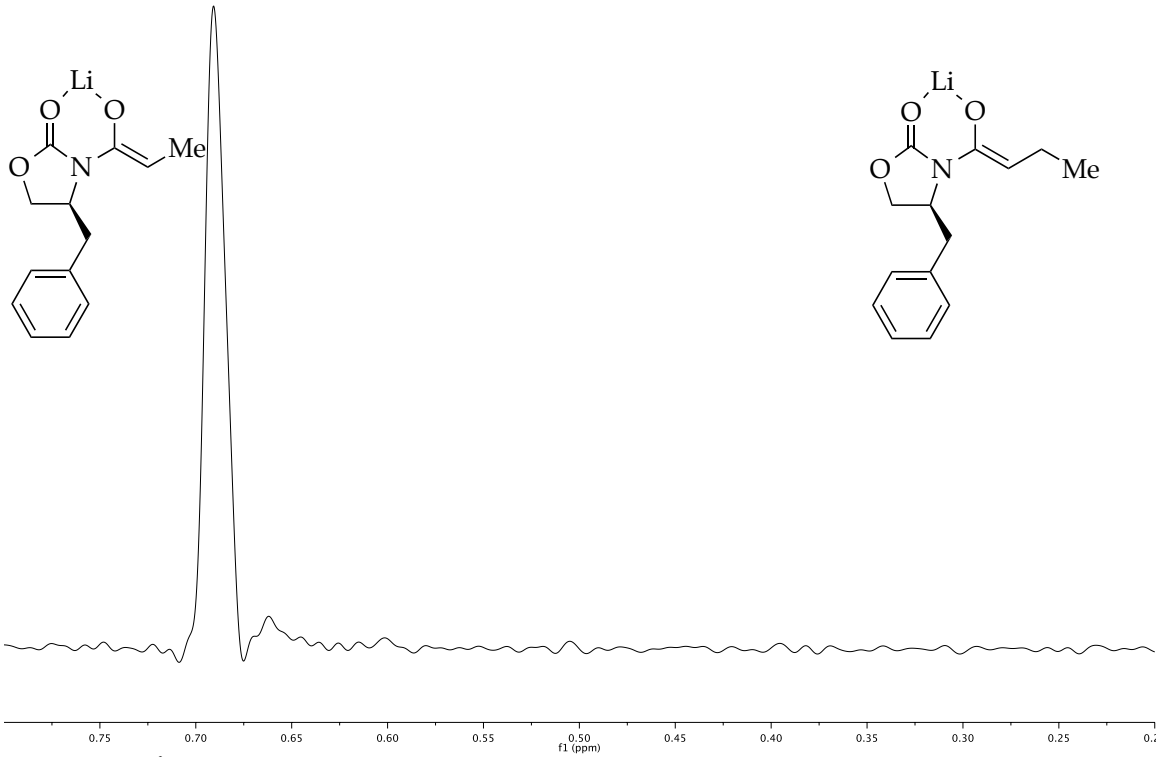


Figure 41. ^{6}Li NMR spectrum of a 9.8: 0.2 mixture of **5** and **6** tetramers (0.098 M **5**, 0.002M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

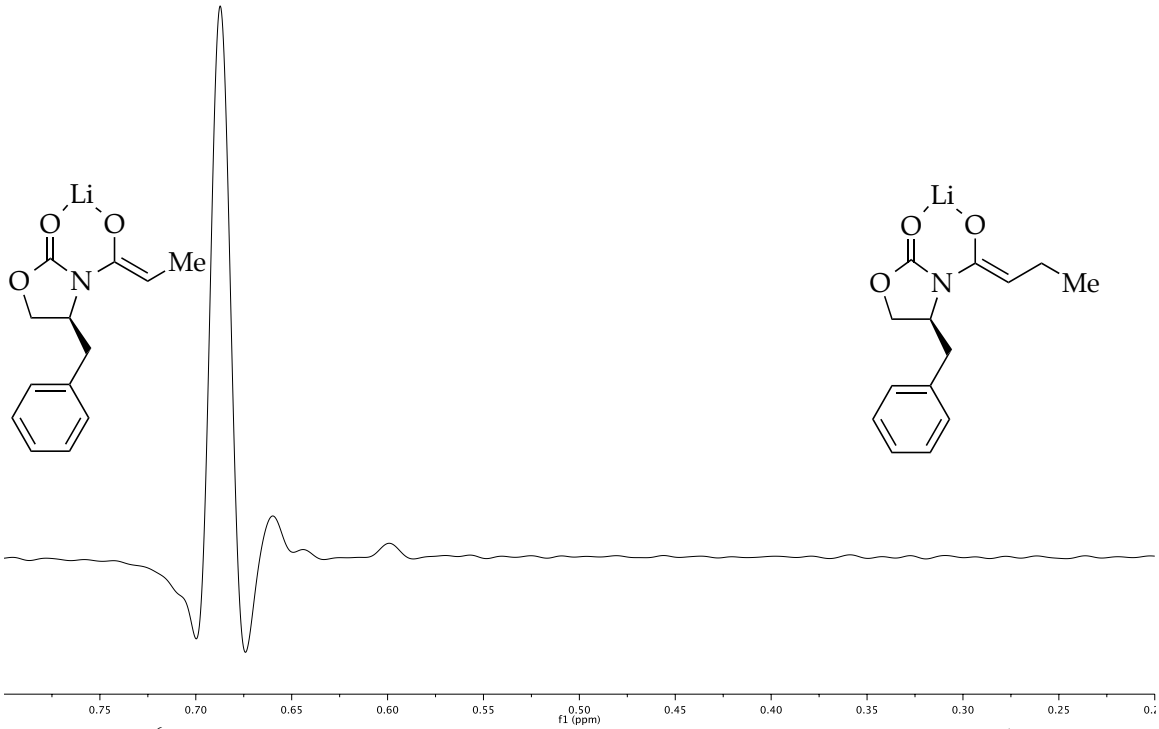


Figure 42. ^{6}Li NMR spectrum of a 9.6: 0.4 mixture of **5** and **6** tetramers (0.096 M **5**, 0.004M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

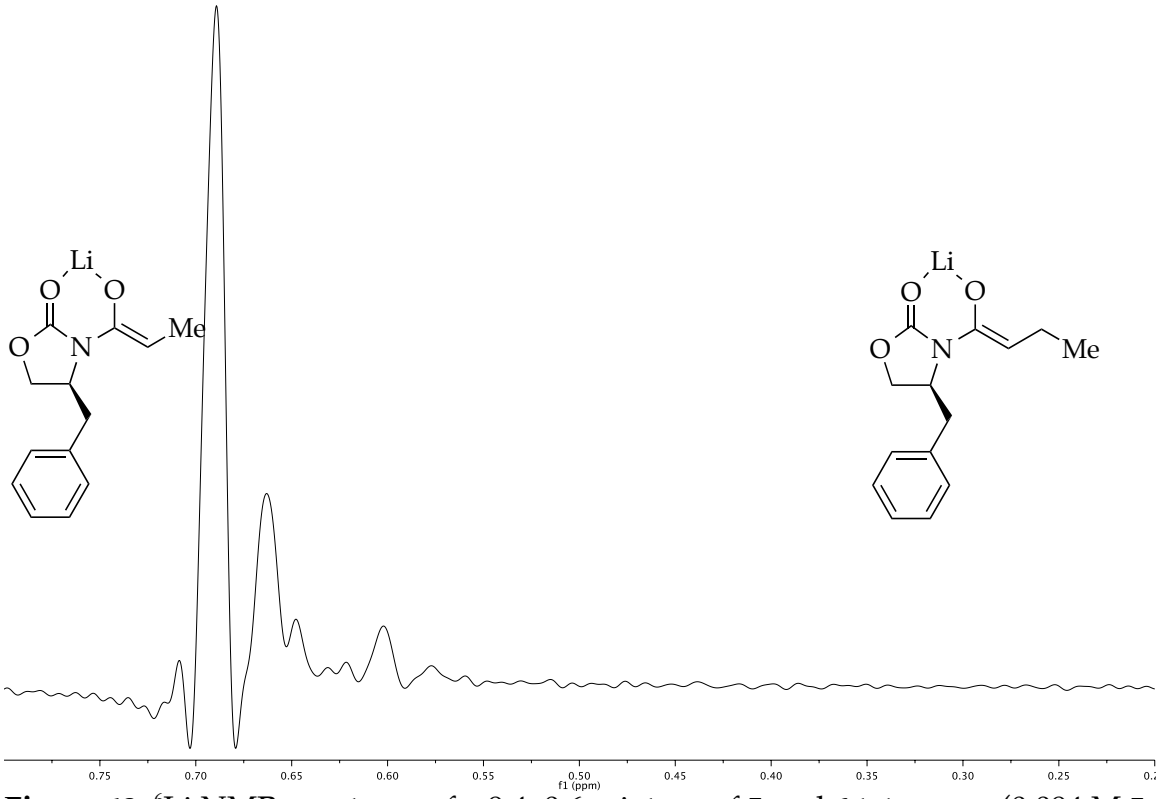


Figure 43. ^{6}Li NMR spectrum of a 9.4: 0.6 mixture of **5** and **6** tetramers (0.094 M **5**, 0.006 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

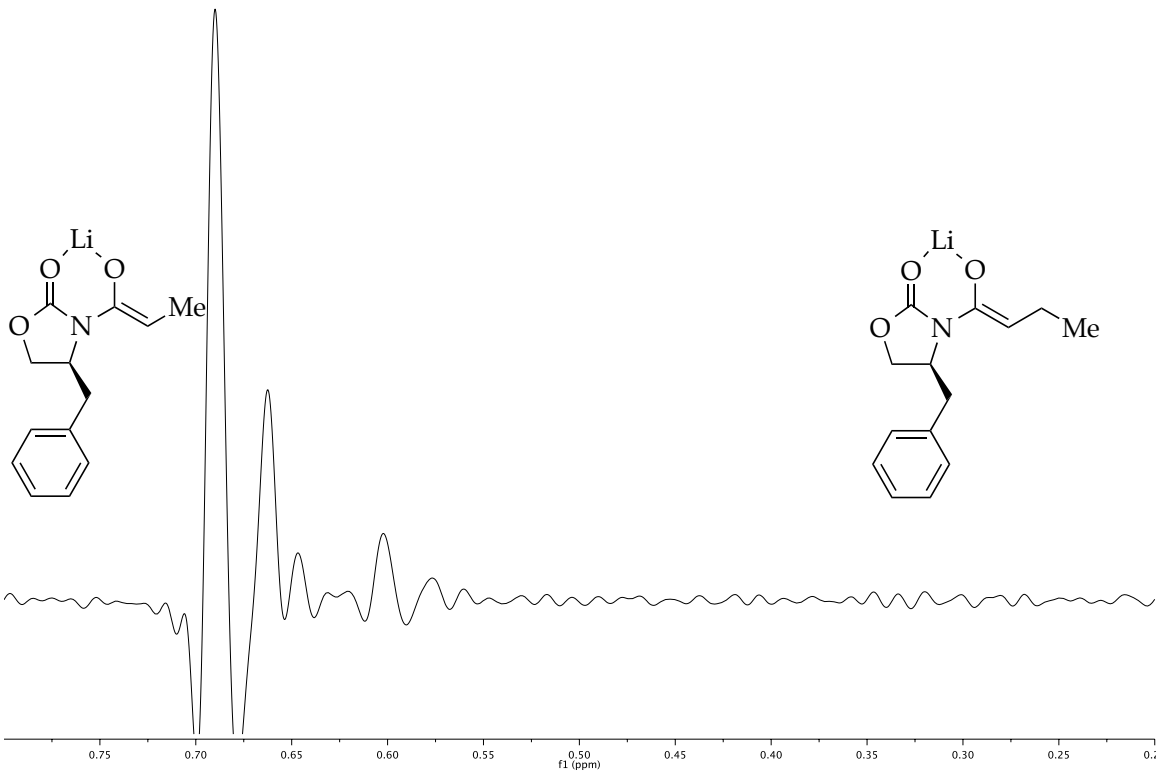


Figure 44. ^{6}Li NMR spectrum of a 9.2: 0.8 mixture of **5** and **6** tetramers (0.092 M **5**, 0.008 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

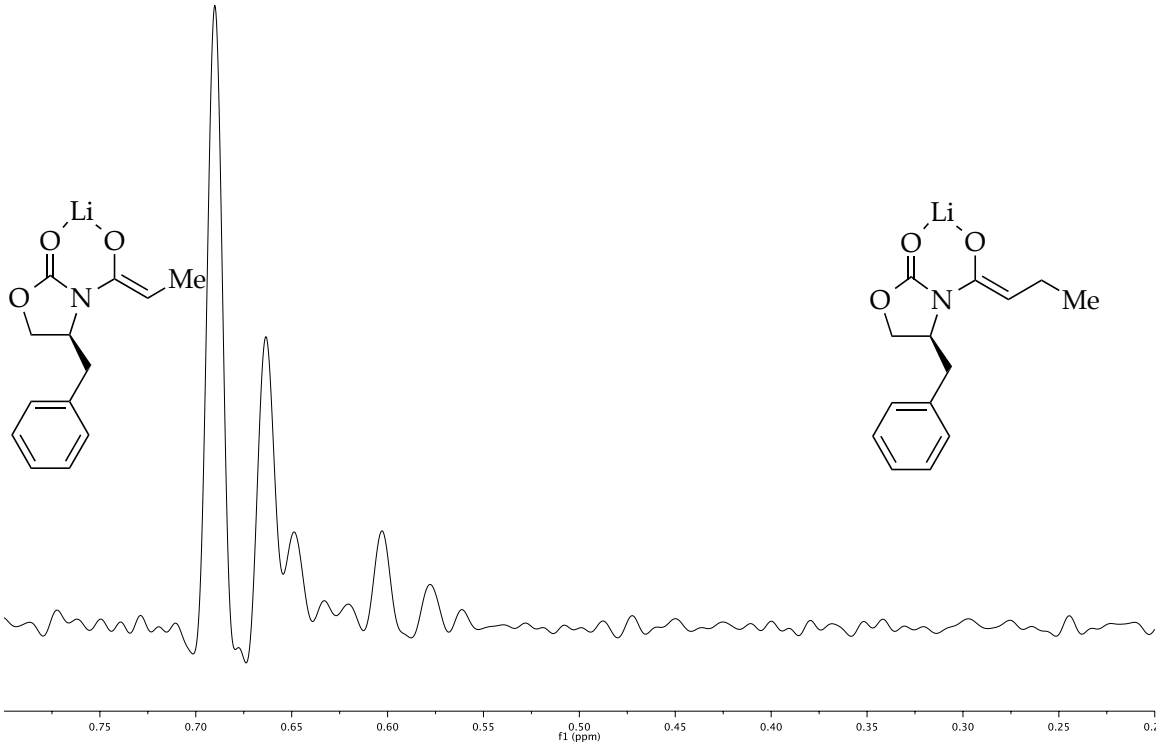


Figure 45. ^{6}Li NMR spectrum of a 9:1 mixture of **5** and **6** tetramers (0.090 M **5**, 0.010 M **6**) with 0.20 M THF and 1. 0 M pyridine in toluene at -60 °C.

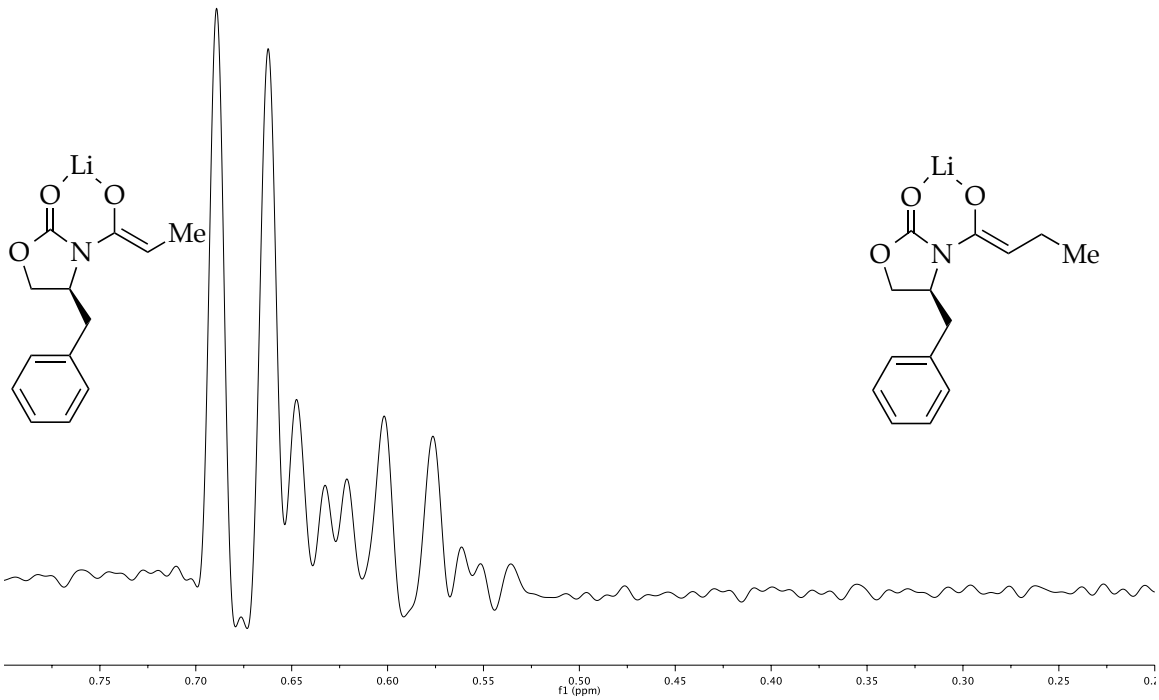


Figure 46. ^{6}Li NMR spectrum of a 8:2 mixture of **5** and **6** tetramers (0.080 M **5**, 0.020 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

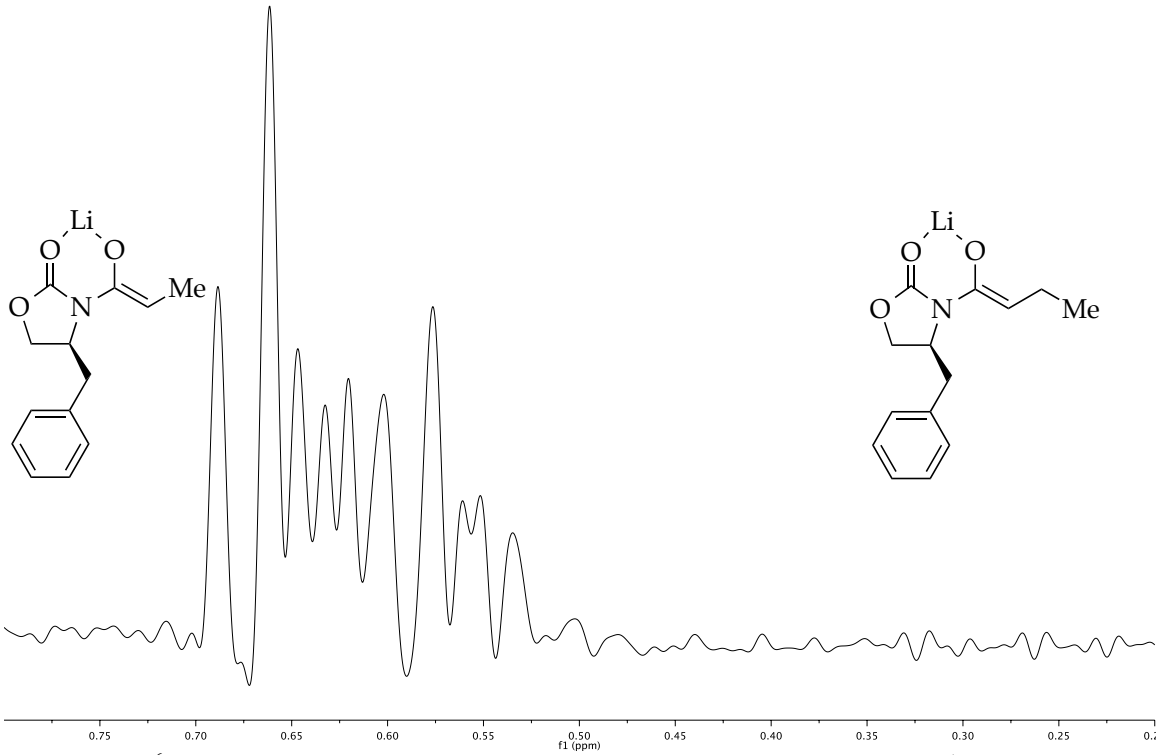


Figure 47. ^{6}Li NMR spectrum of a 7:3 mixture of **5** and **6** tetramers (0.070 M **5**, 0.030 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

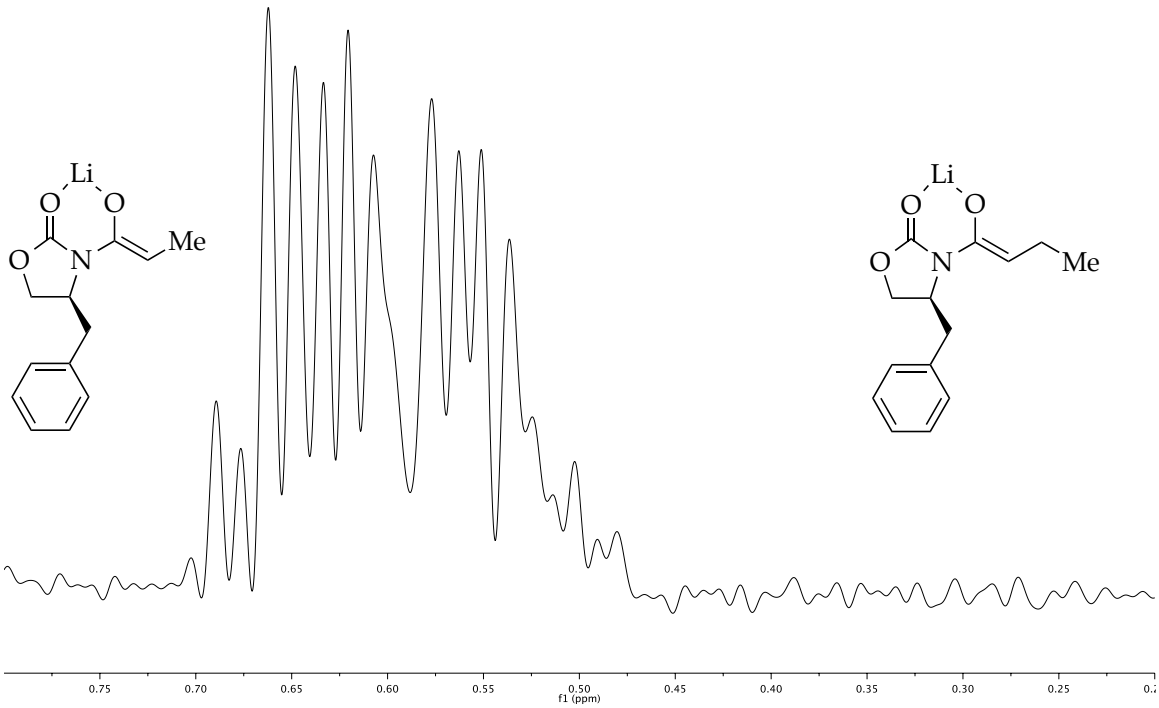


Figure 48. ^{6}Li NMR spectrum of a 6:4 mixture of **5** and **6** tetramers (0.060 M **5**, 0.040 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

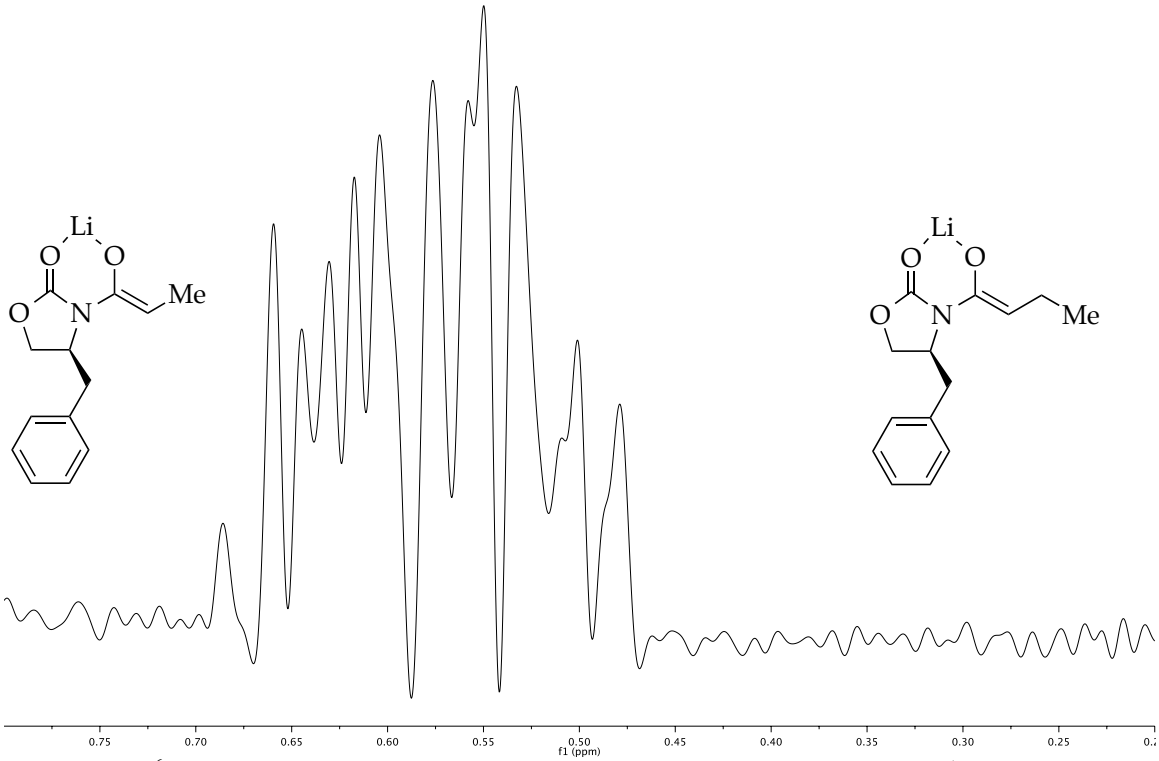


Figure 49. ^{6}Li NMR spectrum of a 5:5 mixture of **5** and **6** tetramers (0.050 M **5**, 0.050 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

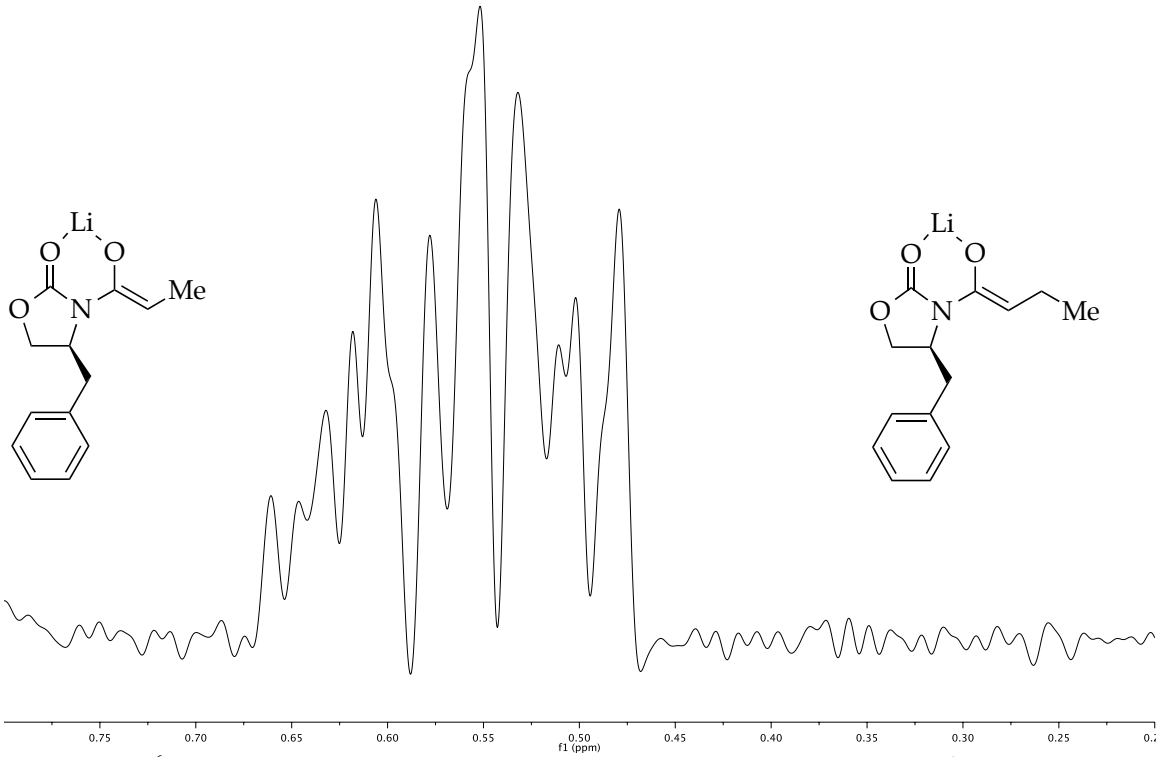


Figure 50. ^{6}Li NMR spectrum of a 4:6 mixture of **5** and **6** tetramers (0.040 M **5**, 0.060 M **6**) with 0.20 M THF and 1. 0 M pyridine in toluene at -60 °C.

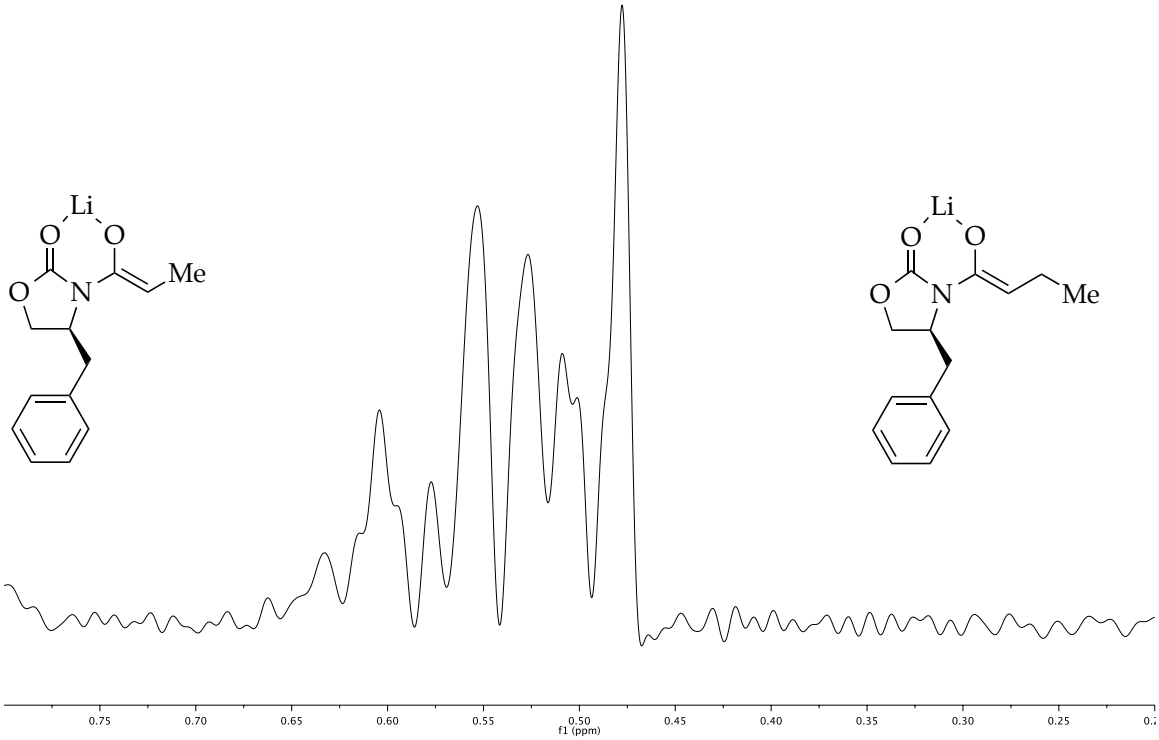


Figure 51. ^{6}Li NMR spectrum of a 3:7 mixture of **5** and **6** tetramers (0.030 M **5**, 0.070 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

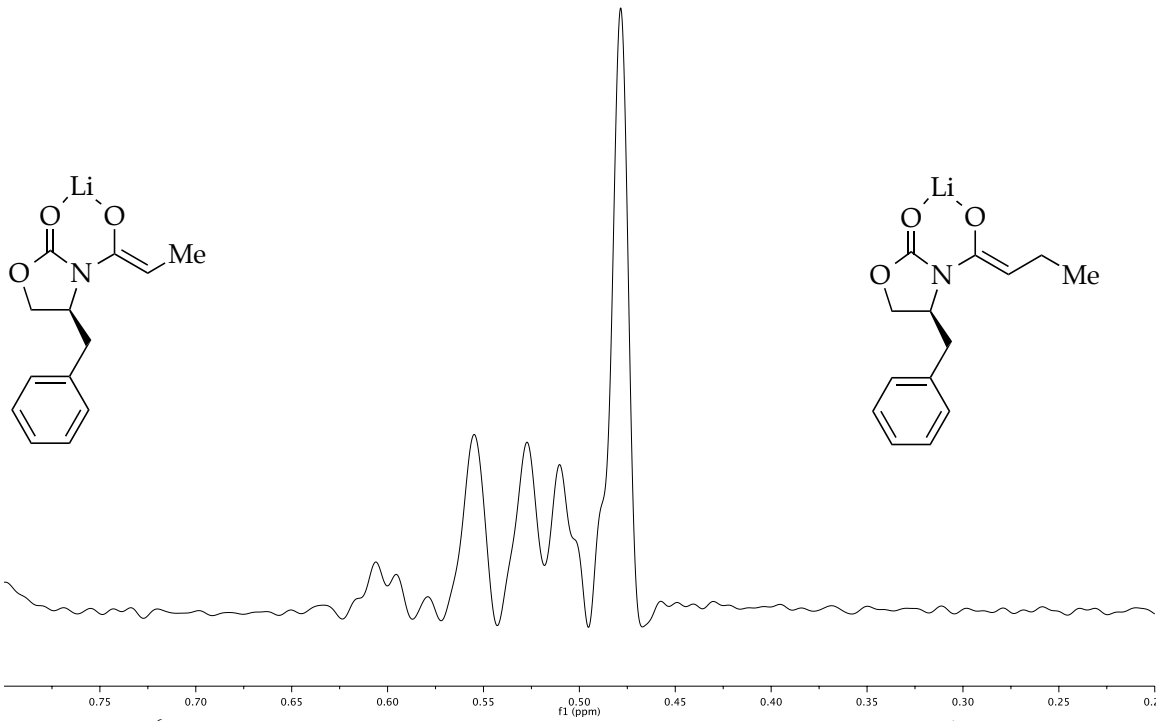


Figure 52. ^{6}Li NMR spectrum of a 2:8 mixture of **5** and **6** tetramers (0.020 M **5**, 0.080 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

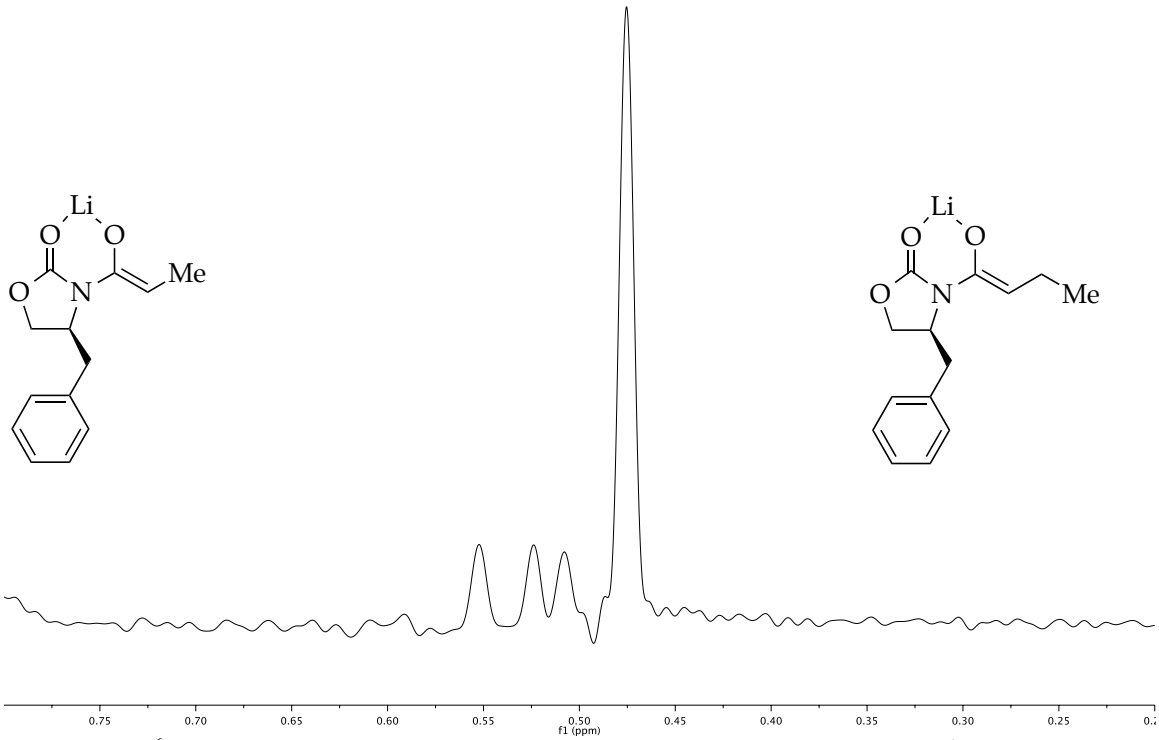


Figure 53. ^{6}Li NMR spectrum of a 1:9 mixture of **5** and **6** tetramers (0.010 M **5**, 0.090 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

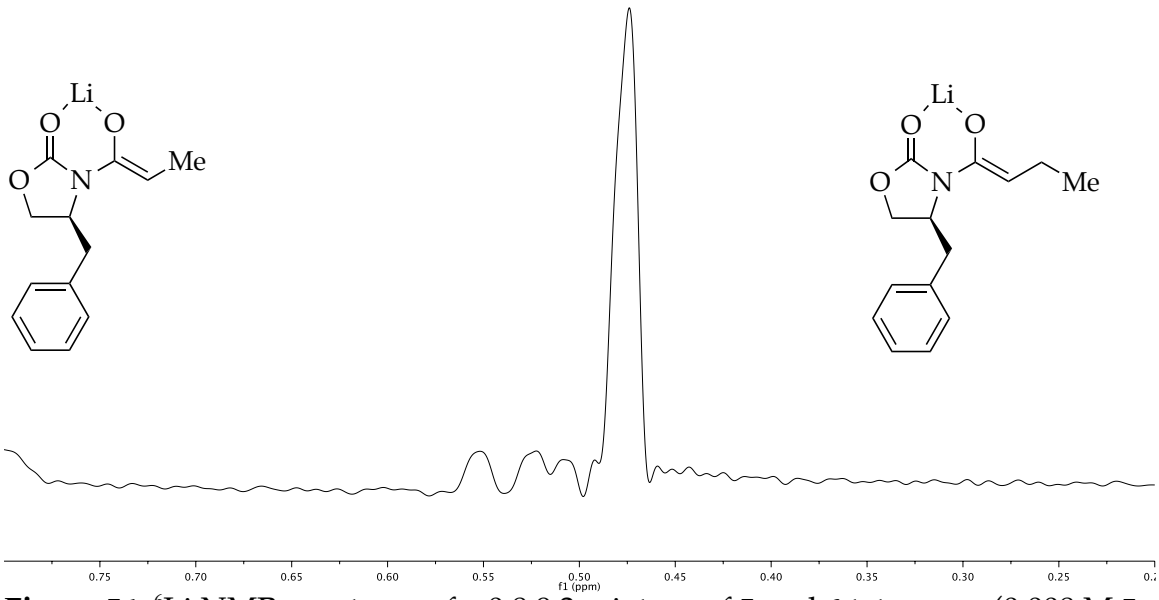


Figure 54. ^{6}Li NMR spectrum of a 0.8:9.2 mixture of **5** and **6** tetramers (0.008 M **5**, 0.092 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

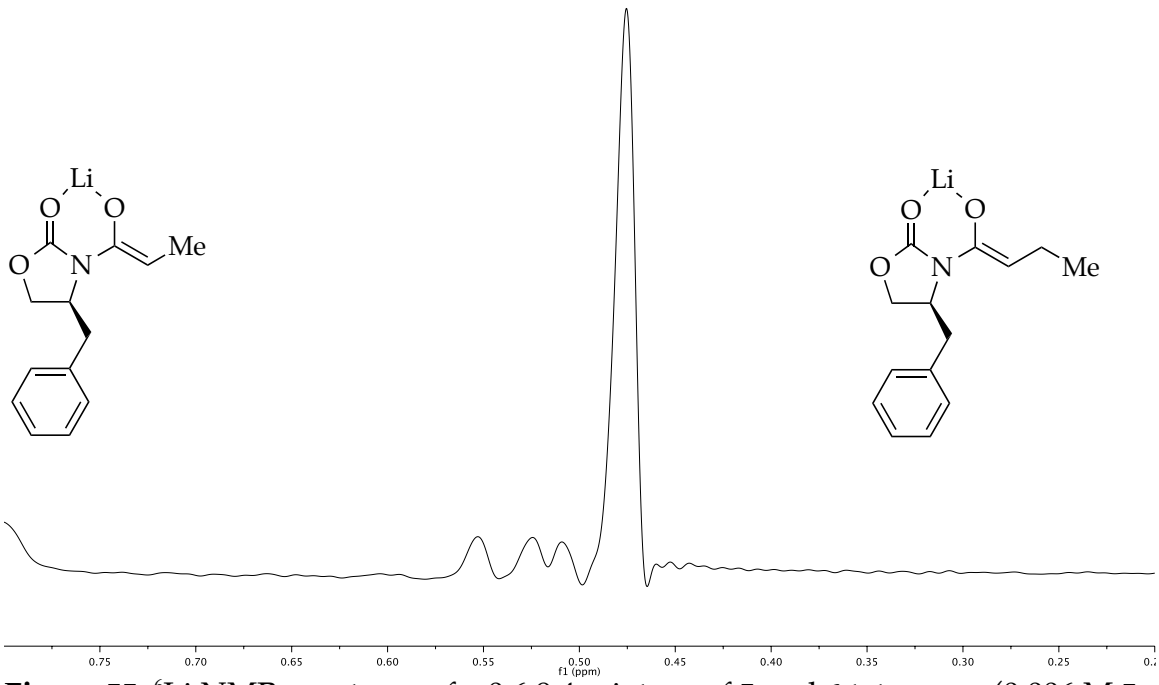


Figure 55. ^{6}Li NMR spectrum of a 0.6:9.4 mixture of **5** and **6** tetramers (0.006 M **5**, 0.094 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

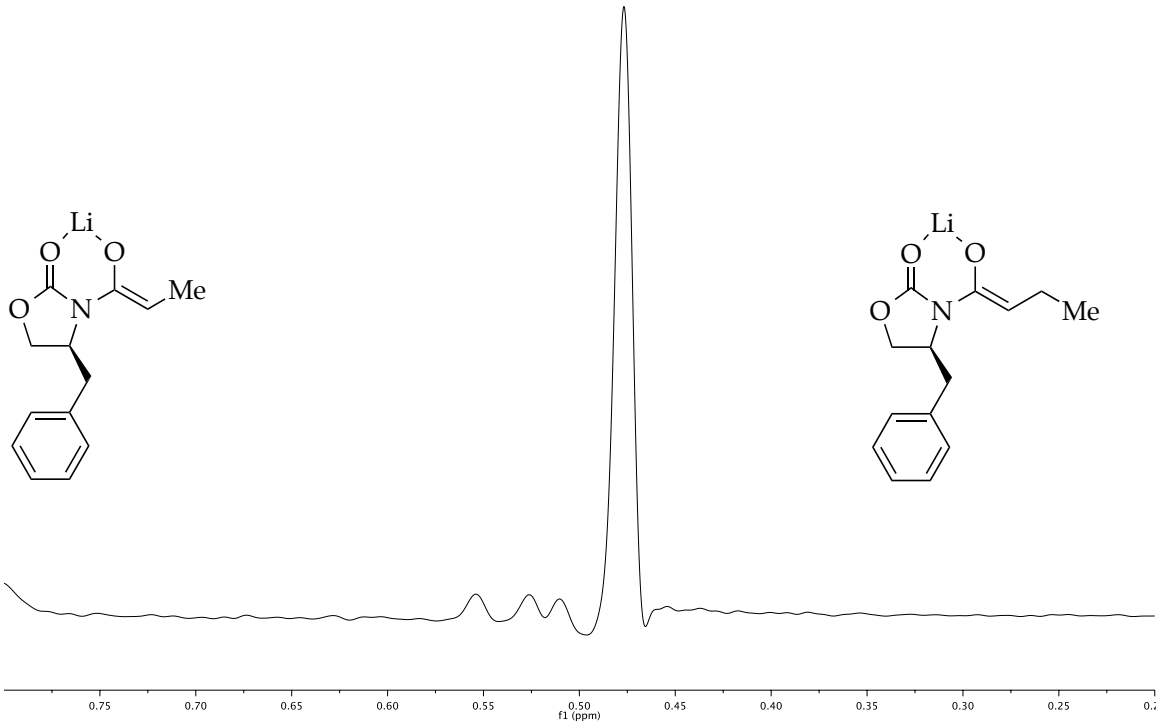


Figure 56. ^{6}Li NMR spectrum of a 0.4:9.6 mixture of **5** and **6** tetramers (0.004 M **5**, 0.096 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

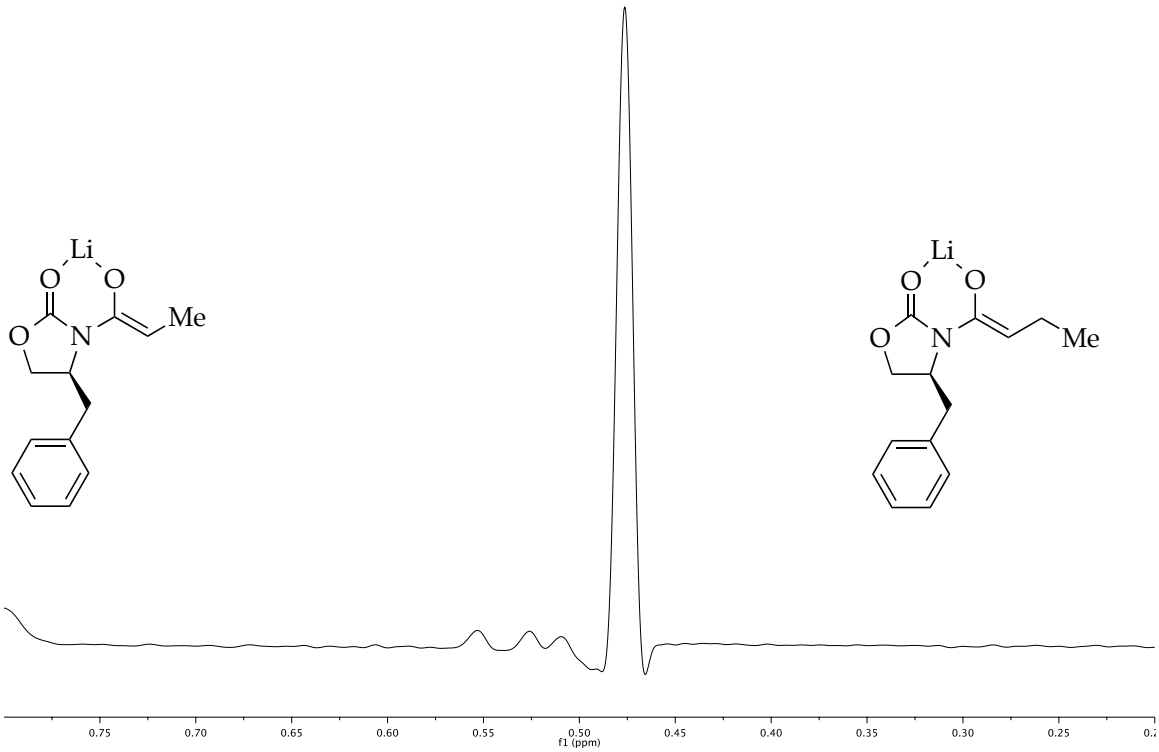


Figure 57. ^{6}Li NMR spectrum of a 0.2:9.8 mixture of **5** and **6** tetramers (0.002 M **5**, 0.098 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

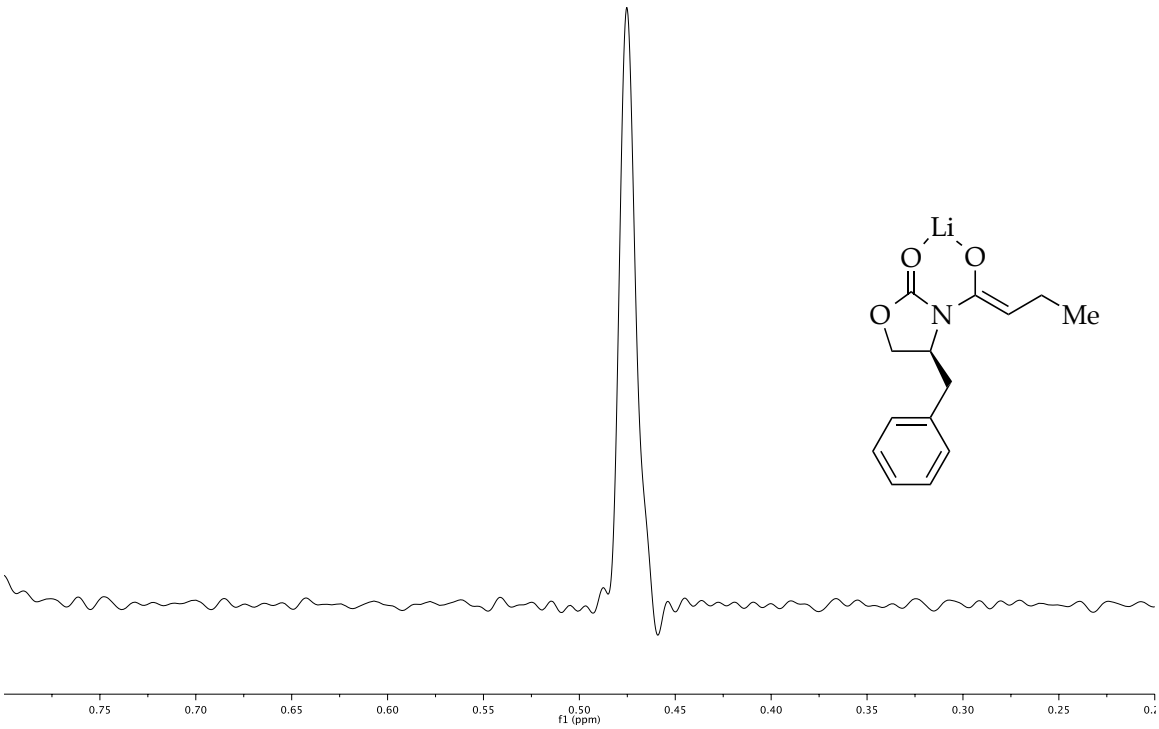


Figure 58. ^{6}Li NMR spectrum of **6** tetramer (0.10 M **6**) with 0.20 M THF and 1.0 M pyridine in toluene at -60 °C.

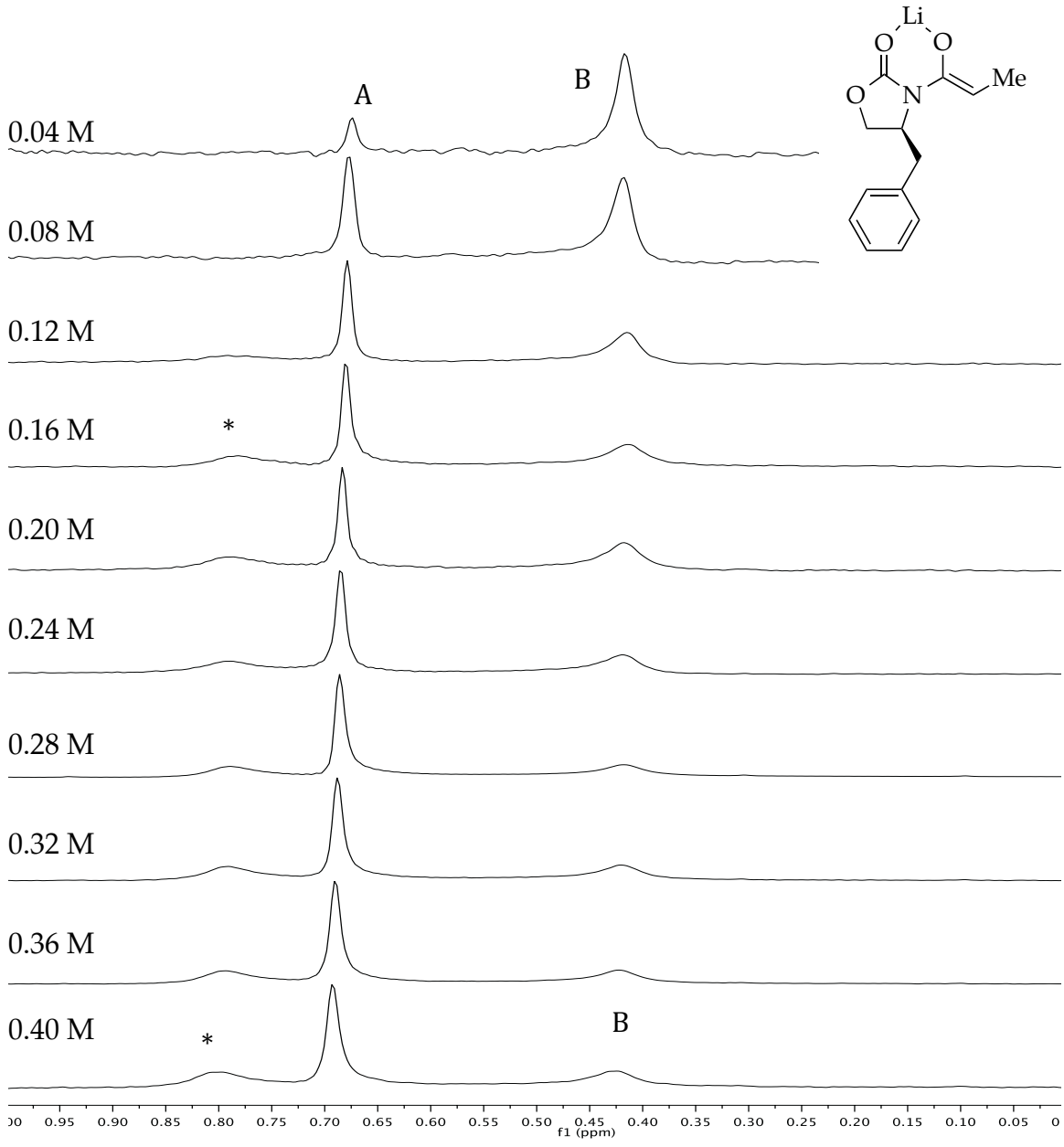


Figure 59. ^{6}Li NMR spectra of **5** (**5**, 1.1 equiv [^{6}Li]LDA) with varying enolate concentrations (as labeled) in neat THF at –60 °C. **A** is the unsolvated tetramer; **B** is the coalesced trisolvated dimers. The mixed aggregate is marked by *.

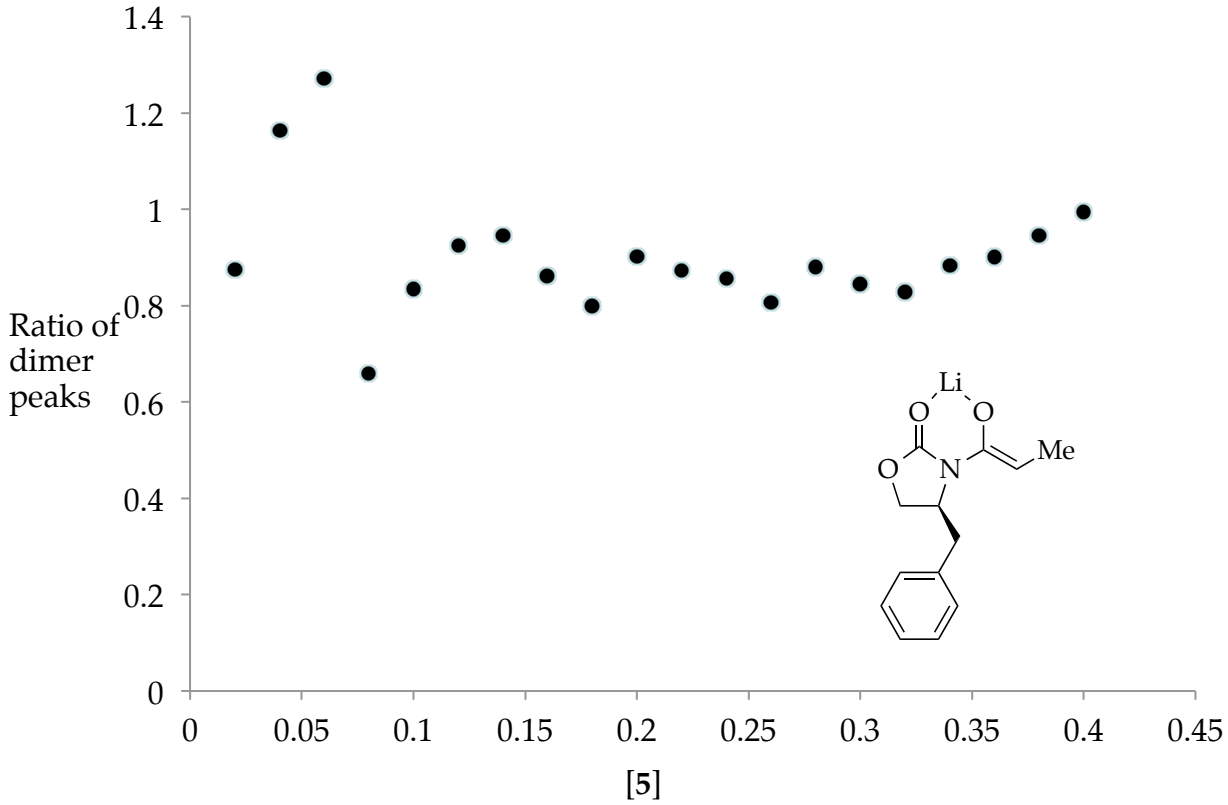


Figure 60. Plot of the relative integrations of the two dimers of **5** at 0.10 M in neat THF at -80°C.

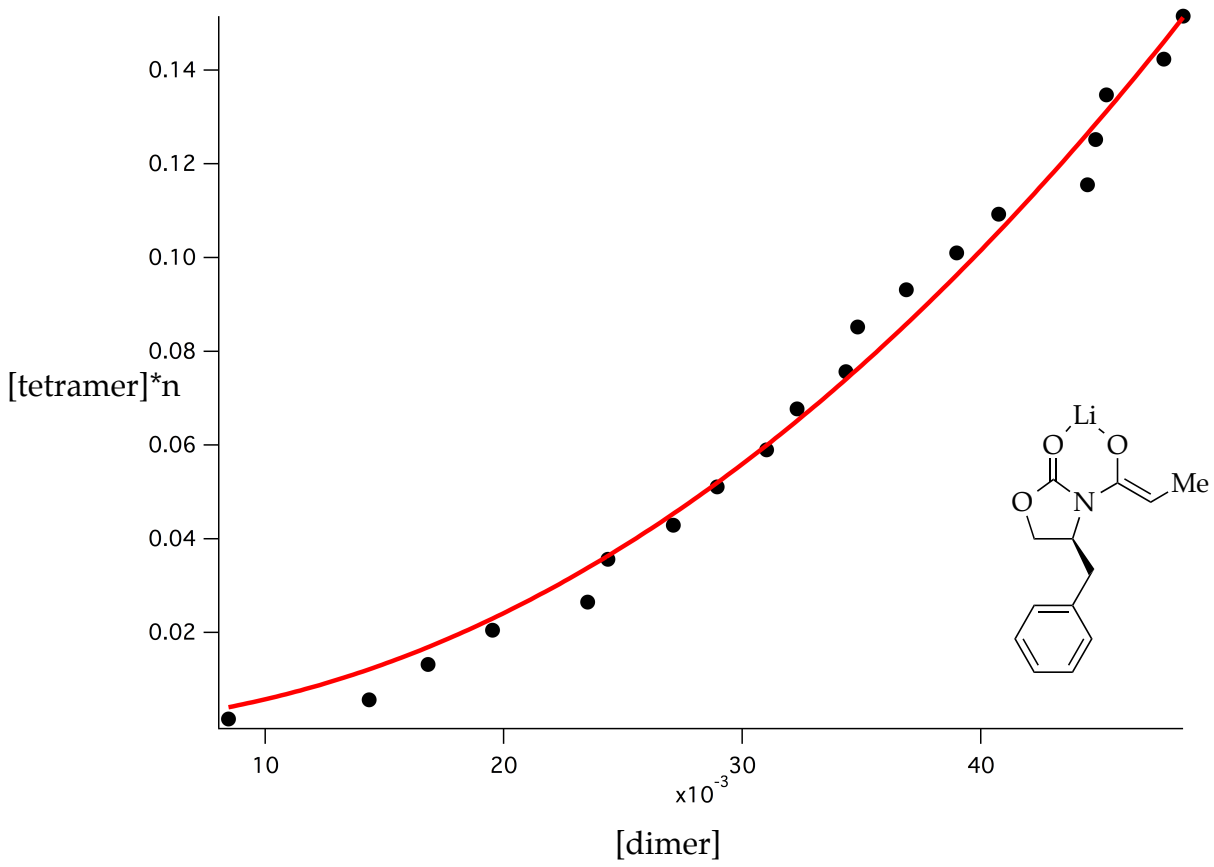


Figure 61. Fit of dimer concentration vs. tetramer concentration for **5** to determine the tetramer aggregation state at –60 °C. The best fit, in red, gives a aggregation number of the higher aggregate, now known to be tetramer, of 4.1 ± 0.2. The fitting equation was $Y = n * {K_{eq}}^{1/2} X^{n/2}$ The derivation of this expression follows (pg. 76).

Equation 1. Explanation for the fitting equation of **Figure 35.**

$$\text{Let } A_n \equiv \text{ Aggregate with aggregation number } n$$
$$\text{Let } A_2 \equiv \text{ Dimer aggregate}$$

$$n\,A_2 \leftrightharpoons 2\,A_n$$
$$\text{Therefore } K_{eq} = \frac{[A_n]^2}{[A_2]^n}$$

$$\text{Let } \chi_{A_2} \equiv \text{ Mole fraction of A in dimer aggregate}$$
$$\text{Let } \chi_{A_n} \equiv \text{ Mole fraction of A in aggregate with aggregation number } n$$

$$\text{Let } I_n \equiv \text{ NMR integration of peak of aggregate with aggregation number } n$$
$$\text{Let } I_D \equiv \text{ NMR integration of peak of dimer aggregate}$$

$$\text{Therefore } \chi_{A_2} = \frac{I_D}{I_D + I_n}$$
$$\text{and } \chi_{A_n} = \frac{I_n}{I_D + I_n}$$

$$\text{Let } C_{tot} \equiv \text{ Total concentration of enolate in solution}$$

$$\text{Therefore } [A_2] = \frac{I_D}{I_D + I_n}\left(\frac{C_{tot}}{2}\right)$$
$$\text{and } [A_n] = \frac{I_n}{I_D + I_n}\left(\frac{C_{tot}}{n}\right)$$

$$\text{Rearrange } K_{eq} \text{ equation to give } [A_n] = {K_{eq}}^{1/2}\,[A_2]^{n/2}$$

$$\text{substitute integrations for concentrations } \frac{I_n}{I_D + I_n}\left(\frac{C_{tot}}{n}\right) = {K_{eq}}^{1/2}\left(\frac{I_D}{I_D + I_n}\left(\frac{C_{tot}}{2}\right)\right)^{n/2}$$

$$\text{multiply by } n \quad \frac{I_n\,C_{tot}}{I_D + I_n} = n * {K_{eq}}^{1/2}\left(\frac{I_D}{I_D + I_n}\left(\frac{C_{tot}}{2}\right)\right)^{n/2}$$

$$\text{Plug in values for } I_n, I_D, \text{ and } C_{tot}$$

This gives you

$$Y = n * {K_{eq}}^{1/2}\,X^{n/2}$$

where

$$Y = \frac{I_n\,C_{tot}}{I_D + I_n} = n * [A_n]\,; \quad X = \frac{I_D}{I_D + I_n}\left(\frac{C_{tot}}{2}\right) = [A_2]$$

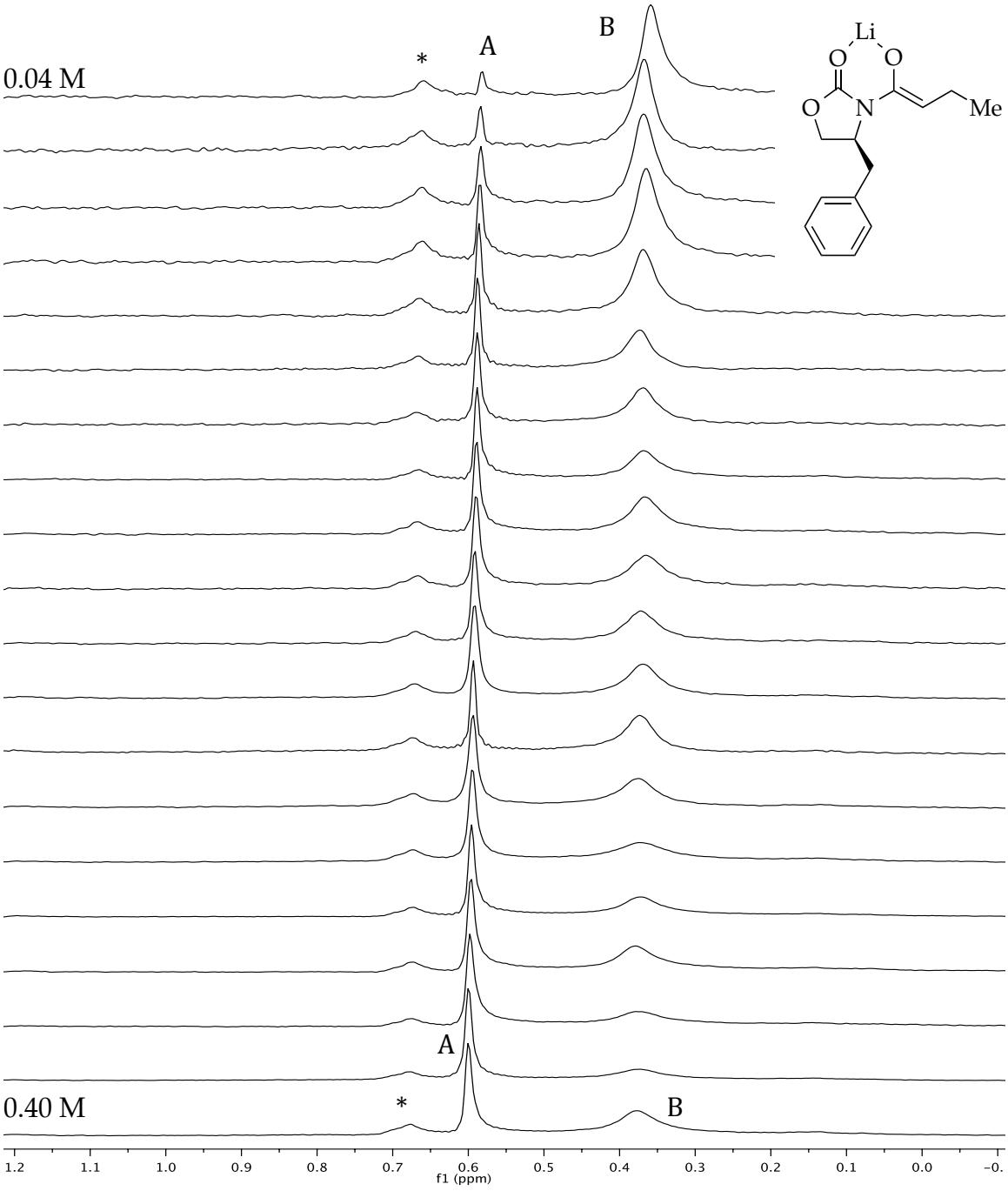


Figure 62. ^{6}Li NMR spectra of **6** with varying enolate concentrations (as labeled) in neat THF at –40 °C. **A** is the unsolvated tetramer; **B** is the coalesced trisolvated dimers. The LDA-**6** mixed dimer is marked *.

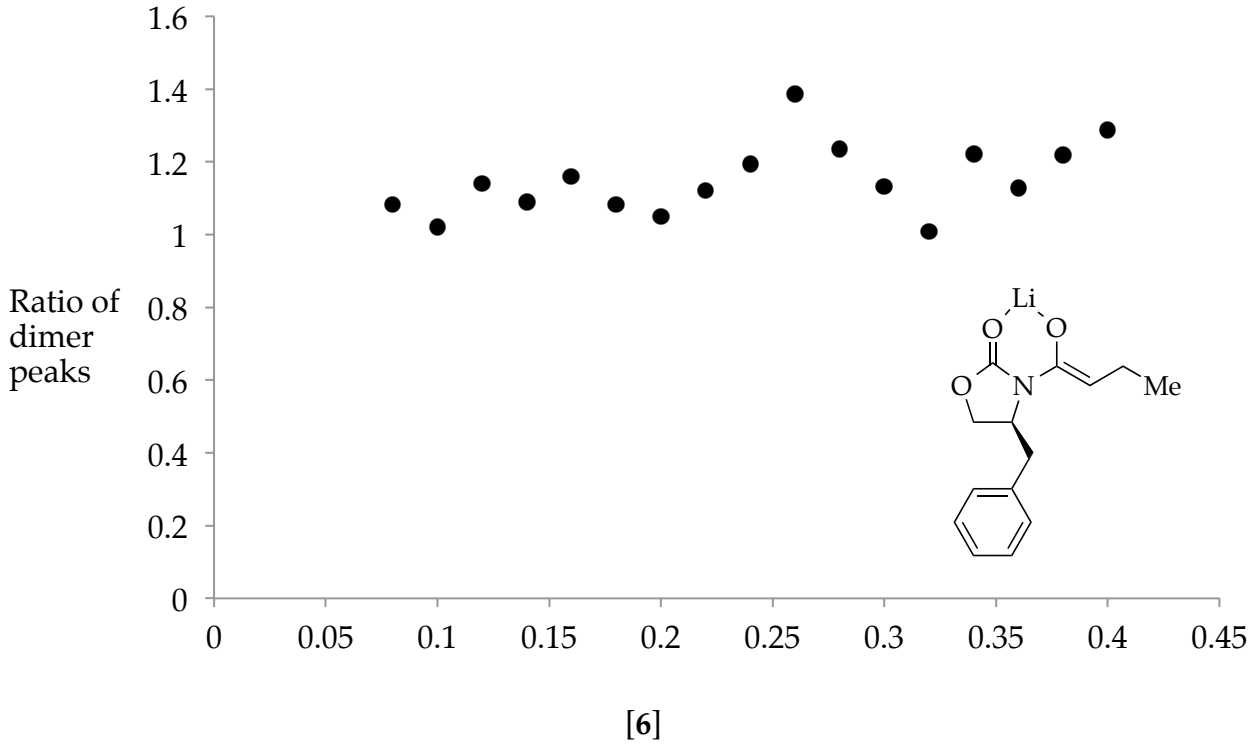


Figure 63. Plot of the relative integrations of the two dimers of **6** at 0.10 M in neat THF at -80°C.

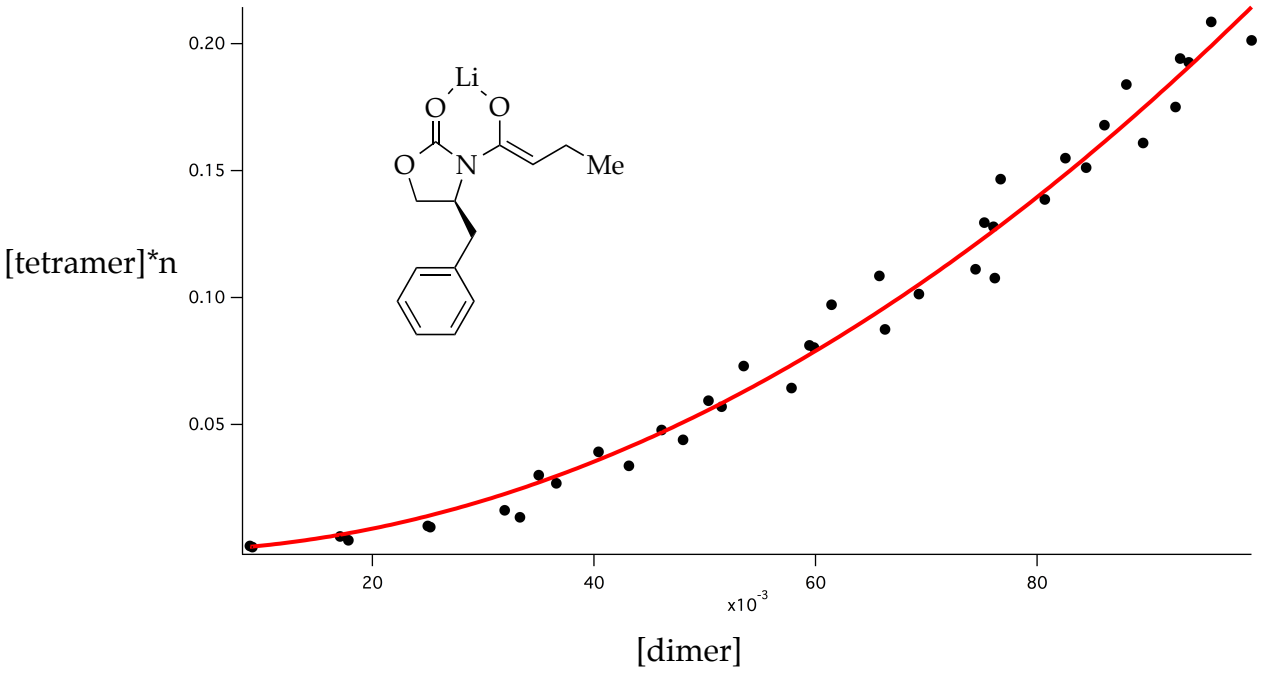


Figure 64. Fit of dimer concentration vs. tetramer concentration for **6** to determine the tetramer aggregation state at –40 °C. The best fit, in red, gives a aggregation number of the higher aggregate, now known to be tetramer, of 4.0 ± 0.1. The fitting equation was $Y = n * {K_{eq}}^{1/2} X^{n/2}$

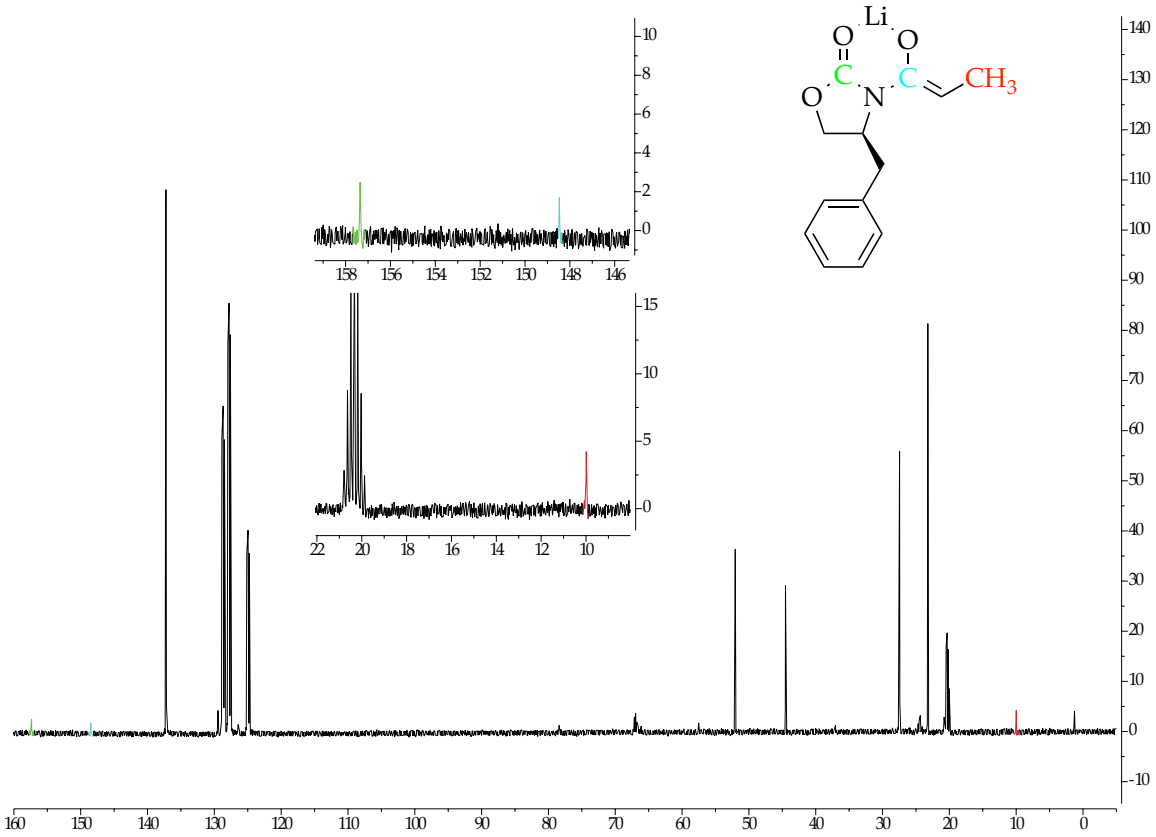


Figure 65. ^{13}C NMR spectrum of **5** tetramer at 0.3 M with 0.60 M D_8 THF in D_8 toluene at –80 °C.

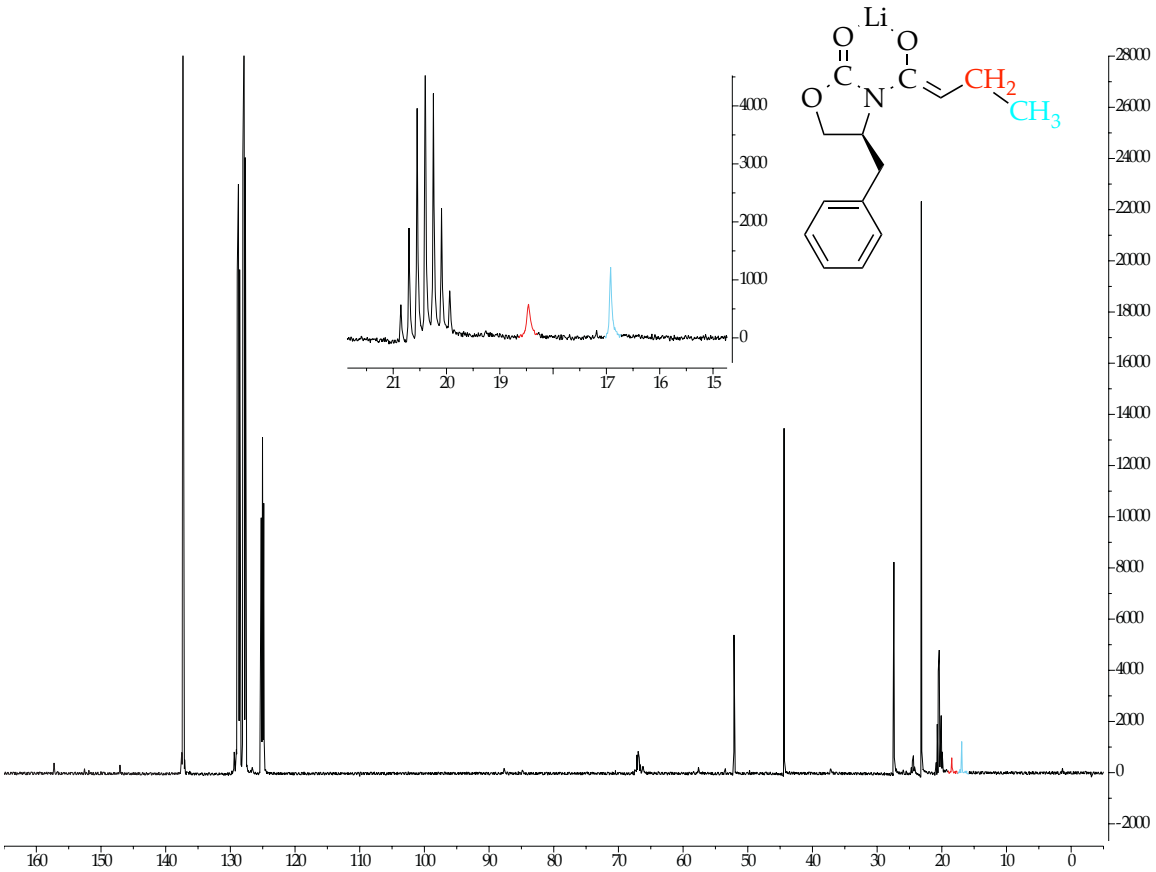


Figure 66. ^{13}C NMR spectrum of **6** tetramer at 0.30 M with 0.60 M D_8 THF in D_8 toluene at –80 °C.

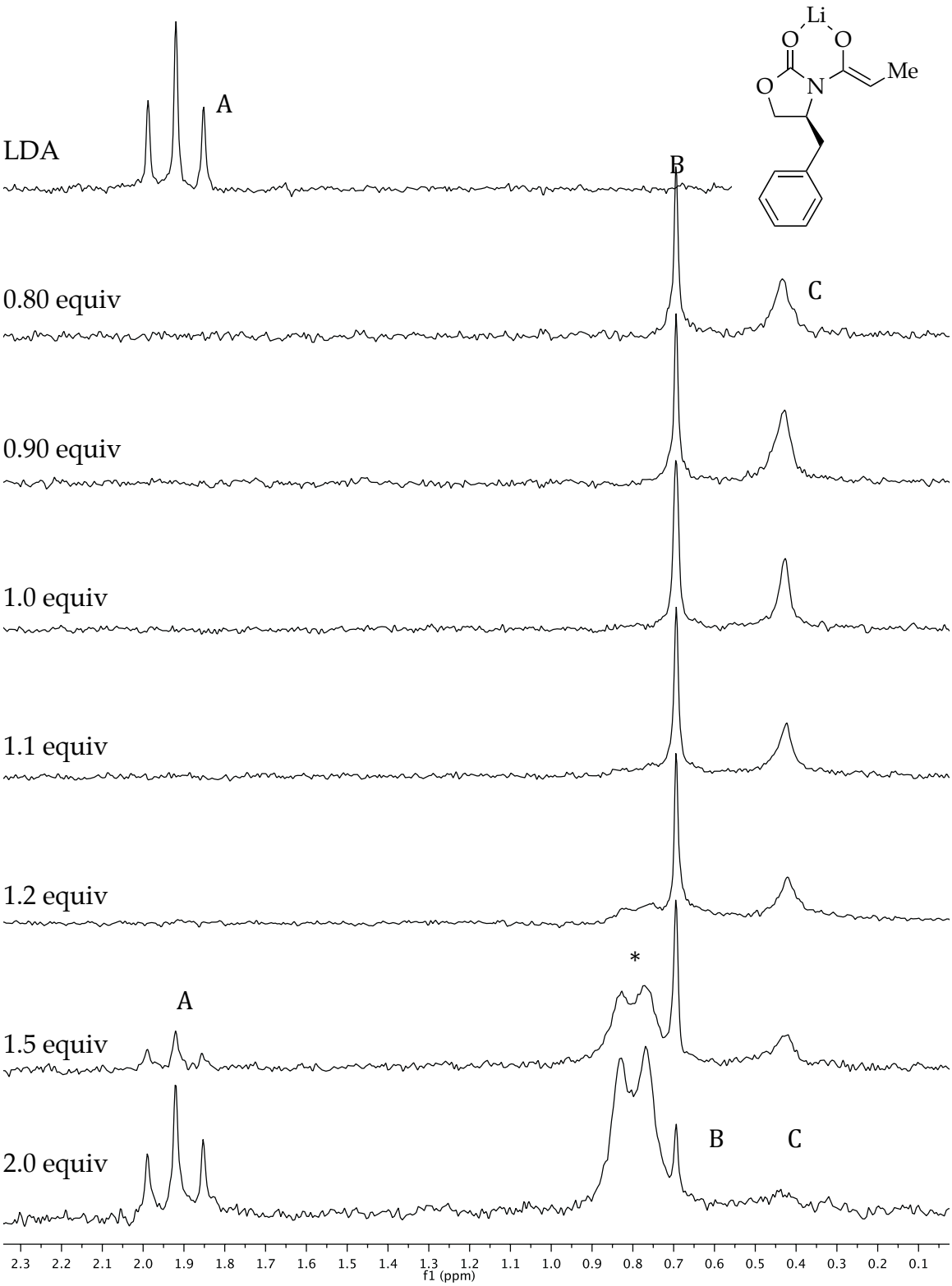


Figure 67. ^{6}Li NMR NMR spectra of **5** (0.20 M) with changing [^{6}Li^{15}N]LDA ratio to the oxazolidinone (as labeled) in THF at –60 °C. **A** is free LDA; **B** is the unsolvated tetramer; **C** is the coalesced trisolvated dimers. The mixed aggregate is labeled *.

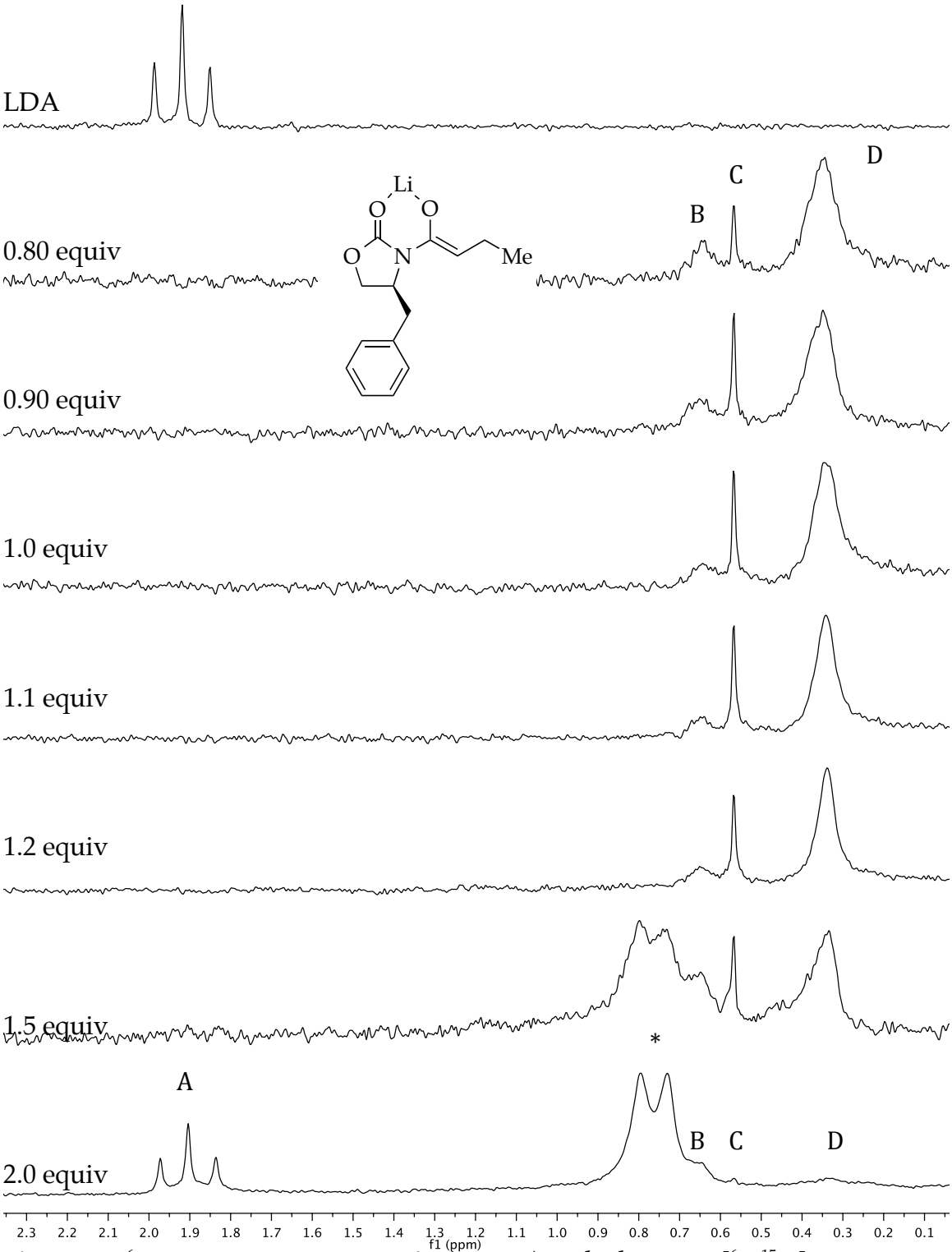
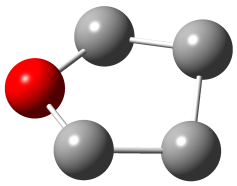


Figure 68. ^{6}Li NMR NMR spectra of **6** (0.20 M) with changing [^{6}Li^{15}N]LDA ratio to the oxazolidinone (as labeled) in THF at –60 °C. **A** is free LDA; **B** is an unidentified dimeric species; **C** is the unsolvated tetramer; **D** is the coalesced trisolvated dimers. The mixed aggregate is labeled *.

Part 5: Dimer Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

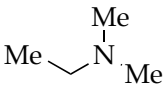
Table 1. Geometric coordinates and thermally corrected MP2 energies for tetrahydrofuran (THF)

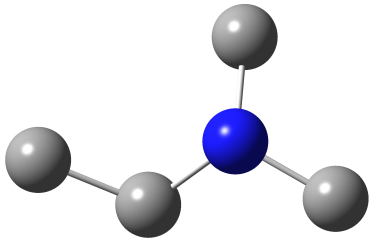


G = -232.349382 Hartree
G_{MP2} = -145312.2903 kcal/mol

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.43133070
C	1.34537191	0.00000000	1.92150203
C	2.24870259	-0.28439627	0.71435321
C	1.43346820	0.33130215	-0.43248249
H	1.58213073	1.41736875	-0.46518645
H	1.68560870	-0.07569023	-1.41670971
H	3.24887201	0.14691464	0.82158362
H	2.35937654	-1.36515207	0.56460786
H	1.57260400	0.98256813	2.36334488
H	1.43285191	-0.75428594	2.71251317
H	-0.30387867	-0.99259206	-0.36803060
H	-0.73798112	0.73090835	-0.35071740

Table 2. Geometric coordinates and thermally corrected MP2 energies for dimethylethylamine (DMEA)

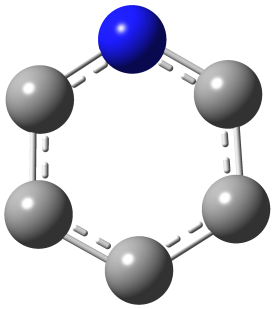




G = -213.656331 Hartree
G_{MP2} = -133573.4354 kcal/mol

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09511810
H	1.04043539	0.00000000	-0.34193630
H	-0.47224561	-0.93380791	-0.32540421
C	-0.75205325	1.19677634	-0.58416956
H	-0.81656889	1.07110229	-1.67205850
H	-1.79673181	1.20085851	-0.20762815
N	-0.09071955	2.47976222	-0.33981037
C	-0.67790172	3.53649446	-1.15184252
H	-1.74296806	3.73451525	-0.91419588
H	-0.12224763	4.46891836	-1.00194973
H	-0.61257345	3.26942003	-2.21241151
C	-0.08827282	2.85432427	1.06791224
H	-1.10807776	2.97189950	1.48856739
H	0.44004187	2.10512460	1.66424416
H	0.43834518	3.80705756	1.19019208

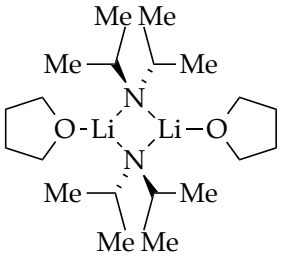
Table 3. Geometric coordinates and thermally corrected MP2 energies for pyridine

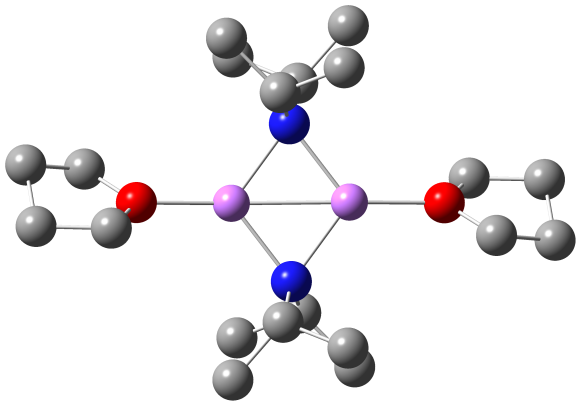


G = -248.212568 Hartree
G_{MP2} = -155252.1531 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000				
C	0.00000000	0.00000000	1.39609960				
C	1.22655027	0.00000000	2.05951808				
C	2.39559516	-0.00004988	1.29934943				
C	2.28298997	-0.00008897	-0.09220166				
N	1.11328009	-0.00003428	-0.74460037				
H	3.17588827	-0.00008126	-0.71582762				
H	3.37453495	-0.00004989	1.76972338				
H	1.27039061	-0.00001990	3.14554958				
H	-0.93779193	0.00002936	1.94392949				
H	-0.94029065	0.00000213	-0.54957532				

Table 4. Geometric coordinates and thermally corrected MP2 energies for lithium diisopropylamide (LDA) with two THF



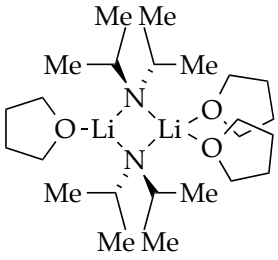


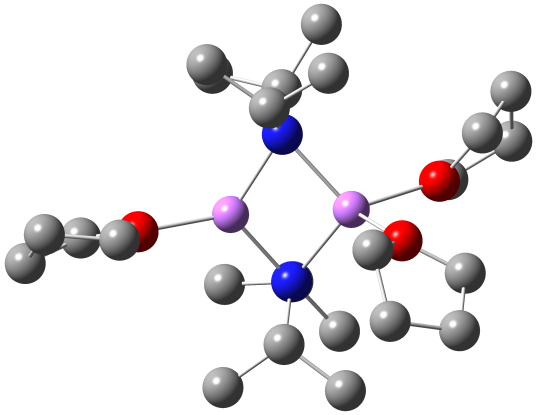
G = -1063.116483 Hartree
G_{MP2} = -664731.8875 kcal/mol
ΔG_{MP2} = 0 kcal/mol vs. LDA with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.01845863	2.50549465	0.96165094
Li	0.00000000	0.00000000	2.39346480	H	-1.81410663	1.86918792	0.52758664
O	0.40731818	0.00000000	4.33666642	C	-0.80797530	3.64048612	-0.06969212
C	-0.31160577	0.75031532	5.34554741	H	-1.76144100	4.13531583	-0.30044256
C	0.59705523	0.76867204	6.57773040	H	-0.12686892	4.41415138	0.30277974
C	1.38039926	-0.54444431	6.42411418	H	-0.38833529	3.25131946	-1.00453270
C	1.58550803	-0.61184065	4.91113852	C	-1.67694186	3.10542503	2.23352810
H	1.66334155	-1.62770125	4.51728807	H	-1.90764523	2.30725174	2.94980958
H	2.46883665	-0.03867321	4.59941701	H	-1.02725739	3.83103093	2.73422227
H	0.77815914	-1.39416582	6.76657132	H	-2.61874741	3.61787491	1.98945185
H	2.32593881	-0.55203312	6.97432432	N	-0.10056751	-1.58942643	1.19475018
H	0.02933285	0.82892055	7.51087129	C	-1.45024064	-2.11026018	0.94660834
H	1.27894121	1.62608966	6.53832804	H	-2.01730929	-1.24034090	0.55530667
H	-0.52831103	1.74382359	4.94463141	C	-2.25393575	-2.53615677	2.20621616
H	-1.25863823	0.23405677	5.54777776	H	-1.88302644	-3.47070131	2.63922295
N	0.10065090	1.58940008	1.19844710	H	-2.18688374	-1.76102302	2.97989617
C	1.45061143	2.11134115	1.44268300	H	-3.31687937	-2.68187367	1.96567937
H	2.01816461	1.24325327	1.83719553	C	-1.61016658	-3.20211490	-0.13915451
C	2.25270052	2.53174806	0.18014310	H	-1.12639271	-2.89814436	-1.07426675
H	1.88051137	3.46383384	-0.25704450	H	-1.17230114	-4.15778508	0.17079101
H	3.31574980	2.67957908	0.41893210	H	-2.67263445	-3.38625648	-0.34991971
H	2.18582944	1.75290378	-0.58986241	C	1.01809177	-2.50661996	1.42936074
C	1.61203409	3.20820544	2.52310583	H	1.81259829	-1.87278768	1.86904874
H	2.67477213	3.39277027	2.73208364	C	0.80533963	-3.64782883	2.45331057
H	1.17436550	4.16264437	2.20909523	H	1.75848838	-4.14330662	2.68391971
H	1.12904002	2.90893149	3.46012848	H	0.38259405	-3.26483646	3.38929575

H	0.12597100	-4.41975376	2.07408838
C	1.67956260	-3.09907875	0.15550803
H	1.91199021	-2.29654468	-0.55533363
H	2.62077364	-3.61310777	0.39856207
H	1.03082423	-3.82148659	-0.35101602
O	-0.40911863	0.00065978	-1.94291869
C	0.32168799	-0.73329970	-2.95513878
C	-0.58918940	-0.76559246	-4.18524867
C	-1.39441703	0.53377791	-4.02789288
C	-1.59749716	0.59561021	-2.51430010
H	-2.47134196	0.00877276	-2.20145036
H	-1.68988997	1.60970501	-2.11891500
H	-2.34108731	0.52609058	-4.57613032
H	-0.80739252	1.39406498	-4.37035596
H	-1.25623881	-1.63457594	-4.14535146
H	-0.02267117	-0.81489229	-5.11976866
H	1.25848431	-0.19892221	-3.15816049
H	0.55777425	-1.72358252	-2.55713091

Table 5. Geometric coordinates and thermally corrected MP2 energies for lithium diisopropylamide (LDA) with three THF



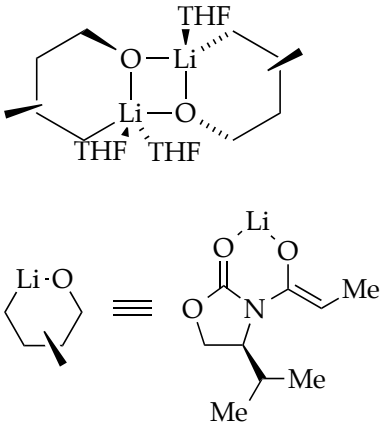


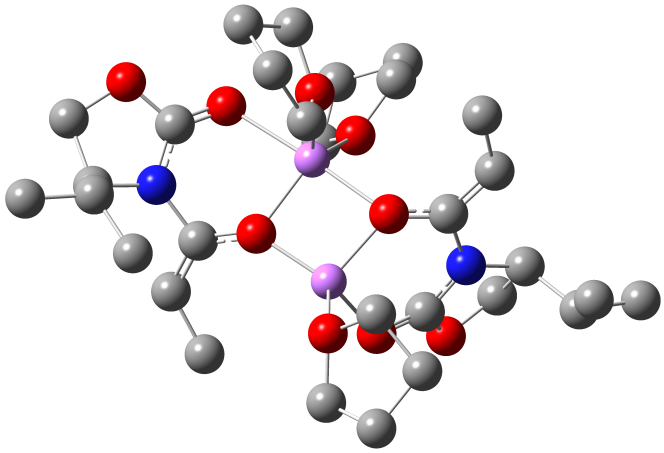
G = -1295.457144 Hartree
G_{MP2} = -810047.7434 kcal/mol
ΔG_{MP2} = 3. 1.782826016 kcal/mol Li vs. LDA with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.87396292	2.59274373	1.48807260
Li	0.00000000	0.00000000	2.45078330	H	1.78043899	1.98652108	1.68124104
O	0.76848937	0.00000000	4.30278586	C	0.77918167	3.54715730	2.70523038
C	0.05243812	-0.35287502	5.51009161	H	1.71765290	4.10407928	2.83848508
C	1.11422368	-0.45211071	6.60812890	H	-0.01888713	4.28875034	2.58550450
C	2.17114282	0.55481747	6.12871645	H	0.57842436	2.98566993	3.62498842
C	2.13508612	0.35175362	4.61320781	C	1.24139344	3.42678721	0.22977099
H	2.79028845	-0.47253419	4.30113315	H	2.19772141	3.95284251	0.36841242
H	2.39179147	1.24830037	4.04276424	H	1.33774558	2.76556180	-0.63844292
H	3.16444475	0.37560221	6.55080826	H	0.48501595	4.18369996	-0.00254504
H	1.87004522	1.57765157	6.38325687	N	-0.25366108	-1.60431767	1.31017524
H	1.53710581	-1.46288735	6.64154945	C	0.87520412	-2.52278726	1.47978528
H	0.71085645	-0.21919600	7.59797483	H	1.75531864	-1.85587890	1.56596750
H	-0.67928690	0.43691403	5.72176425	C	1.21661426	-3.44459026	0.27503715
H	-0.48028717	-1.29042714	5.32984533	H	0.53724126	-4.29906012	0.19391347
N	-0.19534554	1.60798289	1.31467744	H	1.15805401	-2.88047618	-0.66097787
C	-1.59788117	2.04176334	1.34755746	H	2.23471964	-3.85053501	0.37206069
H	-2.16178708	1.19414653	0.91652556	C	0.90531948	-3.38541981	2.76791260
C	-2.22078099	2.22361708	2.76351605	H	0.72978567	-2.76527871	3.65396372
H	-1.82397492	3.10090503	3.28491552	H	0.14436086	-4.17435134	2.74920223
H	-3.31297535	2.33840191	2.70356366	H	1.87998218	-3.88108949	2.88395713
H	-2.01776593	1.34556453	3.39085105	C	-1.62658338	-2.11916070	1.35672220
C	-2.00114156	3.26349110	0.48627836	H	-2.24331366	-1.30390211	0.93829073
H	-3.09486828	3.36313536	0.44607513	C	-1.96121547	-3.35852925	0.49163073
H	-1.60883639	4.20305691	0.89221339	H	-3.04868555	-3.50416451	0.42872341
H	-1.63046072	3.16352344	-0.53908621	H	-1.57074509	-3.24567616	-0.52574629

H	-1.53924533	-4.27923938	0.91121265
C	-2.22377918	-2.34407340	2.77599811
H	-2.08948575	-1.44715473	3.39450064
H	-3.30356843	-2.54666983	2.72376310
H	-1.75524499	-3.18474975	3.29900739
O	-1.15155293	0.09363755	-1.75805537
C	-0.94439464	1.17511625	-2.69666931
C	-2.32736717	1.52442690	-3.25206981
C	-3.05462874	0.17383777	-3.17010425
C	-2.51023443	-0.39140314	-1.85809408
H	-2.48463392	-1.48267101	-1.81948503
H	-3.08227608	-0.02301176	-0.99700184
H	-2.77067747	-0.46776232	-4.01313308
H	-4.14487881	0.26640316	-3.16470015
H	-2.27799881	1.93290062	-4.26609137
H	-2.82180009	2.26210740	-2.61002493
H	-0.46078200	1.99956632	-2.16721399
H	-0.27327676	0.82195565	-3.49033079
O	1.84177836	-0.02817632	-1.08782613
C	2.05959584	-0.70137110	-2.33887026
C	3.42785626	-1.41913872	-2.22636360
C	3.98701297	-0.94448183	-0.86316610
C	3.13384936	0.28777262	-0.55474108
H	3.53044028	1.18883439	-1.04771899
H	3.00783801	0.49901453	0.50858217
H	5.05670128	-0.71589085	-0.89736731
H	3.82387115	-1.70829567	-0.09706728
H	4.08418386	-1.12814200	-3.05269242
H	3.31913055	-2.50648299	-2.25671413
H	1.21399764	-1.37498804	-2.48969236
H	2.06952050	0.03896514	-3.15129439

Table 6. Geometric coordinates and thermally corrected MP2 energies for **10** dimer with three THF



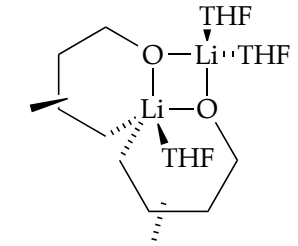


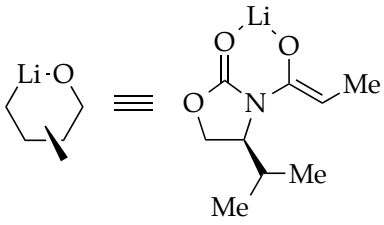
G = -1975.555867 Hartree
G_{MP2} = -1235703.674 kcal/mol
ΔG_{MP2} = 0 kcal/mol vs. **10** dimer with three THF

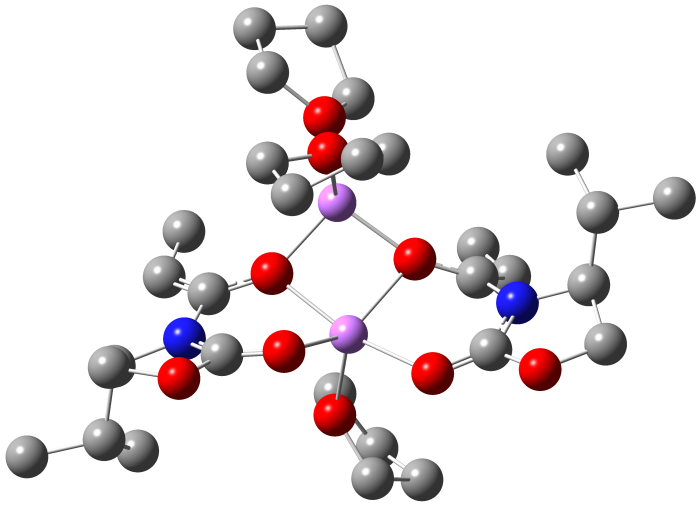
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.31848362	-1.35816036	-0.82029480
O	0.00000000	0.00000000	2.09538850	H	-4.04889854	-0.29429750	-0.20125164
C	1.00759653	0.00000000	2.90760053	H	-5.68943209	0.33531466	-0.45260323
N	1.38005480	-1.32373460	3.43891985	C	-5.85393549	0.08615589	-3.15910380
C	2.65811165	-1.64616838	4.09989224	H	-6.59815680	0.76801996	-2.73328539
C	2.87921840	-3.05665798	3.53476642	H	-5.66954657	0.40744685	-4.19096415
H	3.39305766	-3.04368291	2.56622248	H	-6.30606405	-0.91347606	-3.19678916
H	3.39284972	-3.73870655	4.21380966	C	-2.50222909	-3.07881323	-1.04119118
O	1.54161754	-3.55460899	3.34226257	C	-2.46681311	-4.05573926	0.09932117
C	0.71587370	-2.48292820	3.15277617	H	-3.46622937	-4.24447870	0.52530196
O	-0.44884172	-2.66437721	2.81349445	H	-2.08123614	-5.03153538	-0.22671321
Li	-1.40302230	-1.24180187	1.90212328	H	-1.82081487	-3.70807624	0.91080992
O	-1.58679132	-1.14075907	0.04638654	H	-2.87889909	-3.43737079	-1.99587539
C	-2.09997976	-1.78877575	-0.95916511	O	-3.00789069	-0.87722828	3.07084176
N	-2.27156557	-0.97773833	-2.17300392	C	-3.59579500	-1.99181490	3.78746380
C	-3.50520570	-0.82928926	-2.95369726	C	-3.83758907	-1.50152118	5.22347850
C	-2.91386763	-0.21904667	-4.24398314	C	-2.82165463	-0.35577067	5.36296843
H	-2.69457186	-0.98273852	-4.99934651	C	-2.84184266	0.24797089	3.96060321
H	-3.53469360	0.55993796	-4.68904429	H	-1.91788042	0.75385779	3.67141163
O	-1.67338673	0.38794067	-3.83481295	H	-3.69031690	0.93637060	3.83457129
C	-1.27002753	-0.21267663	-2.66994045	H	-1.82393309	-0.75032355	5.58756705
O	-0.14785624	-0.02860978	-2.21513578	H	-3.08913854	0.36779776	6.13928300
H	-3.94022690	-1.81445501	-3.15214073	H	-3.69573314	-2.29759079	5.96049854
C	-4.58026628	0.07351206	-2.29667560	H	-4.85870164	-1.11783511	5.33458756
H	-4.16612782	1.09369306	-2.27145345	H	-4.51676704	-2.28938720	3.27554262
C	-4.92217023	-0.33645364	-0.85692582	H	-2.88301488	-2.82175680	3.75045306

H	3.42519755	-0.94757040	3.75664831
C	2.58876842	-1.67965667	5.65325446
H	2.00328250	-2.57565374	5.91041831
C	4.00138012	-1.84598551	6.23793817
H	3.95706011	-1.95823619	7.32683929
H	4.52464234	-2.72335464	5.84015303
H	4.61723144	-0.96367838	6.02114182
C	1.88519262	-0.47867842	6.29875845
H	2.47995312	0.43683668	6.21053772
H	0.91094711	-0.28525083	5.84219961
H	1.73362690	-0.67259171	7.36753185
C	1.76434845	1.06718679	3.28619372
H	2.55288207	0.94295598	4.01695117
C	1.50508096	2.46344098	2.79040115
H	0.94347433	2.44766608	1.85241465
H	0.93230836	3.07226835	3.51065974
H	2.44491477	3.00500657	2.61190860
O	1.94914965	-0.65744943	-0.20670993
C	3.01256990	0.31694066	-0.20474241
C	4.22052182	-0.40122255	-0.80687286
C	3.54937300	-1.32410926	-1.83664783
C	2.26382230	-1.73997640	-1.11306394
H	2.40785027	-2.65168739	-0.51856118
H	1.41341426	-1.87983207	-1.78293212
H	4.16618052	-2.18259251	-2.12036323
H	3.30784339	-0.76259312	-2.74652853
H	4.73706033	-0.99164851	-0.03976983
H	4.94461791	0.29045467	-1.24874590
H	2.71776138	1.17549369	-0.82500899
H	3.14724944	0.65301123	0.82667332
O	-0.39936641	2.07179659	-0.14785380
C	-1.62206858	2.49330024	0.50064368
C	-2.15494815	3.68934161	-0.31069300
C	-1.42701649	3.54971513	-1.65906516
C	-0.08325247	2.96865364	-1.22504024
H	0.59349060	3.75709448	-0.86145685
H	0.41625997	2.38328611	-1.99842211
H	-1.32730121	4.49864997	-2.19569920
H	-1.94086887	2.83734983	-2.31421581
H	-1.87937686	4.63489203	0.17077921
H	-3.24508843	3.67079051	-0.40585804
H	-2.30479862	1.63813324	0.49248155
H	-1.39900459	2.74946178	1.54095105

Table 7. Geometric coordinates and thermally corrected MP2 energies for **10** spirocyclic dimer with three THF





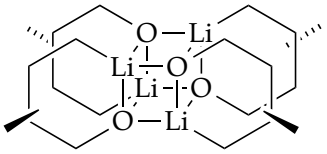


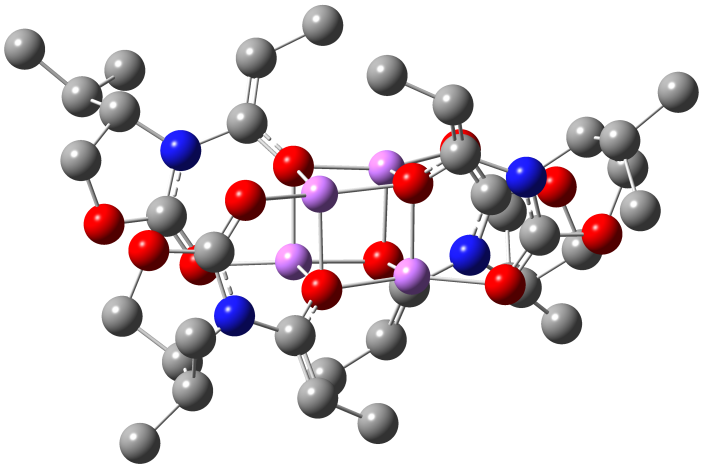
G = -1975.552542 Hartree
G_{MP2} = -1235702.536 kcal/mol
ΔG_{MP2} = 0.568762817 kcal/mol Li vs. **10** dimer with three THF

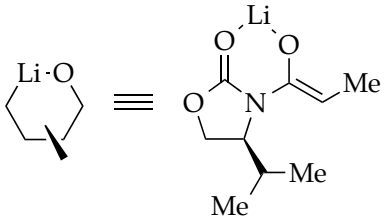
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.87240175	-2.49949474	2.73868255
Li	0.00000000	0.00000000	2.65676290	H	3.99131808	-1.19044940	3.90968418
O	1.42579464	0.00000000	1.44813489	H	2.42000624	-1.59264683	3.19318790
C	2.69318422	0.10879627	1.21043699	O	-1.27944552	-0.69365355	1.48801080
N	3.02272606	1.04180219	0.13010379	C	-2.32055435	-1.37630018	1.12433412
C	2.10301636	1.82024965	-0.52130958	N	-3.26692651	-0.63238635	0.28134959
O	0.89036530	1.70220099	-0.61617484	C	-4.72842247	-0.60697979	0.41314721
O	2.74319268	2.85668521	-1.15066610	C	-5.10436941	-0.04249263	-0.97728844
C	4.11501898	2.86863809	-0.71935063	H	-5.38149305	-0.83421397	-1.68319754
H	4.21802132	3.56923665	0.11871275	H	-5.90034050	0.70334301	-0.94714310
H	4.72751354	3.20845182	-1.55637500	O	-3.91580957	0.60481401	-1.46155723
C	4.37795537	1.41382443	-0.30310616	C	-2.84221626	0.11143820	-0.77573925
H	5.06212132	1.36437205	0.54762389	O	-1.69732618	0.34582101	-1.13534003
C	4.92185162	0.58139536	-1.49889292	H	-5.11223377	-1.62626676	0.53006400
H	4.39220790	0.94830340	-2.39128678	C	-5.25498435	0.26126764	1.58392009
C	4.65143793	-0.92551767	-1.40713551	H	-4.96449597	1.30020110	1.36369656
H	5.17313674	-1.38374695	-0.56074560	C	-4.65607484	-0.12637776	2.94328124
H	3.58279087	-1.12816363	-1.29622969	H	-4.90664665	-1.16121212	3.20511231
H	5.00063722	-1.41592299	-2.32430931	H	-3.56791974	-0.03503951	2.95122935
C	6.42179032	0.86221531	-1.68194397	H	-5.06144350	0.52524276	3.72734832
H	6.80089883	0.37351343	-2.58616753	C	-6.79016730	0.18629405	1.65004164
H	6.64079492	1.93342239	-1.77168175	H	-7.17047373	0.83287864	2.44838609
H	6.99595697	0.47550649	-0.82996126	H	-7.27462641	0.49983550	0.71832201
C	3.71384134	-0.51855567	1.85852269	H	-7.12025311	-0.83749385	1.86982111
H	4.73965502	-0.35459232	1.55285600	C	-2.64357775	-2.66436574	1.40397073
C	3.48791711	-1.49515884	2.97751417	C	-1.83920113	-3.55229210	2.30824731

H	-1.60232521	-4.51598924	1.83403544
H	-0.89255956	-3.07397523	2.57653245
H	-2.36860335	-3.79305444	3.24491917
H	-3.54734285	-3.08101646	0.96785922
O	-0.41963833	1.98442345	3.10811737
C	-1.74384110	2.46875897	2.77152115
C	-1.57204816	3.93115159	2.34201756
C	-0.11816196	3.96143371	1.84439533
C	0.56228887	3.00328175	2.82009641
H	0.83783383	3.50968687	3.75740517
H	1.44105813	2.50086901	2.41100415
H	0.32211451	4.96355183	1.86413718
H	-0.04831392	3.56656085	0.82615312
H	-1.69936860	4.60378905	3.19914600
H	-2.29444052	4.22209819	1.57355287
H	-2.12913439	1.83993430	1.96325406
H	-2.38849128	2.35082337	3.64948439
O	0.25845346	-0.61596501	4.56065220
C	-0.02928207	-1.87610753	5.19959847
C	0.33426980	-1.67719247	6.67128463
C	1.52399437	-0.70969273	6.57080599
C	1.10820321	0.19447542	5.40651637
H	1.95266976	0.54587917	4.80682610
H	0.52786301	1.06082980	5.74419544
H	2.43932238	-1.25790697	6.31998805
H	1.70547252	-0.14627786	7.49104793
H	0.58014242	-2.61770839	7.17345932
H	-0.49774066	-1.20848719	7.21037075
H	-1.08276908	-2.11002290	5.02834067
H	0.58458727	-2.66123241	4.73808152
O	0.80558503	-1.53668786	-1.13115832
C	1.06994691	-2.74441633	-0.36968466
C	0.62389827	-3.91798554	-1.25600513
C	-0.38561579	-3.25551359	-2.20766534
C	0.24941901	-1.88228317	-2.41407962
H	-0.45358649	-1.09305373	-2.68626142
H	1.05525136	-1.92561420	-3.16242784
H	-1.35652440	-3.14676811	-1.71077539
H	-0.52806218	-3.80541311	-3.14361093
H	0.19154565	-4.73455576	-0.66979307
H	1.47153272	-4.32216271	-1.82284886
H	2.13420766	-2.77044512	-0.11603133
H	0.49110125	-2.67851413	0.55461308

Table 8. Geometric coordinates and thermally corrected MP2 energies for **10** D_{2d} tetramer





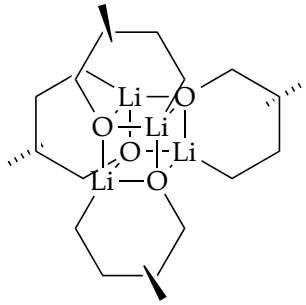


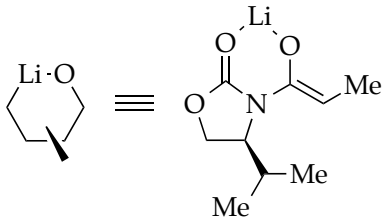
G = -2557.052041 Hartree
G_{MP2} = -1599531.467 kcal/mol
ΔG_{MP2} = 0.53453263 kcal/mol Li vs. **10** dimer with three THF

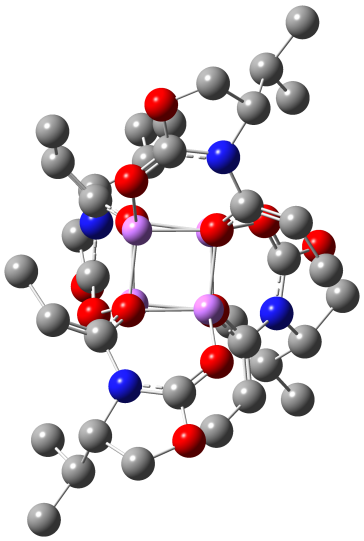
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.28322963	1.66548900	-2.11428320
O	0.00000000	0.00000000	1.90431030	C	-2.51124346	1.81203379	-1.56463394
C	1.06056664	0.00000000	2.52461150	H	-3.17815228	2.57783436	-1.93688088
O	1.12404446	-0.56766431	3.76019418	C	-2.99585821	0.98088527	-0.40750049
C	2.50653940	-0.60311222	4.17898911	H	-2.53362807	-0.01297514	-0.39355384
H	2.90294560	-1.59695633	3.95104903	H	-2.78977109	1.44742350	0.56873066
H	2.53126284	-0.42782219	5.25526511	H	-4.08078495	0.82810957	-0.46100570
C	3.18084865	0.49976047	3.34601741	O	-0.36541643	0.80500138	-1.73194704
H	4.16988159	0.18280570	3.00224313	Li	-0.04943499	-1.00198316	-2.50528689
N	2.27265708	0.52342754	2.18567012	O	-0.31190737	-1.01873279	-4.39210153
C	2.66925567	0.88731244	0.83623963	C	0.61760098	-0.75572995	-5.15148705
C	3.77093228	1.65069749	0.64874663	O	0.36480376	-0.19559933	-6.36565784
H	4.30048131	2.05347946	1.50264962	C	1.62282122	0.18847500	-6.96401824
C	4.29357523	2.00732434	-0.71684046	H	1.78497009	1.25008711	-6.75601566
H	3.85365681	2.93545016	-1.11445376	H	1.54171506	0.02567583	-8.03946905
H	5.37968311	2.15737757	-0.69415423	C	2.65944897	-0.70872894	-6.26792476
H	4.09520491	1.21678746	-1.45057685	H	3.57676852	-0.15342869	-6.05073296
O	1.91674595	0.37423421	-0.11223207	N	1.95673881	-0.95778636	-4.99676956
Li	1.57793089	0.94525864	-1.93801876	C	2.61509433	-1.20100167	-3.72487599
O	1.42593614	2.23628707	-3.33430043	C	3.88450722	-1.66959061	-3.71024775
C	0.33118975	2.48068509	-3.83361116	H	4.37236964	-1.93807596	-4.63854789
O	0.24747463	2.86078165	-5.13934359	C	4.66240293	-1.87599377	-2.43826040
C	-1.15037346	2.85297549	-5.51678065	H	4.49882584	-2.87012935	-1.99332191
H	-1.38364308	1.87057716	-5.93828121	H	5.74001042	-1.78477039	-2.61946736
H	-1.29083081	3.63180120	-6.26694226	H	4.40301856	-1.13462886	-1.67256832
C	-1.87110691	3.11983053	-4.18777359	O	1.90141107	-0.87895679	-2.66825319
H	-2.82936891	2.59704920	-4.12948247	Li	1.96915293	-1.48937499	-0.82499351
N	-0.91417462	2.46576984	-3.27169108	O	2.35854636	-2.74621689	0.55463312

C	1.44734403	-3.22547855	1.22501688
O	1.67153431	-3.58877928	2.51748804
C	0.40631164	-3.93886226	3.12243490
H	0.04268566	-3.06634882	3.67297142
H	0.58631307	-4.76660302	3.80957563
C	-0.49633136	-4.29671127	1.92935530
H	-1.50960042	-3.90974078	2.07224646
N	0.15894178	-3.50062282	0.87630279
C	-0.52122719	-2.92993688	-0.27430563
C	-1.66724853	-3.49618502	-0.71763670
C	-2.47921666	-2.92624814	-1.84907271
H	-2.39566407	-1.83441234	-1.90453082
H	-2.18037964	-3.32354899	-2.83161506
H	-3.54368792	-3.15925543	-1.72437905
H	-2.02034488	-4.41621089	-0.26952370
O	0.04156922	-1.84300031	-0.75611664
C	-0.57452848	-5.81713598	1.62435290
H	-1.12574976	-5.91928603	0.68297544
C	0.79661541	-6.47758502	1.41763336
H	1.35237546	-6.00701067	0.59986337
H	1.41921135	-6.43475115	2.31927310
H	0.66647163	-7.53470203	1.16001610
C	-1.39036264	-6.53328146	2.71262160
H	-2.38316094	-6.08354516	2.83466468
H	-1.53196277	-7.58778322	2.45226562
H	-0.88782270	-6.50576844	3.68772199
C	3.02255517	-1.99553508	-7.05693510
H	3.64435656	-2.60418736	-6.39110724
C	1.80533263	-2.84996724	-7.44263809
H	1.23414240	-3.15980059	-6.56127749
H	1.12405973	-2.32121235	-8.11967965
H	2.13631292	-3.75987727	-7.95575763
C	3.87576774	-1.63827180	-8.28450885
H	4.76195111	-1.05590412	-8.00434050
H	4.22036764	-2.54730580	-8.78919797
H	3.31009313	-1.05405527	-9.02138163
C	-2.04478831	4.64706959	-3.95139945
H	-1.10333888	5.11228727	-4.28069496
C	-3.18210552	5.18500536	-4.83586974
H	-4.14632761	4.75872036	-4.53060228
H	-3.25805168	6.27389250	-4.74357701
H	-3.03897326	4.95645477	-5.89846140
C	-2.26474755	5.06147273	-2.49060589
H	-3.25439083	4.76219986	-2.12771649
H	-1.51555654	4.62427653	-1.82531679
H	-2.20184989	6.15274915	-2.40637036
C	3.31221016	1.86271200	4.07798751
H	3.66826651	2.58329057	3.33328460
C	1.98228223	2.40123859	4.62604162
H	1.23857147	2.52553601	3.83199766
H	1.55262294	1.74630178	5.39339022
H	2.13892171	3.38381011	5.08516906
C	4.38242056	1.77111361	5.17743533
H	5.34266158	1.42253137	4.77836980
H	4.54779907	2.75345787	5.63290101
H	4.08617485	1.08709122	5.98277780

Table 9. Geometric coordinates and thermally corrected MP2 energies for **10** S_4 tetramer





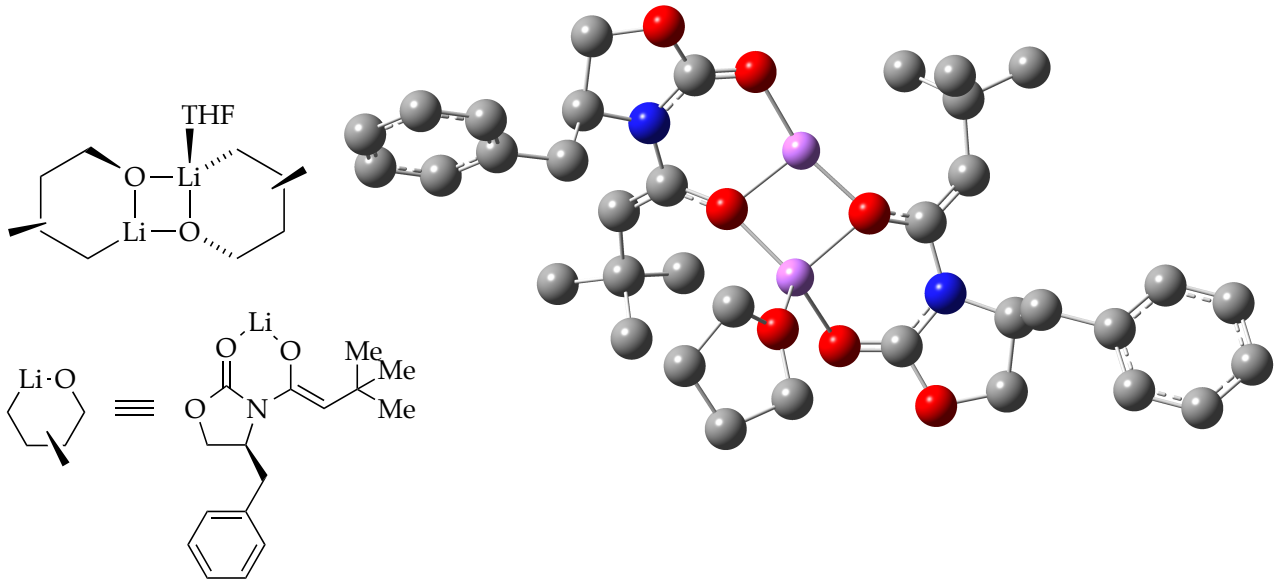


G = -2557.053052 Hartree
G_{MP2} = -1599531.983 kcal/mol
ΔG_{MP2} = 0.405721001 kcal/mol Li vs. **10** dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.84544025	-5.45349744	-1.67610379
O	0.00000000	0.00000000	1.91500780	C	-2.27020570	-5.65748562	-1.61435655
C	1.06008305	0.00000000	2.53560933	H	-2.51421622	-6.09421494	-0.63932396
N	2.29572449	-0.40347828	2.13077013	H	-2.53831680	-6.35991733	-2.40426094
C	3.31241475	-0.05156651	3.13793916	C	-2.87769651	-4.25193196	-1.79808775
C	2.39931884	0.12407952	4.36608335	H	-3.72555485	-4.10867785	-1.12247261
H	2.29648811	-0.79999923	4.94636658	N	-1.73616700	-3.43240975	-1.35417303
H	2.69874352	0.93797510	5.02729227	C	-1.81845652	-2.05273635	-0.89030842
O	1.11132850	0.45957573	3.81365473	O	-0.81939770	-1.28037156	-1.27313032
H	4.00114695	-0.88790856	3.28271896	Li	-0.31754809	-0.04069395	-2.65427822
C	4.11609769	1.23094232	2.80323746	O	-1.02189181	1.10317705	-3.99578943
H	3.41188985	2.07376771	2.87805830	C	-0.60795611	2.26069363	-4.02972019
C	4.70861860	1.23572976	1.38782427	O	-0.57108859	2.95288363	-5.19540809
H	5.39938045	0.39847964	1.23851583	C	-0.25954642	4.33050712	-4.91175853
H	3.93407995	1.16903409	0.61977410	H	-1.17817467	4.91670181	-5.01935003
H	5.26419926	2.16615241	1.22143147	H	0.46669434	4.66209762	-5.65529639
C	5.22863746	1.43195280	3.84628715	C	0.29182907	4.34970259	-3.46328817
H	5.75496889	2.37559222	3.66743847	H	-0.21528763	5.12256461	-2.87563525
H	4.84931529	1.45918063	4.87468794	N	-0.14239672	3.01938106	-3.00517313
H	5.96860369	0.62348338	3.78463652	C	-0.23352323	2.57809755	-1.61077720
C	2.54923120	-1.11260226	0.88345490	O	0.30141012	1.39600732	-1.37690523
O	1.83835738	-0.69300595	-0.14362961	Li	2.03252629	0.49950367	-1.64694503
Li	1.03907565	-1.95142186	-1.42597316	O	3.56850421	1.02006889	-2.59287920
O	0.57185909	-3.78086874	-1.18557003	C	3.84215726	0.59974428	-3.71413363
C	-0.58172111	-4.15488448	-1.37840513	O	4.91242263	1.11890102	-4.37304043

C	5.15618784	0.34820669	-5.56027393
H	5.99448633	-0.32952685	-5.36544680
H	5.43201870	1.03703392	-6.36031931
C	3.84209204	-0.40988474	-5.82019537
H	4.06724283	-1.45287774	-6.06146614
N	3.22397227	-0.34334948	-4.48266971
C	2.08429720	-1.16613378	-4.09112342
O	1.47149221	-0.79499918	-2.98896040
C	1.74892371	-2.21579229	-4.87982667
H	2.35602438	-2.45758844	-5.74341376
C	0.55775621	-3.09758894	-4.63210761
H	-0.14470321	-2.63066827	-3.93512437
H	0.01486620	-3.29353582	-5.56688646
H	0.83496961	-4.07532380	-4.21174458
C	2.95004077	0.17585408	-6.94250181
H	2.00947994	-0.38469082	-6.89791975
C	3.58936222	-0.08212567	-8.31552347
H	2.92003783	0.24720981	-9.11752556
H	4.53452363	0.46304775	-8.43805399
H	3.79549311	-1.14816231	-8.47167445
C	2.61411774	1.66041330	-6.74335693
H	2.09733451	1.82954156	-5.79373717
H	3.50887299	2.29539878	-6.76916749
H	1.94484253	2.00245867	-7.54025373
C	-0.83565730	3.42000004	-0.74455476
H	-1.27525819	4.32877782	-1.14696489
C	-0.94483429	3.21635091	0.73821814
H	-0.36095757	2.35856425	1.08073443
H	-0.59057646	4.10050327	1.28755183
H	-1.98392273	3.04675933	1.05552967
C	1.81817994	4.59753365	-3.39147638
H	2.29695223	3.87299657	-4.06702271
C	2.13857509	6.01869346	-3.88795313
H	3.22053385	6.18750484	-3.87867205
H	1.78822665	6.20784975	-4.90928785
H	1.68162067	6.77225706	-3.23320875
C	2.40114333	4.39682972	-1.98604324
H	1.93449873	5.07694458	-1.26326094
H	2.26642522	3.37465778	-1.62843601
H	3.47758175	4.60209763	-2.00044899
C	-2.88500515	-1.68757584	-0.14841784
H	-3.59521684	-2.44893130	0.15872636
C	-3.14779906	-0.27711150	0.30151259
H	-2.82042552	-0.09812126	1.33562236
H	-2.63173465	0.45031102	-0.33626468
H	-4.21986156	-0.04441674	0.25907733
C	-3.33126327	-3.97963986	-3.25509447
H	-2.51468746	-4.31776259	-3.91067794
C	-4.58721525	-4.81079832	-3.56953615
H	-4.87947062	-4.67835267	-4.61664032
H	-4.44267887	-5.88502097	-3.40418144
H	-5.43179688	-4.48767309	-2.94724944
C	-3.59451646	-2.49743493	-3.55414114
H	-4.37986101	-2.09120407	-2.90711425
H	-2.69997197	-1.88500036	-3.41726333
H	-3.91963149	-2.38185918	-4.59474885
C	3.47344184	-2.09685721	0.87825696
H	3.93159052	-2.39506075	1.81587303
C	3.89427834	-2.83457852	-0.36308561
H	3.35897766	-3.78641110	-0.49063472
H	3.71283642	-2.23506461	-1.26334609
H	4.96638725	-3.06874987	-0.33727682

Table 10. Geometric coordinates and thermally corrected MP2 energies for **7** dimer with one THF

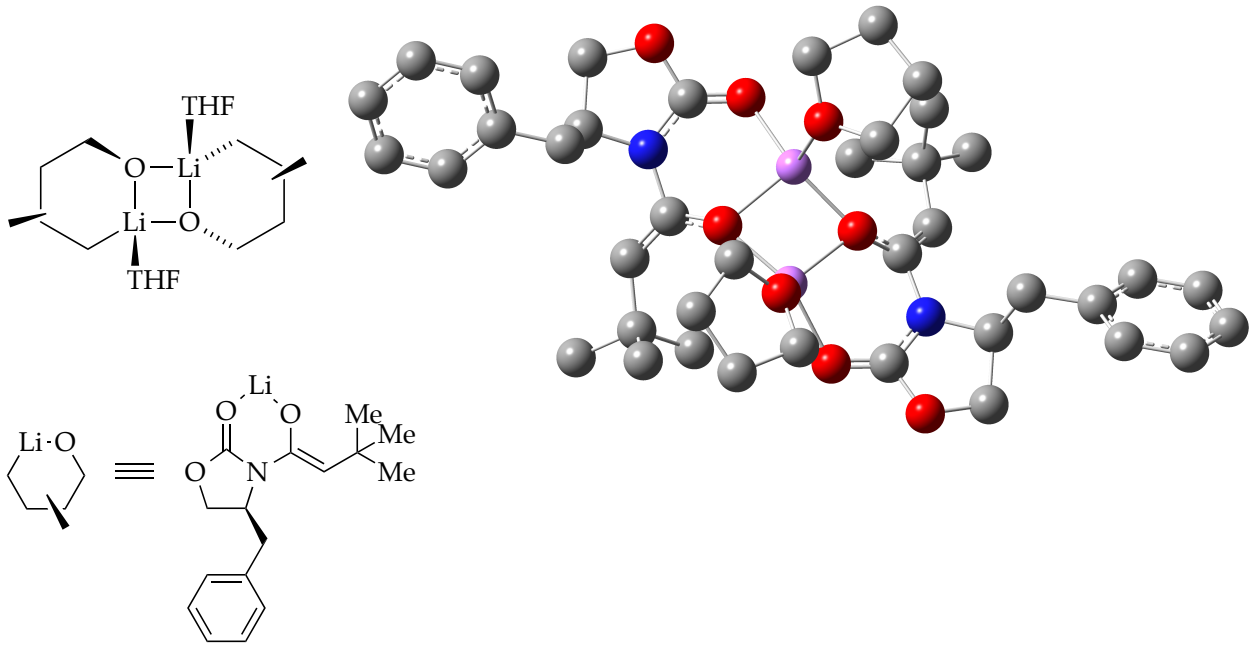


G = -2051.379484 Hartree
G_{MP2} = -1283129.296 kcal/mol
ΔG_{MP2} = 5.0148607 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.87258049	-4.57413317	0.95957619
O	0.00000000	0.00000000	1.92260770	H	5.50770081	-4.53773435	-0.69576575
C	1.09396447	0.00000000	2.48293739	O	1.72609290	-0.87935987	-0.15136577
O	1.25846683	0.66394343	3.66060471	Li	1.00249923	-1.53275845	-1.70832712
C	2.55341986	0.33614194	4.19965109	O	0.91219292	-2.04924331	-3.51136410
H	2.42093194	-0.42949517	4.97185969	C	-0.11763020	-1.81504192	-4.14482585
H	2.97846839	1.23460102	4.65012190	O	-0.10162706	-1.81864943	-5.50234133
C	3.35629479	-0.18663605	2.99631529	C	-1.45818975	-1.73864050	-5.98194037
H	3.94862897	-1.05635945	3.28826229	H	-1.77664364	-2.74364541	-6.27866537
N	2.26128616	-0.58310882	2.10094156	H	-1.47848455	-1.08184224	-6.85307025
C	2.46622009	-1.29622629	0.83506967	C	-2.26861514	-1.20045602	-4.78837251
C	3.41567838	-2.26681380	0.84736800	H	-3.20889295	-1.74848750	-4.69253538
H	3.85869420	-2.51621986	1.80664564	N	-1.36383211	-1.53497047	-3.68176675
C	3.89489060	-3.09932494	-0.33562722	C	-1.70174848	-1.35366292	-2.26119908
C	4.32724685	-2.21309120	-1.52539714	C	-2.96215988	-1.69347051	-1.89546733
H	5.15260358	-1.55388832	-1.23122780	C	-3.57081445	-1.55511527	-0.50515285
H	4.66601585	-2.82921152	-2.36811692	C	-2.78473034	-2.38646692	0.53482858
H	3.51336411	-1.57539799	-1.88203386	H	-1.74400169	-2.05838253	0.60262535
C	2.80623949	-4.10123256	-0.78998497	H	-3.23485060	-2.29322837	1.53207146
H	1.88433724	-3.59690389	-1.10016132	H	-2.78582143	-3.44766723	0.25897970
H	3.15120142	-4.70488604	-1.63977480	C	-3.61494068	-0.07521407	-0.05895212
H	2.53999478	-4.77990263	0.02835115	H	-4.22824713	0.51780626	-0.74941712
C	5.12475882	-3.91346293	0.12056622	H	-4.04952288	0.01752727	0.94520260
H	5.93542550	-3.24980172	0.44656827	H	-2.61432398	0.36611773	-0.03492063

C	-5.01861784	-2.08588391	-0.55883741
H	-5.62190864	-1.51968455	-1.28029880
H	-5.04080615	-3.14140294	-0.85720556
H	-5.50226982	-2.00330424	0.42189940
H	-3.59523025	-2.14869051	-2.65143057
O	-0.73434614	-0.86584415	-1.53685445
C	-2.56910999	0.31491169	-4.84757215
H	-2.93308509	0.60654801	-3.85570261
H	-1.62873032	0.85170139	-5.02452895
C	-3.58820544	0.66978912	-5.90766597
C	-3.20240556	1.25525763	-7.12082261
C	-4.14599497	1.55267486	-8.10660555
C	-5.49470304	1.26752326	-7.89263213
C	-5.89394704	0.68761778	-6.68599512
C	-4.94880237	0.39297591	-5.70398252
H	-5.26878074	-0.04857253	-4.76222105
H	-6.94364703	0.46970336	-6.50736304
H	-6.23099809	1.49982556	-8.65722894
H	-3.82610797	2.01090030	-9.03876848
H	-2.15406907	1.49237183	-7.29047761
C	4.28266588	0.86148647	2.33747735
H	4.60053118	0.44724756	1.37415722
H	3.69660541	1.76459345	2.12696788
C	5.48583085	1.19667985	3.19081945
C	6.54906507	0.28778325	3.30470830
C	7.65033795	0.57119987	4.11158128
C	7.71021191	1.77379699	4.82008763
C	6.66309194	2.68912286	4.71206911
C	5.56109924	2.40050252	3.90394241
H	4.75422861	3.12517793	3.81536134
H	6.70360750	3.63110231	5.25282023
H	8.56960929	1.99693715	5.44652287
H	8.46564381	-0.14404283	4.18261384
H	6.51569131	-0.64515602	2.74544962
O	-0.18737861	1.96082510	-0.34823997
C	-0.51100878	2.51906603	-1.62846383
C	-1.72477424	3.42725703	-1.36801758
C	-1.57826687	3.81993134	0.12943390
C	-0.34834708	3.02059914	0.60688354
H	-0.46052265	2.55601137	1.58711864
H	0.55703435	3.64564154	0.60390595
H	-2.47078188	3.53554137	0.69361484
H	-1.42912210	4.89527544	0.26591359
H	-2.65440759	2.87398286	-1.52885774
H	-1.73203072	4.29531215	-2.03411383
H	0.34929668	3.09602838	-2.00014618
H	-0.70238483	1.68152173	-2.30058349

Table 11. Geometric coordinates and thermally corrected MP2 energies for **7** dimer with two THF

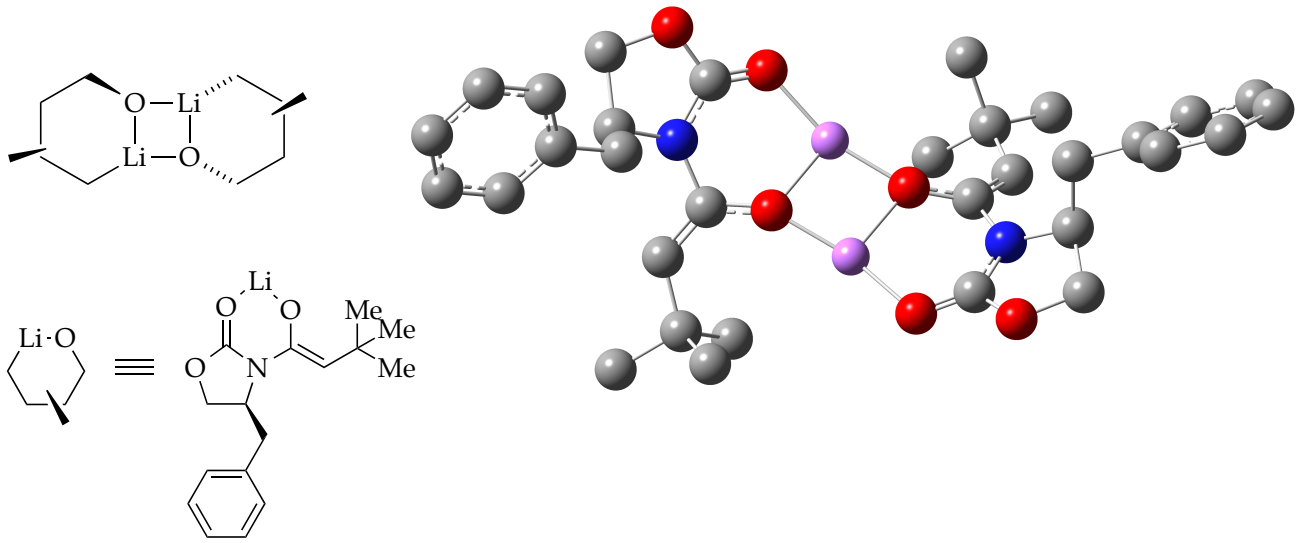


G = -2283.730227 Hartree
G_{MP2} = -1428451.616 kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	-4.66925269	-4.41904120	-0.01401512
H	0.00000000	0.00000000	1.09537450	H	-3.72182571	-4.93635951	-0.21296859
H	1.03011798	0.00000000	-0.36064894	H	-4.68132760	-4.13564370	1.04589756
C	-0.85531882	-1.14218826	-0.57896199	H	-5.48499639	-5.13317415	-0.17996165
H	-0.99817980	-1.92532402	0.16931261	Li	-5.51424410	-0.37042111	-3.35667891
N	-2.11413144	-0.43051174	-0.82592207	O	-7.35468906	-0.88387963	-3.64729111
C	-1.92225781	0.91152408	-0.81372251	C	-8.16261886	0.01186076	-3.88525048
O	-0.64215527	1.20815025	-0.45228537	O	-9.22663135	-0.22070833	-4.70443802
O	-2.71645939	1.81132643	-1.08076626	C	-10.11060631	0.91575522	-4.64444531
Li	-4.06299760	1.44416347	-2.41772777	H	-10.94294721	0.66900371	-3.97648882
O	-3.94217587	-0.49034573	-2.27897576	H	-10.49718907	1.10652572	-5.64712629
C	-3.34990428	-1.08861353	-1.28847501	C	-9.24358791	2.06140591	-4.09027017
C	-3.66303965	-2.23865245	-0.63809628	H	-9.80385597	2.63614234	-3.34905497
H	-3.04776425	-2.49563012	0.21950086	N	-8.17300361	1.29392946	-3.44456407
C	-4.82656940	-3.18001599	-0.92080690	C	-7.09896750	1.90410652	-2.63934360
C	-4.82667510	-3.65993709	-2.38967182	C	-7.51468387	2.83812051	-1.74578248
H	-3.90049113	-4.20299602	-2.61733301	C	-6.65382005	3.68980877	-0.82196415
H	-5.67204508	-4.33448415	-2.57962894	C	-5.96547330	2.81882917	0.25478497
H	-4.90222659	-2.82230370	-3.08817415	H	-5.30436302	2.07191215	-0.19305640
C	-6.17877686	-2.50591279	-0.59071797	H	-5.36150341	3.43618019	0.93353069
H	-6.34191999	-1.61120637	-1.19767904	H	-6.71440791	2.28606503	0.85229839
H	-7.01626480	-3.19241979	-0.77489891	C	-5.58890528	4.48585082	-1.60947527
H	-6.20901801	-2.20444004	0.46282946	H	-6.06789576	5.16156875	-2.32957265

H	-4.97423443	5.09210190	-0.93095251
H	-4.92046337	3.82423866	-2.16688522
C	-7.57564691	4.70193968	-0.10918359
H	-8.08729954	5.34850211	-0.83374391
H	-8.34298667	4.18717670	0.48249448
H	-7.00239531	5.34423162	0.57037823
H	-8.58826414	2.95920690	-1.63250493
O	-5.90287529	1.48483135	-2.92800990
C	-8.68949333	3.02794142	-5.16214475
H	-7.91943885	3.63516917	-4.67267635
H	-8.19566915	2.43932446	-5.94517126
C	-9.75746580	3.91634318	-5.76025457
C	-10.26873661	3.67996737	-7.04324603
C	-11.27533298	4.48876900	-7.57565569
C	-11.78839875	5.54982537	-6.82932870
C	-11.28553772	5.79921408	-5.55003897
C	-10.27958107	4.99030086	-5.02286100
H	-9.88487621	5.19793117	-4.03019522
H	-11.67344251	6.62857528	-4.96434378
H	-12.57035289	6.18145452	-7.24208947
H	-11.65446447	4.29063070	-8.57485121
H	-9.86607756	2.86154048	-7.63668104
C	-0.29337137	-1.77794752	-1.87130776
H	-1.09461075	-2.39435280	-2.29480546
H	-0.07754777	-0.97901724	-2.59144109
C	0.94040110	-2.61727625	-1.62454360
C	0.82895393	-3.87903939	-1.02016878
C	1.96060747	-4.65076331	-0.75937949
C	3.22875362	-4.17459125	-1.10100793
C	3.35416459	-2.92427152	-1.70685524
C	2.21813796	-2.15376843	-1.96497146
H	2.32394141	-1.18462064	-2.44837670
H	4.33556057	-2.54765788	-1.98328957
H	4.11097712	-4.77655125	-0.90074193
H	1.85238546	-5.62718948	-0.29437457
H	-0.15645695	-4.26171712	-0.76168720
C	-3.91091044	2.87558153	-5.11650334
O	-3.17397868	2.38651061	-3.98311014
C	-1.94809238	3.13072075	-3.94162162
C	-2.35896794	4.56898132	-4.28079358
C	-3.58462004	4.38388118	-5.21615081
H	-4.42685805	4.99583331	-4.88185652
H	-3.35959360	4.66788936	-6.24901184
H	-2.64905459	5.09792164	-3.36809375
H	-1.54545985	5.13005987	-4.75082498
H	-1.52495250	3.00290073	-2.94493826
H	-1.25104056	2.72652998	-4.69258396
H	-3.57972085	2.33777196	-6.01688856
H	-4.95946634	2.64593933	-4.92662408
C	-5.53346938	-1.43411927	-6.27345637
O	-4.79458212	-0.83561344	-5.19911647
C	-3.40861824	-1.13213489	-5.44050349
C	-3.38151224	-2.53311924	-6.09501100
C	-4.85950681	-2.79407556	-6.49299415
H	-4.96726883	-3.14630751	-7.52345963
H	-5.30849002	-3.54218341	-5.83288755
H	-2.71455943	-2.54612501	-6.96283966
H	-3.02548631	-3.29320971	-5.39420745
H	-2.99292443	-0.37051076	-6.11627827
H	-2.90579683	-1.06818631	-4.47543740
H	-6.57574196	-1.48993422	-5.95829669
H	-5.45285187	-0.79867899	-7.16952327

Table 12. Geometric coordinates and thermally corrected MP2 energies for **7** dimer with no THF

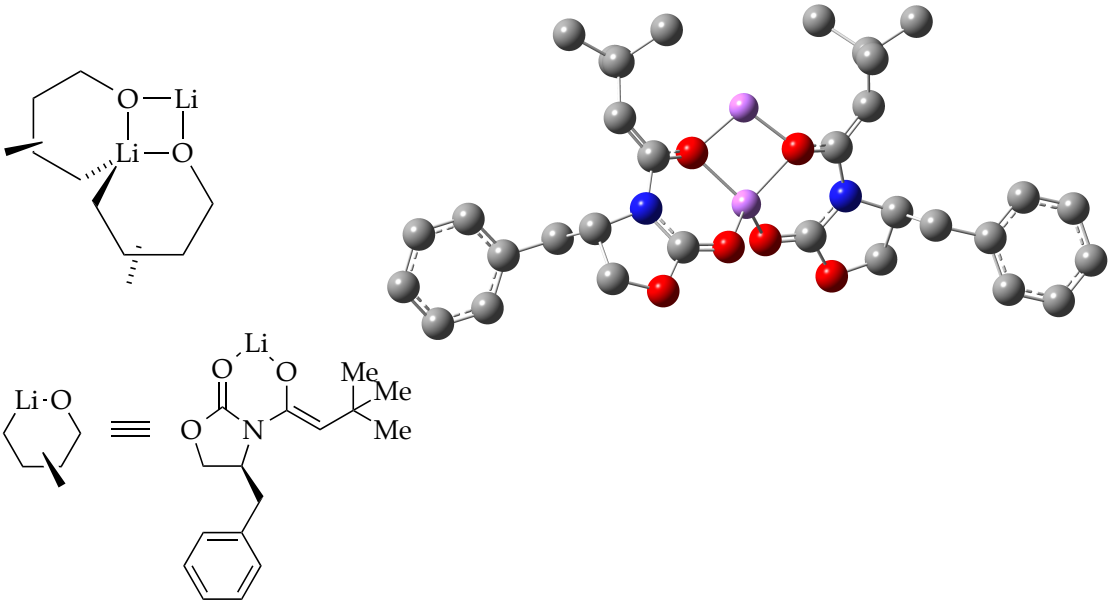


G = -1819.027824 Hartree
G_{MP2} = -1137807.868 kcal/mol
ΔG_{MP2} = 9.583721399 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-4.88744133	-4.10141279	0.91457656
H	0.00000000	0.00000000	1.09511520	H	-5.65240959	-5.06058254	-0.36576223
H	1.02901134	0.00000000	-0.36250291	Li	-5.19715922	-0.31027790	-3.57962985
C	-0.85766544	-1.13754322	-0.58264398	O	-6.10528749	-0.62681764	-5.18075358
H	-0.99800161	-1.92488821	0.16160902	C	-6.41648767	0.33840088	-5.88150498
N	-2.11890100	-0.41974403	-0.81556747	O	-6.61682071	0.18036692	-7.21268210
C	-1.91408489	0.92368953	-0.81292138	C	-7.16044518	1.40366933	-7.74953015
O	-0.64034538	1.21154616	-0.44978959	H	-8.24103746	1.27315642	-7.87021606
O	-2.70389367	1.83102888	-1.08214940	H	-6.70579501	1.58301109	-8.72493000
Li	-4.15667583	1.44851335	-2.19184255	C	-6.81670013	2.47901564	-6.70331949
O	-3.98137906	-0.42649255	-2.21655678	H	-7.66840879	3.14645800	-6.55286579
C	-3.34811718	-1.07172078	-1.27405057	N	-6.61070676	1.63358495	-5.51883404
C	-3.66646944	-2.25372911	-0.69479834	C	-6.36007196	2.16714241	-4.17765590
H	-3.04006859	-2.59425222	0.12432653	C	-7.11798627	3.21892337	-3.78608268
C	-4.85048730	-3.14368190	-1.05590823	C	-6.99070040	3.98096297	-2.47177666
C	-4.76354753	-3.62252810	-2.52348221	C	-7.24746803	3.05262112	-1.26188137
H	-3.84689908	-4.20065172	-2.68949369	H	-6.54835596	2.21022659	-1.24908317
H	-5.61894234	-4.26073928	-2.78029454	H	-7.14148951	3.60013678	-0.31615344
H	-4.75175119	-2.78262911	-3.22587970	H	-8.26048989	2.63609346	-1.30268874
C	-6.19139458	-2.40874670	-0.82476636	C	-5.59778700	4.63881627	-2.33894559
H	-6.24994765	-1.48881543	-1.41540253	H	-5.42429634	5.34882931	-3.15614529
H	-7.04210495	-3.04643630	-1.09871889	H	-5.50925303	5.18423542	-1.39044955
H	-6.30146161	-2.12811842	0.22903828	H	-4.79246517	3.89774485	-2.37355590
C	-4.81679164	-4.38657556	-0.14240425	C	-8.05341930	5.09936162	-2.45704434
H	-3.88515846	-4.95063048	-0.27741592	H	-7.90732288	5.79384574	-3.29410675

H	-9.06528261	4.68323886	-2.53761653
H	-8.00073198	5.67859783	-1.52745296
H	-7.91247277	3.53911124	-4.45359693
O	-5.40416718	1.56090549	-3.52619947
C	-5.56191774	3.31951451	-7.03266365
H	-5.29315201	3.86694843	-6.12212987
H	-4.73238520	2.63897537	-7.26039809
C	-5.78935685	4.28140591	-8.17805391
C	-5.26726282	4.03048580	-9.45391068
C	-5.50607954	4.90972495	-10.51250295
C	-6.27431450	6.05636349	-10.31003184
C	-6.79802137	6.32074556	-9.04212564
C	-6.55595816	5.44122919	-7.98760141
H	-6.95588988	5.66096142	-6.99964657
H	-7.38995838	7.21643675	-8.87302275
H	-6.45948119	6.74282588	-11.13173226
H	-5.08738855	4.69942508	-11.49315821
H	-4.65621009	3.14508985	-9.61698549
C	-0.30333822	-1.75936927	-1.88473296
H	-1.10405616	-2.37112959	-2.31552934
H	-0.09052181	-0.95284004	-2.59701119
C	0.93266965	-2.59932457	-1.64884080
C	0.82592409	-3.86483562	-1.05198861
C	1.95999096	-4.63650988	-0.80183557
C	3.22545286	-4.15571537	-1.14708086
C	3.34595731	-2.90152746	-1.74578847
C	2.20760672	-2.13104240	-1.99322638
H	2.30897755	-1.15943617	-2.47240240
H	4.32523901	-2.52213666	-2.02557304
H	4.10960710	-4.75767284	-0.95569804
H	1.85583679	-5.61643718	-0.34342369
H	-0.15754653	-4.25187881	-0.79263478

Table 13. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer with no THF

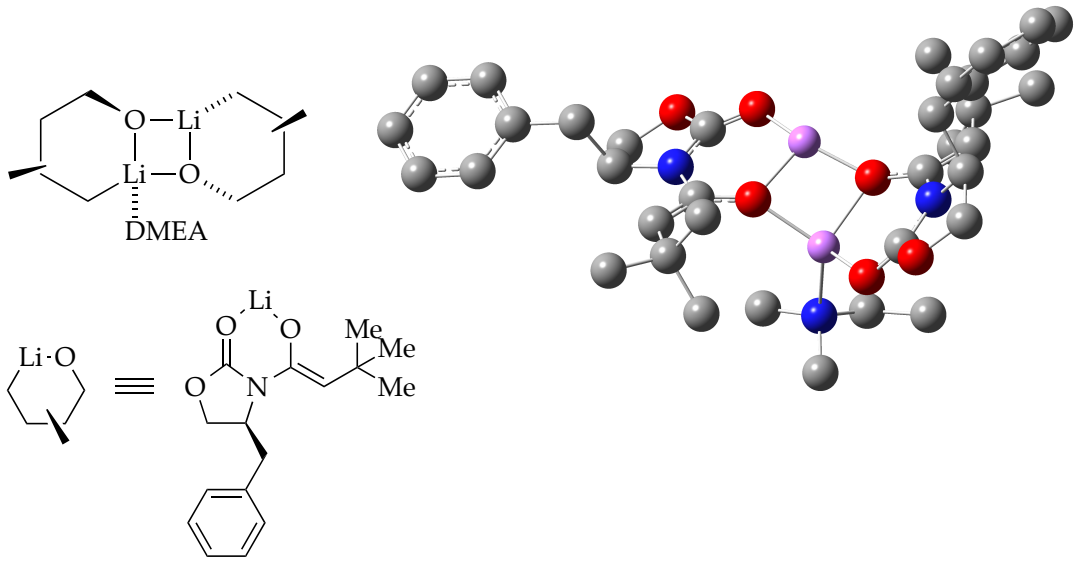


G = -1819.015172 Hartree
G_{MP2} = -1137799.956 kcal/mol
ΔG_{MP2} = 13.5397214 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.43434397	-1.19715468	-1.85099942
O	0.00000000	0.00000000	1.91159690	H	5.10406105	-0.90838965	-1.36775299
C	1.06485233	0.00000000	2.51790693	H	4.73546315	-2.22504798	-2.49921889
O	1.15247234	0.58063063	3.74385225	O	1.70546531	-0.95494870	-0.05881879
C	2.43455103	0.27440131	4.31938165	Li	0.83118684	-1.93313998	-1.27266838
H	2.30752528	-0.55257587	5.02681272	O	-0.78559940	-1.17599694	-1.35116840
H	2.79341846	1.15552245	4.85341520	C	-1.66285262	-0.90647629	-2.27859895
C	3.31450270	-0.11728123	3.12209970	N	-2.26859981	0.41444461	-2.18395222
H	3.94306148	-0.97054810	3.38551733	C	-3.62932158	0.72515559	-2.64534866
N	2.28115586	-0.51346727	2.15422188	C	-3.61248117	2.25837898	-2.54008710
C	2.56680515	-1.18499742	0.89402773	H	-3.35140563	2.73490800	-3.49149479
C	3.68731228	-1.95097084	0.82661939	H	-4.54832952	2.67935840	-2.16950313
H	4.26143805	-2.09965529	1.73430594	O	-2.57379221	2.54716212	-1.58784020
C	4.22001844	-2.66208972	-0.41255571	C	-1.74250588	1.47560917	-1.49738242
C	5.61170397	-3.23705773	-0.07189462	O	-0.69830085	1.55753189	-0.86118945
H	6.30137641	-2.43592745	0.22003541	H	-3.76100779	0.42497348	-3.68707410
H	5.55303994	-3.95060932	0.75957807	C	-4.70104669	0.03440856	-1.77015148
H	6.04628817	-3.75854628	-0.93330863	H	-4.46007736	-1.03407798	-1.75019094
C	3.31547437	-3.85040831	-0.82046117	H	-4.60724348	0.40908434	-0.74360002
H	2.30452101	-3.52374888	-1.10232793	C	-6.10588292	0.25144163	-2.28771654
H	3.72835537	-4.38992066	-1.68306667	C	-6.97504023	1.16228468	-1.67240039
H	3.19817558	-4.55896270	0.00666701	C	-8.25938285	1.38117665	-2.17545503
C	4.37844269	-1.69406340	-1.60681394	C	-8.69540328	0.68990216	-3.30598755

C	-7.84134766	-0.22482616	-3.92676309
C	-6.56012983	-0.44104294	-3.42062214
H	-5.90514262	-1.16428745	-3.90266400
H	-8.17590540	-0.77484788	-4.80251700
H	-9.69506427	0.85711478	-3.69778465
H	-8.91920453	2.08857609	-1.68001128
H	-6.64739051	1.69552339	-0.78245314
C	-2.07690708	-1.71882439	-3.28616016
C	-1.64293095	-3.16219620	-3.51624664
C	-1.83983823	-4.03075330	-2.25316333
H	-1.49878146	-5.06001718	-2.42636161
H	-1.29758340	-3.62392845	-1.39373461
H	-2.89951376	-4.06736049	-1.97628219
C	-0.16885096	-3.24384556	-3.98225222
H	0.52650216	-2.84487196	-3.23029223
H	0.13204490	-4.28115671	-4.18011552
H	-0.01138363	-2.65851409	-4.89471218
C	-2.51754819	-3.75088135	-4.64396787
H	-3.57798481	-3.72614706	-4.36553769
H	-2.40022555	-3.18131135	-5.57438775
H	-2.24764828	-4.79357103	-4.85103150
H	-2.76297749	-1.31296473	-4.02132465
C	4.19914085	1.02785576	2.57624057
H	4.58391679	0.70164288	1.60385106
H	3.56368302	1.90396138	2.39823647
C	5.33884845	1.37973205	3.50668637
C	6.45933647	0.54067953	3.60608592
C	7.50110269	0.83725599	4.48426920
C	7.44198559	1.98337568	5.28076295
C	6.33695258	2.82978438	5.18824220
C	5.29534065	2.52847623	4.30803206
H	4.44337357	3.20084217	4.23202378
H	6.28532638	3.72851845	5.79722134
H	8.25453079	2.21708888	5.96335499
H	8.36249809	0.17697580	4.54279895
H	6.51859828	-0.34758522	2.98002933

Table 14. Geometric coordinates and thermally corrected MP2 energies for **7** dimer with one DMEA

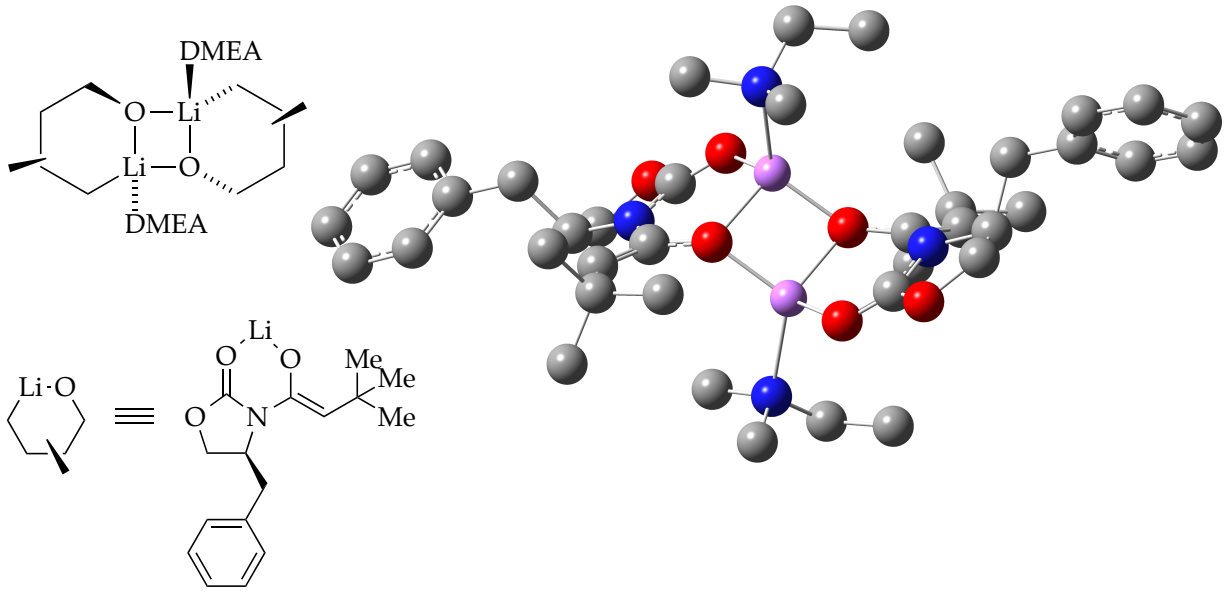


G = -2032.681005 Hartree
G_{MP2} = -1271390.477 kcal/mol
ΔG_{MP2} = 4.996905257 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.79333060	2.91653347	0.27473601
O	0.00000000	0.00000000	1.94657030	C	-5.69391841	3.27619941	-0.68064383
C	0.72237635	0.00000000	3.02896452	C	-5.70197203	4.64200704	-0.36709466
N	0.61242558	-1.22854888	3.82785311	C	-6.82308151	5.43228989	-0.63004953
C	1.45165878	-1.55792610	4.99155024	C	-7.95693604	4.86641039	-1.21332667
C	1.24007578	-3.07420212	5.03878757	C	-7.96434530	3.50516242	-1.52725157
H	1.95491966	-3.61698353	4.40994568	C	-6.84338500	2.71934887	-1.26198690
H	1.24766052	-3.48839272	6.04753050	H	-6.86155101	1.65716422	-1.49820197
O	-0.08145915	-3.24779578	4.48618391	H	-8.84666579	3.05384585	-1.97354826
C	-0.35902813	-2.17780832	3.69508275	H	-8.83105811	5.47901907	-1.41681442
O	-1.38680973	-2.17304776	3.01706958	H	-6.81027145	6.48853155	-0.37416153
Li	-1.61447307	-0.86624440	1.70436378	H	-4.82646516	5.08822971	0.10003835
O	-1.87971823	-0.53100090	-0.05712323	C	-3.73041250	-0.90820880	-1.53213531
C	-2.72392800	-0.18176577	-0.98748816	C	-4.16369385	-2.30829830	-1.11058341
N	-2.56418821	1.19230385	-1.47565137	C	-3.00760914	-3.32492652	-1.24238445
C	-3.69152787	2.10064076	-1.72571335	H	-2.15590239	-3.02289935	-0.62661722
C	-2.94505781	3.30148972	-2.33182631	H	-3.32811444	-4.32592335	-0.92440625
H	-2.93667871	3.27187617	-3.42697216	H	-2.66826855	-3.39174199	-2.28278084
H	-3.32948355	4.26687573	-1.99923569	C	-4.68034415	-2.31185976	0.34735565
O	-1.58932229	3.16460132	-1.86481723	H	-5.52234761	-1.61941782	0.46628884
C	-1.38725896	1.87734122	-1.47697084	H	-5.02019781	-3.31347927	0.64193106
O	-0.25826766	1.48264668	-1.19660162	H	-3.89441065	-2.01253013	1.04877722
H	-4.37557747	1.67056500	-2.46092304	C	-5.31680988	-2.75333014	-2.03366611
C	-4.47218972	2.42030401	-0.42955810	H	-6.17170586	-2.06903949	-1.95797021
H	-4.76279968	1.46188986	0.01554272	H	-4.99565030	-2.77413641	-3.08250636

H	-5.66740177	-3.75801178	-1.76849508
H	-4.29061407	-0.45737416	-2.34608363
H	2.49225799	-1.30281923	4.77914204
C	0.96935268	-0.85242533	6.28596642
H	0.88650379	0.21877984	6.08042582
H	-0.04175001	-1.21212703	6.51333426
C	1.88684333	-1.10060855	7.46386807
C	3.13528317	-0.46434523	7.54208676
C	3.99719921	-0.70656875	8.61122067
C	3.62497584	-1.59114852	9.62629723
C	2.38498445	-2.22709776	9.56441084
C	1.52538262	-1.98263740	8.49116333
H	0.55473270	-2.47310568	8.45676073
H	2.08214740	-2.91108608	10.35286986
H	4.29478457	-1.77801336	10.46124904
H	4.95773168	-0.19990901	8.65512406
H	3.43007163	0.23651448	6.76357472
C	1.55544427	0.97298900	3.48207150
H	2.10010394	0.79800994	4.40168269
C	1.76409160	2.34768794	2.85381730
C	0.41964378	3.09332103	2.69112773
H	-0.06205347	3.23779268	3.66578923
H	0.57290992	4.08141250	2.23701385
H	-0.26355652	2.52345659	2.05553301
C	2.46149528	2.25608041	1.47792831
H	1.83538766	1.72854510	0.75361451
H	2.65936642	3.25734203	1.07247629
H	3.42001488	1.72878620	1.56090108
C	2.66807407	3.16777998	3.79811261
H	2.21127672	3.27220015	4.79037177
H	3.64676100	2.68717203	3.92648903
H	2.83911145	4.17484107	3.39923860
N	1.61656175	-1.23428135	-0.80498958
C	1.10177759	-2.33317082	-1.65279623
C	0.29654428	-1.87808240	-2.86752160
H	0.90880838	-1.33337707	-3.59319750
H	-0.54316250	-1.24343063	-2.57114403
H	-0.11117086	-2.75802960	-3.37699823
H	0.46316476	-2.95456541	-1.01465363
H	1.94382342	-2.97091204	-1.98351306
C	2.54108713	-0.36706074	-1.55289549
H	2.96336011	0.37884264	-0.87457381
H	3.37128600	-0.94214131	-2.00128566
H	2.00749125	0.16499979	-2.34221905
C	2.31385443	-1.80918167	0.35511646
H	2.66418929	-1.00773214	1.01084347
H	1.62189650	-2.43725060	0.92407930
H	3.17927205	-2.42588254	0.05230676

Table 15. Geometric coordinates and thermally corrected MP2 energies for **7** dimer with two DMEA

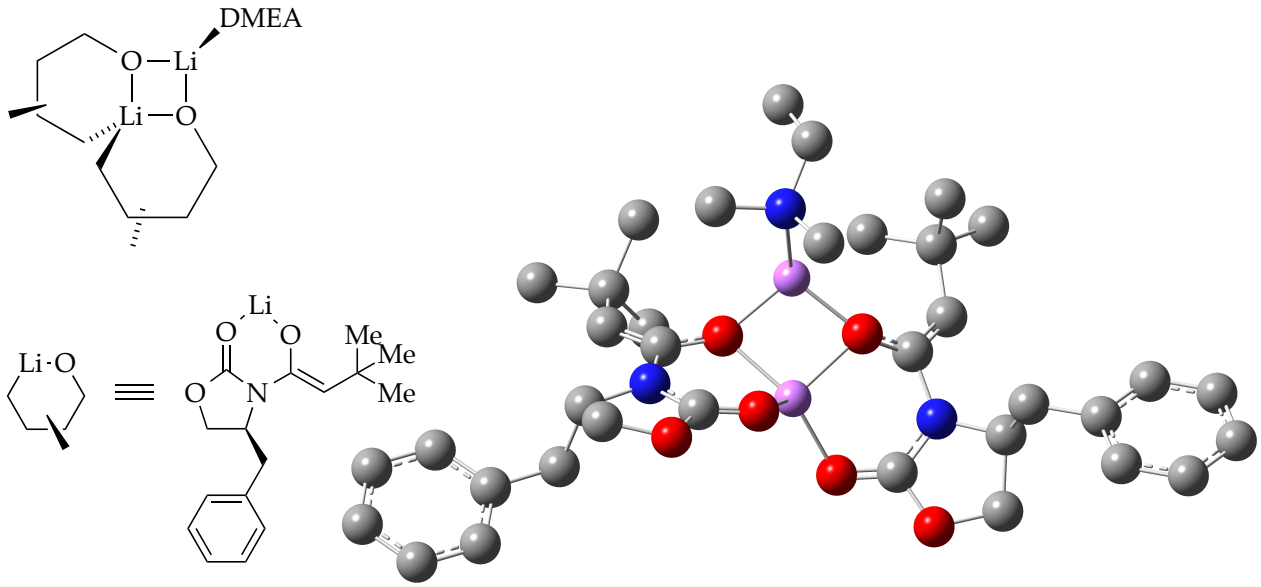


G = -2246.337074 Hartree
G_{MP2} = -1404975.289 kcal/mol
ΔG_{MP2} = -0.691410886 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.41120346	3.29284334	-1.70716893
O	0.00000000	0.00000000	1.93453380	O	1.90946313	-0.04362314	-0.10544682
C	1.05513034	0.00000000	2.55895082	Li	1.64865901	-1.68747188	-1.05822450
O	1.06267267	-0.31781088	3.88591564	O	1.57208007	-1.84263060	-3.00785304
C	2.43306485	-0.39801127	4.32587095	C	0.51172859	-1.87135862	-3.62319287
H	2.75735777	-1.44399275	4.27590748	O	0.50257831	-1.77918145	-4.97912996
H	2.48416126	-0.04634816	5.35712369	C	-0.85813539	-1.73767149	-5.44092440
C	3.18229846	0.49198896	3.32892262	H	-0.94560754	-2.38055227	-6.31796821
H	4.18258964	0.10885406	3.11389787	H	-1.09315356	-0.70613532	-5.72749696
N	2.32087663	0.31902137	2.15028252	C	-1.71005690	-2.20462777	-4.24437470
C	2.73469123	0.48350813	0.74552756	H	-1.94880799	-3.27294201	-4.34275551
C	3.91505849	1.12481767	0.52780327	N	-0.75895921	-2.01091145	-3.14255549
H	4.44993888	1.49264544	1.39752583	C	-1.02635338	-2.30781846	-1.72391041
C	4.62829065	1.46244074	-0.77423724	C	-1.98950266	-3.22475850	-1.44841366
C	3.88344087	1.03640812	-2.05189270	C	-2.45160601	-3.65489834	-0.05860165
H	2.89177045	1.49345174	-2.11077576	C	-1.28683490	-4.25906096	0.75802989
H	4.45738031	1.35037080	-2.93357274	H	-0.48829619	-3.52161382	0.87892030
H	3.74397486	-0.04573536	-2.11071388	H	-1.62621218	-4.56835447	1.75581947
C	6.02463588	0.79309527	-0.76677423	H	-0.87309697	-5.14019572	0.25273280
H	5.93564445	-0.29937923	-0.75317683	C	-3.04698369	-2.46815917	0.73181178
H	6.60563302	1.07573165	-1.65480677	H	-3.89820838	-2.03096322	0.19604240
H	6.60177973	1.09021339	0.11834018	H	-3.40200355	-2.79581259	1.71823061
C	4.83326116	2.99726370	-0.82134670	H	-2.29675835	-1.68783335	0.88936933
H	3.86942394	3.51846718	-0.85366756	C	-3.54496062	-4.72944933	-0.22838845
H	5.37499507	3.35363173	0.06415969	H	-4.40397330	-4.33531001	-0.78674253

H	-3.16140306	-5.60121451	-0.77385710
H	-3.90965377	-5.07621052	0.74609731
H	-2.46461397	-3.72887439	-2.28489496
O	-0.28293031	-1.63593086	-0.89765108
C	-3.02010188	-1.41204089	-4.08661344
H	-3.47044291	-1.69227974	-3.12919639
H	-2.77397500	-0.34486954	-4.02705329
C	-3.98413424	-1.66716284	-5.22651072
C	-4.17687927	-0.72010389	-6.24108752
C	-5.04621402	-0.97279054	-7.30431681
C	-5.73867831	-2.18205506	-7.36982051
C	-5.56001167	-3.13361903	-6.36298187
C	-4.69232420	-2.87638420	-5.30206296
H	-4.56968358	-3.61826863	-4.51567303
H	-6.10211814	-4.07489807	-6.40045502
H	-6.41719359	-2.38009323	-8.19513484
H	-5.18404886	-0.22229777	-8.07832394
H	-3.64921059	0.23011665	-6.19280627
N	3.06345588	-3.30056740	-0.49135464
C	2.47999521	-4.65874809	-0.42186359
C	1.79096856	-5.13154782	-1.69969663
H	2.48561770	-5.21864399	-2.54082654
H	0.97971711	-4.45659516	-1.98514743
H	1.35887206	-6.12355314	-1.52566252
H	1.74771226	-4.64881117	0.39256126
H	3.26782832	-5.38279094	-0.13747882
C	4.14635416	-3.23475305	-1.48544005
H	4.60414766	-2.24207505	-1.45398932
H	4.93183980	-3.98671564	-1.28746959
H	3.74877815	-3.38580717	-2.49014134
C	3.59428140	-2.94451099	0.83267273
H	4.02297553	-1.93914970	0.80078268
H	2.78212055	-2.95277898	1.56656369
H	4.37419129	-3.65224847	1.16836335
C	3.25751561	1.96828219	3.80175837
H	3.54472512	2.58985060	2.94843006
H	2.24889803	2.28244442	4.09745437
C	4.22258164	2.16865261	4.95049160
C	5.60824978	2.13214698	4.73126547
C	6.50557618	2.29147043	5.78669761
C	6.03255948	2.49239025	7.08567416
C	4.65779925	2.53522289	7.31822556
C	3.76271873	2.37387247	6.25827763
H	2.69210103	2.42032056	6.44657970
H	4.27891519	2.69823312	8.32377995
H	6.73109264	2.61949470	7.90825413
H	7.57497553	2.26422057	5.59441963
H	5.98757616	1.98740240	3.72163468
N	-0.80104906	1.92316863	-0.63128111
C	-2.21168038	2.15483221	-0.25682667
C	-3.20145486	1.18415425	-0.89762257
H	-4.18851120	1.31735750	-0.44123485
H	-2.89521297	0.14481352	-0.74402940
H	-3.31518964	1.35560786	-1.97305101
H	-2.50135490	3.19461940	-0.50197829
H	-2.26619055	2.05672402	0.83342001
C	0.05397804	2.88350575	0.08244589
H	-0.09174932	2.76768540	1.16032518
H	1.10387122	2.68262791	-0.14649572
H	-0.17846454	3.92765668	-0.19394437
C	-0.58389295	2.05241442	-2.07766194
H	-1.14248471	1.28224072	-2.61426735
H	-0.88925332	3.04439739	-2.45827944
H	0.47856817	1.90832884	-2.29338579

Table 16. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer with one DMEA

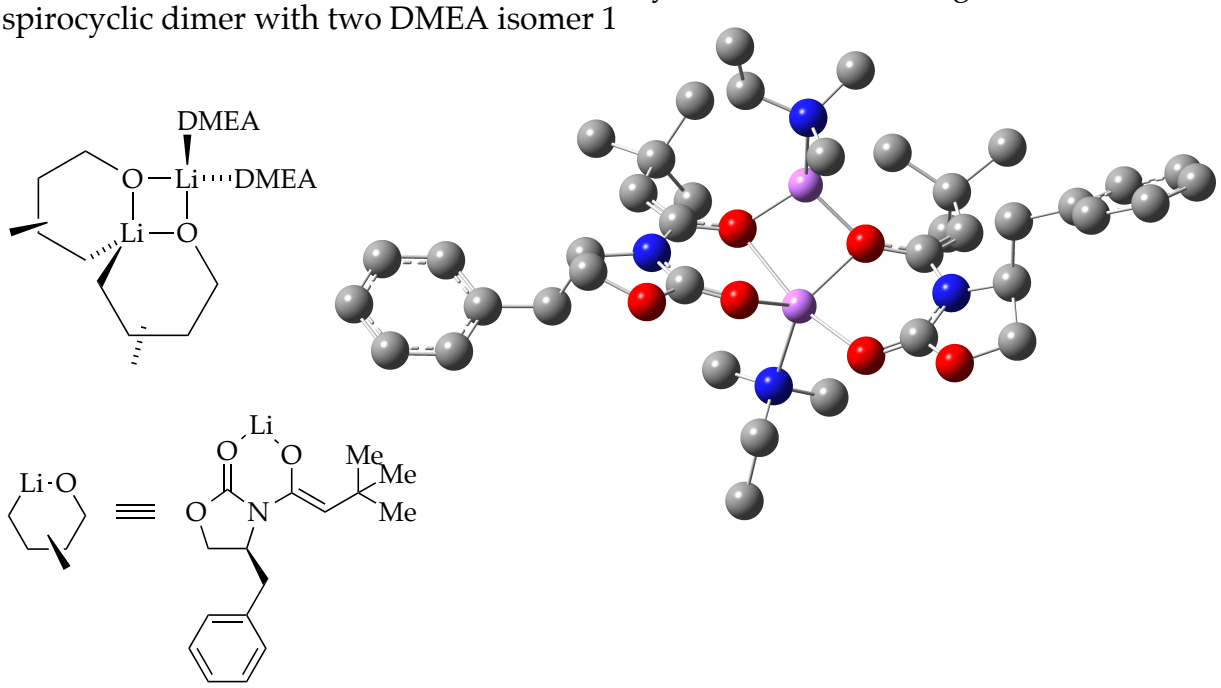


G = -2032.678376 Hartree
G_{MP2} = -1271389.192 kcal/mol
ΔG_{MP2} = 5.639405257 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.84667535	-0.70213760	-2.09681042
O	0.00000000	0.00000000	1.95671960	H	4.32185991	0.26513194	-1.94647049
C	1.08036405	0.00000000	2.53801937	H	4.29547935	-1.13822251	-3.03358753
O	1.15468488	0.40244680	3.83697226	O	1.57028495	-1.12380627	0.02371978
C	2.48559379	0.15087292	4.32529136	Li	0.27668343	-2.39214028	-0.34687779
H	2.48233007	-0.79782222	4.87460055	O	-1.06041848	-1.29847934	-1.00041083
H	2.76437694	0.96182943	4.99941827	C	-1.79657847	-0.87778643	-1.99181705
C	3.34297245	0.08397080	3.05548993	N	-2.47527889	0.40136260	-1.75734604
H	4.11727715	-0.68080322	3.15062182	C	-3.91534209	0.60609373	-1.93781834
N	2.32594154	-0.34644886	2.08454954	C	-4.00328576	2.12946062	-1.72308722
C	2.62119226	-0.90069934	0.76134223	H	-3.99868743	2.67984999	-2.67010858
C	3.91996962	-1.13021823	0.43716724	H	-4.86691354	2.43695476	-1.13116853
H	4.68823138	-0.91468813	1.17024263	O	-2.80762113	2.47276249	-0.99521374
C	4.41527753	-1.65585539	-0.90680495	C	-1.90504566	1.46686251	-1.13586005
C	5.95765329	-1.65277974	-0.88377832	O	-0.75260534	1.58814104	-0.72844884
H	6.34577432	-0.63914289	-0.72315981	H	-4.21378826	0.34681152	-2.95667966
H	6.34385058	-2.29296787	-0.07994269	C	-4.74393972	-0.23590834	-0.94000686
H	6.36515032	-2.02159684	-1.83284005	H	-4.42886078	-1.27901710	-1.06133546
C	3.93766534	-3.10508151	-1.15657191	H	-4.47886563	0.06669005	0.08027787
H	4.29680908	-3.77735198	-0.36741754	C	-6.23483525	-0.10814067	-1.16290455
H	2.84430016	-3.15408748	-1.17512397	C	-7.03343612	0.66551496	-0.31006877
H	4.30872009	-3.48369673	-2.11862933	C	-8.40390427	0.80500398	-0.54013617
C	3.93817856	-0.75472702	-2.06830126	C	-8.99844741	0.17077829	-1.63117958

C	-8.21511888	-0.60688973	-2.48749976
C	-6.84734831	-0.74450613	-2.25344706
H	-6.24555262	-1.36063729	-2.91874769
H	-8.67127665	-1.11109405	-3.33551735
H	-10.06489162	0.27645928	-1.81105866
H	-9.00587705	1.40609494	0.13635530
H	-6.57914545	1.15328495	0.54979636
C	-2.05402585	-1.45684500	-3.19144837
C	-1.57511165	-2.81904554	-3.67309290
C	-2.06517212	-3.93619523	-2.72538536
H	-1.69822280	-4.92107199	-3.04525930
H	-1.72331064	-3.75417615	-1.70187521
H	-3.16089900	-3.97305682	-2.70534413
C	-0.03362845	-2.86405139	-3.78327388
H	0.44612015	-2.64464113	-2.82334666
H	0.31246639	-3.84980546	-4.12326867
H	0.32503624	-2.11314860	-4.49603491
C	-2.16494240	-3.07708303	-5.07473749
H	-3.26177270	-3.06707638	-5.04780276
H	-1.83938174	-2.30820636	-5.78606317
H	-1.84596216	-4.05204404	-5.46325432
H	-2.64867066	-0.88161221	-3.89536267
N	-0.00976746	-4.01578820	0.99506133
C	-0.30968063	-5.35711661	0.44443519
H	-1.28443422	-5.29073784	-0.04940268
H	-0.41915639	-6.08211858	1.27167503
C	0.72285064	-5.86680010	-0.55873743
H	1.70649052	-6.02587116	-0.10656194
H	0.39072271	-6.82726973	-0.96777346
H	0.83982900	-5.17032287	-1.39650200
C	1.18194563	-4.05555855	1.86138544
H	2.06661949	-4.33029992	1.28392461
H	1.35461507	-3.06294343	2.28327750
H	1.05627724	-4.77629462	2.68831259
C	-1.16403783	-3.53387989	1.77991283
H	-0.95967119	-2.52655412	2.15423775
H	-2.04869393	-3.48644191	1.13889104
H	-1.38034092	-4.19550590	2.63620307
C	3.97728879	1.44304451	2.66788625
H	4.34587497	1.35652364	1.64085335
H	3.18556219	2.20238799	2.66170374
C	5.09281968	1.85778227	3.60221521
C	6.34458757	1.22584414	3.54346559
C	7.37058627	1.58503684	4.41689805
C	7.16420493	2.58760583	5.36752981
C	5.92674846	3.22813208	5.43437888
C	4.90143552	2.86408833	4.55873950
H	3.94375862	3.37807077	4.60830230
H	5.75812575	4.01544534	6.16442172
H	7.96445853	2.87066127	6.04595242
H	8.33438594	1.08691258	4.35097068
H	6.52101006	0.45419375	2.79668635

Table 17. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer with two DMEA isomer 1

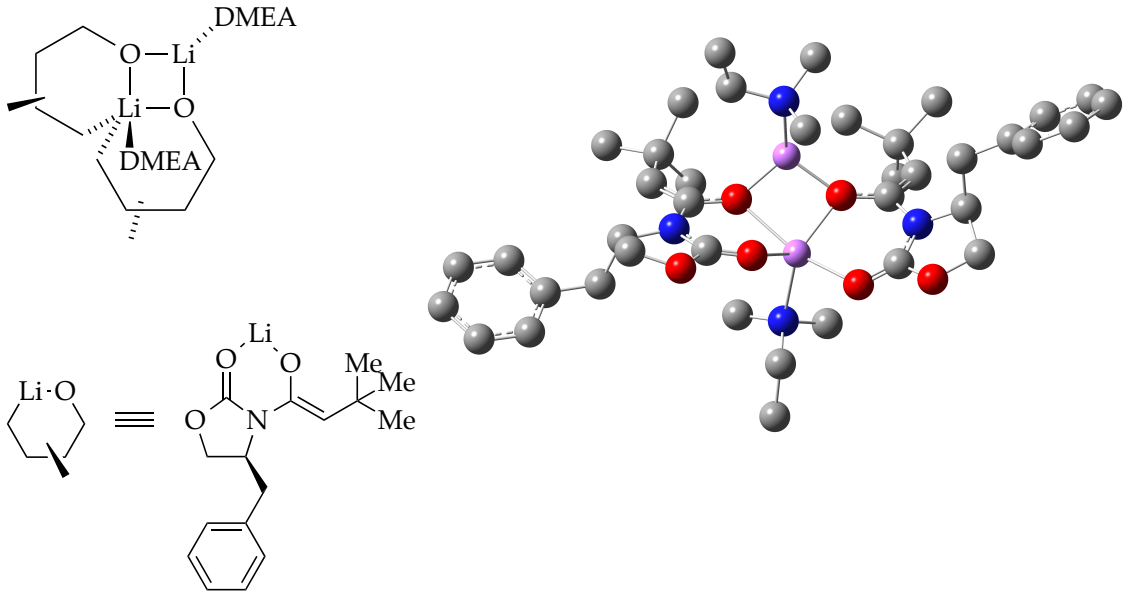


G = -2246.325941 Hartree
G_{MP2} = -1404966.831 kcal/mol
ΔG_{MP2} = 3.537589114 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	7.90140022	4.99677255	-2.38320371
Li	0.00000000	0.00000000	2.62675760	H	9.60107942	4.76416667	-0.58109499
O	1.53835750	0.00000000	1.66662966	H	9.15735218	3.24372480	1.33855253
C	2.68534935	0.59860524	1.70774919	H	7.03818022	1.97709659	1.45597111
N	2.75255641	1.83734729	0.92184947	C	3.80628670	0.22271062	2.38513012
C	1.72731167	2.35148855	0.17339717	H	4.68489799	0.85455062	2.33466071
O	0.62287435	1.89344246	-0.08550586	C	3.94543071	-1.01926334	3.25960934
O	2.09257207	3.56778542	-0.33440993	C	5.41911767	-1.12978571	3.70309585
C	3.33560475	3.96712345	0.26713908	H	5.57400183	-2.00920071	4.34021913
H	3.12014528	4.64712933	1.10002583	H	6.08361068	-1.22177496	2.83483748
H	3.93166488	4.49036187	-0.48219926	H	5.72964609	-0.24390831	4.27233062
C	3.96251205	2.65092886	0.74298239	C	3.56946460	-2.30694372	2.49374187
H	4.46804790	2.78759092	1.70185330	H	4.22043076	-2.43923524	1.62132584
C	4.93801844	2.02344409	-0.28436681	H	3.67926167	-3.19161469	3.13550866
H	5.11135911	0.98619970	0.01989675	H	2.53573959	-2.25783939	2.14171179
H	4.43773325	1.99731864	-1.26050198	C	3.06728426	-0.91519925	4.52983302
C	6.24727628	2.77454165	-0.38616893	H	3.33558033	-0.02894262	5.11766321
C	7.21867766	2.64859848	0.61891644	H	2.00738807	-0.83986371	4.26351741
C	8.41631278	3.35963874	0.55189596	H	3.18934804	-1.79850451	5.17179847
C	8.66685307	4.21186893	-0.52625296	O	-1.16337166	-0.74877407	1.45400127
C	7.71295349	4.34287266	-1.53570687	C	-2.28932252	-1.38259962	1.31924370
C	6.51439114	3.62961272	-1.46397913	N	-3.23645161	-0.73616545	0.40309331
H	5.78145444	3.72808105	-2.26208582	C	-4.67974427	-0.63077999	0.63135701

C	-5.12806405	-0.02068446	-0.70989850
H	-5.48547860	-0.78518298	-1.40903269
H	-5.89229682	0.75110061	-0.60181887
O	-3.94372218	0.58168709	-1.25911989
C	-2.84856820	0.03151006	-0.65616341
O	-1.72400077	0.24399477	-1.08460548
H	-5.12466010	-1.62042682	0.76271769
C	-5.00872626	0.23710395	1.86871235
H	-4.43977956	-0.17799388	2.70889953
H	-4.63869581	1.25404507	1.68882285
C	-6.48513782	0.26192484	2.19616909
C	-7.28012018	1.37493171	1.89130793
C	-8.64875088	1.37771470	2.16943068
C	-9.24547302	0.26266449	2.75830630
C	-8.46431482	-0.85256935	3.07088240
C	-7.09791612	-0.85077933	2.79274088
H	-6.49394751	-1.71886189	3.04939657
H	-8.91906572	-1.72287177	3.53690881
H	-10.30987838	0.26322024	2.97703189
H	-9.24621210	2.25316563	1.92863585
H	-6.82052903	2.25283134	1.44189772
C	-2.71831249	-2.53119471	1.90393143
C	-2.00241917	-3.44614159	2.88593395
C	-0.84437089	-2.77427484	3.64917132
H	-0.03297439	-2.48942123	2.97411660
H	-1.19046415	-1.88051272	4.18381972
H	-0.43414790	-3.46703563	4.39526424
C	-1.44114151	-4.67051389	2.12126359
H	-0.97044198	-5.38893837	2.80653325
H	-2.23827380	-5.19421182	1.57984832
H	-0.69021258	-4.35546252	1.38797425
C	-3.03741373	-3.94697984	3.92041775
H	-3.87980205	-4.44704547	3.42563341
H	-2.58644387	-4.66555945	4.61682732
H	-3.44189822	-3.11249114	4.50624149
H	-3.67505665	-2.92278691	1.56589431
N	-0.62300060	1.56210040	3.92037637
C	0.58043712	2.27468463	4.41205939
C	0.35265818	3.55448365	5.22931574
H	-0.16996247	4.32585643	4.65402269
H	1.32273748	3.96731541	5.52822319
H	-0.21850879	3.36605390	6.14465014
H	1.19155262	2.50535790	3.53242687
H	1.15436727	1.55790064	5.01039288
C	-1.46629700	1.05969929	5.01355078
H	-1.94848973	1.86420268	5.59198566
H	-2.25500399	0.42473764	4.59735003
H	-0.86139493	0.45571012	5.69822900
C	-1.41746291	2.38017898	2.98729248
H	-1.89115875	3.24618538	3.47624788
H	-0.77888482	2.73368122	2.17257536
H	-2.20097549	1.75714635	2.54753990
N	0.98814530	-1.18390513	-1.61150162
C	0.90830800	-0.34554229	-2.82822451
C	1.43465142	-0.95514837	-4.13698693
H	2.49712116	-1.21622768	-4.07811935
H	1.31921205	-0.22565288	-4.94698061
H	0.88060089	-1.85502485	-4.42601933
H	1.45789475	0.57859032	-2.61191927
H	-0.14127330	-0.06059618	-2.94635558
C	0.17787072	-2.40252030	-1.71277619
H	0.56608896	-3.12323897	-2.45255330
H	0.15346755	-2.89979726	-0.73729472
H	-0.84619137	-2.13341181	-1.98533398
C	2.36808648	-1.50975321	-1.24029173
H	2.86425567	-2.18136282	-1.96179955
H	2.95287820	-0.58795411	-1.16470832
H	2.37531438	-1.98992428	-0.25919776

Table 18. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer with two DMEA isomer 2

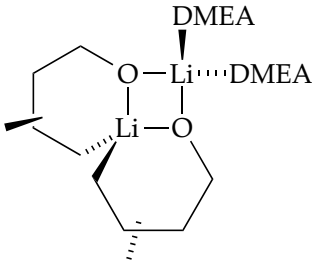


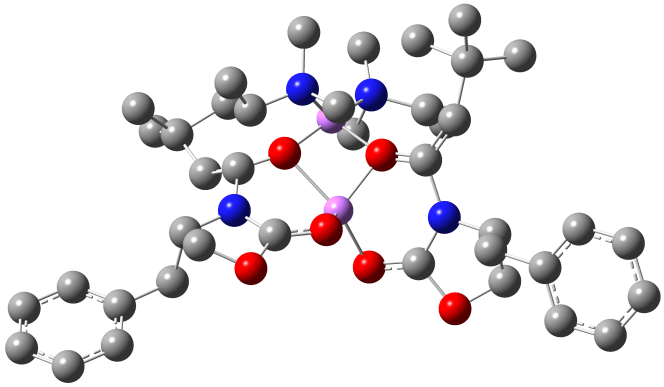
G = -2246.325937 Hartree
G_{MP2} = -1404966.828 kcal/mol
ΔG_{MP2} = 3.539089114 kcal/mol Li vs. **7** dimer with two THF

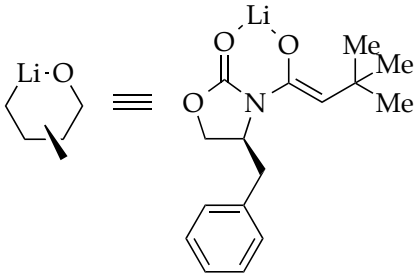
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.78160378	3.72811927	-2.26186534
Li	0.00000000	0.00000000	2.62682900	H	7.90154311	4.99682740	-2.38292840
O	1.53841196	0.00000000	1.66683480	H	9.60114788	4.76428563	-0.58074214
C	2.68536740	0.59867925	1.70799309	H	9.15736068	3.24388359	1.33892111
N	2.75260416	1.83734003	0.92197359	H	7.03820396	1.97722037	1.45627355
C	1.72739471	2.35145412	0.17344771	C	3.80619701	0.22299916	2.38566883
O	0.62294740	1.89344484	-0.08548101	H	4.68475287	0.85492299	2.33530563
O	2.09267837	3.56774894	-0.33435456	C	3.94523488	-1.01872919	3.26051834
C	3.33565194	3.96711999	0.26728680	C	5.41879917	-1.12891173	3.70448944
H	3.12011558	4.64711133	1.10016540	H	5.57361051	-2.00810038	4.34194118
H	3.93175580	4.49037944	-0.48200322	H	6.08356574	-1.22108449	2.83645997
C	3.96256049	2.65094034	0.74315697	H	5.72903586	-0.24280848	4.27353558
H	4.46804749	2.78761140	1.70205178	C	3.56969708	-2.30667068	2.49487780
C	4.93812172	2.02349003	-0.28416090	H	4.22096549	-2.43910523	1.62270896
H	5.11147552	0.98624470	0.02008766	H	3.67941384	-3.19115305	3.13691788
H	4.43786931	1.99736919	-1.26031344	H	2.53607749	-2.25781191	2.14250417
C	6.24736312	2.77462062	-0.38591297	C	3.06667547	-0.91446007	4.53044535
C	7.21872370	2.64871351	0.61921719	H	3.33451108	-0.02790813	5.11803269
C	8.41635187	3.35976862	0.55223202	H	2.00683967	-0.83953691	4.26378522
C	8.66692642	4.21197725	-0.52592804	H	3.18880602	-1.79749565	5.17276816
C	7.71306899	4.34294408	-1.53542589	O	-1.16334888	-0.74879157	1.45402830
C	6.51451142	3.62967273	-1.46372940	C	-2.28928577	-1.38264083	1.31925016

N	-3.23643067	-0.73619688	0.40311725
C	-4.67974046	-0.63094291	0.63133715
C	-5.12806394	-0.02074212	-0.70986947
H	-5.48540987	-0.78519709	-1.40908509
H	-5.89235033	0.75098260	-0.60173708
O	-3.94374484	0.58175544	-1.25900358
C	-2.84857165	0.03157895	-0.65607956
O	-1.72401357	0.24413010	-1.08452100
H	-5.12457917	-1.62064082	0.76256832
C	-5.00886784	0.23675846	1.86877987
H	-4.43991159	-0.17838533	2.70893813
H	-4.63895407	1.25377074	1.68904605
C	-6.48529696	0.26132638	2.19616863
C	-7.28045527	1.37421510	1.89133686
C	-8.64910908	1.37672091	2.16934596
C	-9.24567661	0.26151008	2.75807594
C	-8.46434141	-0.85360885	3.07062005
C	-7.09792001	-0.85154150	2.79259144
H	-6.49381352	-1.71954134	3.04920236
H	-8.91897177	-1.72403750	3.53652552
H	-10.31010077	0.26185127	2.97670653
H	-9.24671491	2.25208005	1.92857358
H	-6.82099081	2.25223459	1.44203271
C	-2.71825985	-2.53126443	1.90389842
C	-2.00237445	-3.44623475	2.88589231
C	-0.84430392	-2.77440827	3.64912065
H	-0.03293451	-2.48953778	2.97404519
H	-1.19036810	-1.88066245	4.18381143
H	-0.43406095	-3.46720384	4.39517133
C	-1.44112830	-4.67061798	2.12121835
H	-0.97043529	-5.38905179	2.80648494
H	-2.23826730	-5.19430548	1.57980327
H	-0.69019002	-4.35558539	1.38792903
C	-3.03737353	-3.94704568	3.92038841
H	-3.87979127	-4.44706541	3.42560977
H	-2.58642577	-4.66565417	4.61678155
H	-3.44180867	-3.11254515	4.50623050
H	-3.67499253	-2.92285888	1.56583202
N	-0.62303694	1.56207582	3.92044617
C	0.58038514	2.27461397	4.41223184
C	0.35257282	3.55443464	5.22944234
H	-0.16991311	4.32583759	4.65406527
H	1.32263365	3.96720845	5.52848937
H	-0.21874323	3.36605115	6.14469418
H	1.19160154	2.50523777	3.53265570
H	1.15421709	1.55781338	5.01063781
C	-1.46643000	1.05968962	5.01354962
H	-1.94867444	1.86421204	5.59191627
H	-2.25509613	0.42471616	4.59728997
H	-0.86158806	0.45571955	5.69829382
C	-1.41740111	2.38018886	2.98731101
H	-1.89111629	3.24620359	3.47623159
H	-0.77874108	2.73367776	2.17265086
H	-2.20089462	1.75718470	2.54748137
N	0.98795038	-1.18386878	-1.61163248
C	0.90789196	-0.34554889	-2.82837310
C	1.43410169	-0.95519113	-4.13716774
H	2.49660771	-1.21615263	-4.07843646
H	1.31846502	-0.22576668	-4.94719888
H	0.88010233	-1.85514815	-4.42604855
H	1.45744694	0.57862656	-2.61217370
H	-0.14172356	-0.06068094	-2.94636821
C	0.17769717	-2.40250692	-1.71276089
H	0.56580966	-3.12321640	-2.45260422
H	0.15347543	-2.89975433	-0.73725950
H	-0.84642125	-2.13342811	-1.98514349
C	2.36797232	-1.50967389	-1.24068679
H	2.86400371	-2.18128910	-1.96228231
H	2.95275887	-0.58786050	-1.16524635
H	2.37541952	-1.98982091	-0.25958525

Table 19. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer unsymmetric with two DMEA isomer 1





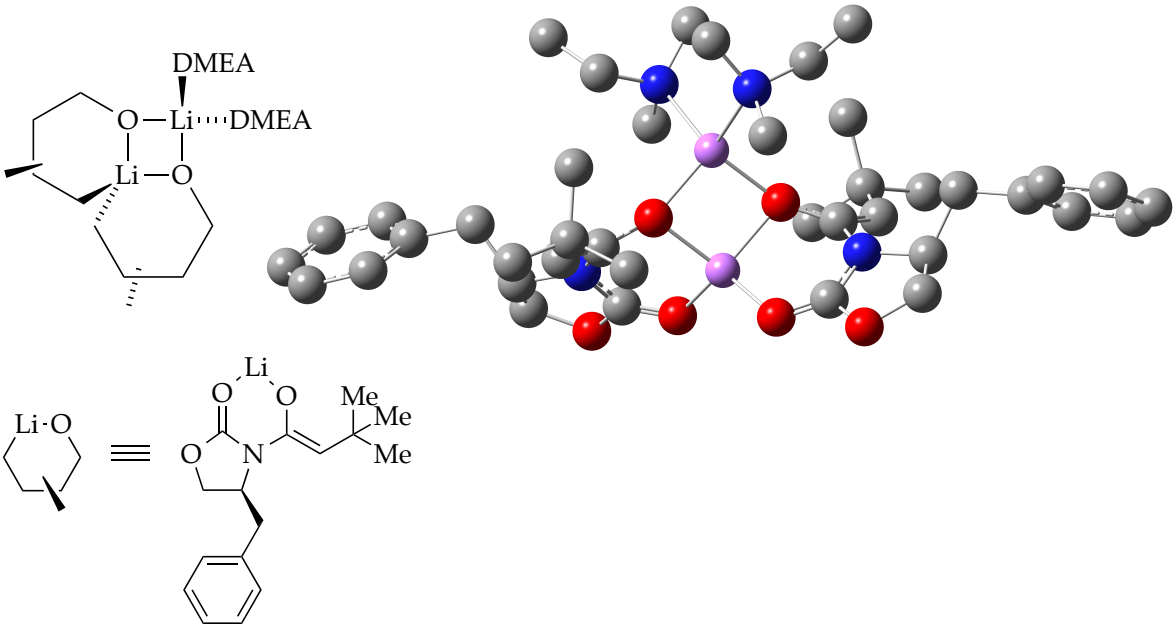


G = -2246.320131 Hartree
G_{MP2} = -1404965.182 kcal/mol
ΔG_{MP2} = 4.362089114 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.97572311	2.59171249	3.41590780
Li	0.00000000	0.00000000	2.46866470	H	8.16132947	3.01174811	4.47760867
O	1.20200552	0.00000000	1.10374828	H	8.62586329	2.12051009	6.73625691
C	2.32532366	0.37491804	1.48820188	H	6.90116268	0.80142448	7.92431806
N	2.64547604	-0.20719815	2.85722849	H	4.71074794	0.37920923	6.84971374
C	3.90227098	-0.02799573	3.50790365	C	3.18186192	1.14399555	0.76973316
C	3.97572274	-1.32166531	4.32000952	C	3.66866938	1.88127742	-0.49555210
H	4.15128744	-2.14654393	3.66592651	C	2.42838400	1.48297640	-1.31655144
H	4.75016286	-1.29415229	5.05807134	H	2.32985517	0.49940755	-0.91204186
O	2.65559257	-1.45661899	4.87503712	H	1.53755237	2.04305394	-1.11482185
C	1.85212937	-1.02274139	3.73319263	H	2.57758717	1.42164486	-2.37482727
O	0.57770834	-1.32525276	3.57960279	C	4.95697651	1.07817335	-0.78716574
H	4.73140173	0.07049382	2.83733573	H	5.10576840	1.00763025	-1.84125721
C	3.85007815	1.24165518	4.37069623	H	5.79646322	1.57110866	-0.33867089
H	3.65234050	2.08766539	3.74385448	H	4.86148636	0.09392884	-0.37058324
H	3.07455760	1.14390627	5.09760147	C	3.77724025	3.29640589	-1.08959006
C	5.20028226	1.46431584	5.06562320	H	4.60935645	3.80675040	-0.65217410
C	5.45869531	0.94953228	6.34097203	H	3.91705513	3.22729718	-2.14785904
C	6.69995522	1.18836010	6.94597416	H	2.87854557	3.83948896	-0.88359473
C	7.67833793	1.93697128	6.27480669	H	4.08759753	1.50057240	1.21289848
C	7.41778715	2.44315145	4.99409138	O	-1.21529023	0.51754939	0.98062745
C	6.17931232	2.20508529	4.39400163	C	-2.41342202	0.62416379	1.30206925

N	-2.54694166	1.30837981	2.65470186
C	-3.80366127	1.65199511	3.23574513
C	-3.40057718	2.88263054	4.04910512
H	-3.20124295	3.69853938	3.39059853
H	-4.15949689	3.17617091	4.74417618
O	-2.16539227	2.49359887	4.67519125
C	-1.54176434	1.75811165	3.57621156
O	-0.24565385	1.52910896	3.49308661
H	-4.56829703	1.87831233	2.52095096
C	-4.30296226	0.47999186	4.09379555
H	-4.42438121	-0.38563390	3.47434941
H	-3.59067009	0.27515346	4.86194928
C	-5.66480577	0.82140280	4.71377198
C	-5.76355856	1.41778783	5.97585926
C	-7.02729233	1.69973867	6.51184032
C	-8.18615810	1.38811632	5.78517617
C	-8.08176236	0.79869619	4.51788619
C	-6.82113770	0.51722947	3.98665927
H	-6.73720885	0.06521513	3.01906688
H	-8.96200757	0.56206332	3.95924032
H	-9.15130538	1.60221256	6.19393272
H	-7.10892778	2.15109951	7.47981059
H	-4.87819428	1.65413182	6.52702319
C	-3.31441920	-0.34537610	1.00285653
C	-3.98752100	-0.85106837	-0.29048155
C	-2.65041598	-0.98982968	-1.04140455
H	-2.19145685	-0.11884107	-0.62730098
H	-2.06583441	-1.85317460	-0.79469542
H	-2.70843350	-0.89227861	-2.10586921
C	-4.83566103	0.39117846	-0.64717857
H	-4.88987025	0.49709627	-1.70739891
H	-5.82359714	0.27820770	-0.24706369
H	-4.37984199	1.26419155	-0.22118197
C	-4.61680741	-2.11755249	-0.89651563
H	-5.60430873	-2.24961035	-0.50715136
H	-4.66313892	-2.01657295	-1.96043029
H	-4.01850758	-2.96832934	-0.64503751
H	-4.30882787	-0.30701421	1.39474987
H	-1.91679076	1.96062460	1.29304985
C	-1.89798928	2.04990876	0.29132357
N	-0.55671273	1.79166572	-0.22158612
C	-0.38655455	2.16354761	-1.59889026
H	-0.61395676	3.20106387	-1.72934297
H	0.62239855	1.97873750	-1.90548617
H	-1.05348528	1.57475822	-2.19422299
C	0.37607782	2.60238146	0.64639547
H	0.15004978	3.63987163	0.52413937
H	0.26091236	2.33337044	1.67736024
H	1.38370620	2.41799138	0.34064819
C	-2.24199647	3.54518035	0.04956110
H	-1.56518010	4.13470877	0.63362542
H	-3.24494520	3.74168403	0.35906169
H	-2.13021806	3.79577253	-0.98485064
H	-2.59497022	1.46138125	-0.33731527
N	0.97684147	-1.18090193	-0.95094106
C	2.34961951	-1.42708747	-0.49231247
C	2.66832607	-2.92694797	-0.65088178
H	1.97849937	-3.50138386	-0.06699974
H	3.66446350	-3.11896145	-0.31748658
H	2.57596846	-3.20058768	-1.68136250
H	2.44069235	-1.14887808	0.53807713
H	3.03500577	-0.85333980	-1.07771032
C	0.84949139	-1.57822312	-2.36603288
H	1.07628285	-2.61900263	-2.46857253
H	-0.15274198	-1.39782000	-2.69637838
H	1.52965030	-1.00475469	-2.96135482
C	0.36180556	-2.43487128	-0.40910515
H	0.60379957	-3.29763345	-0.47668192
H	0.29474181	-2.18469912	0.69096332
H	-0.77856799	-2.08807995	-0.63567948

Table 20. Geometric coordinates and thermally corrected MP2 energies for **7** spirocyclic dimer unsymmetric with two DMEA isomer 2

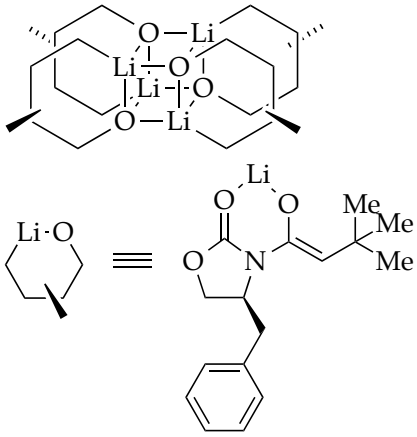


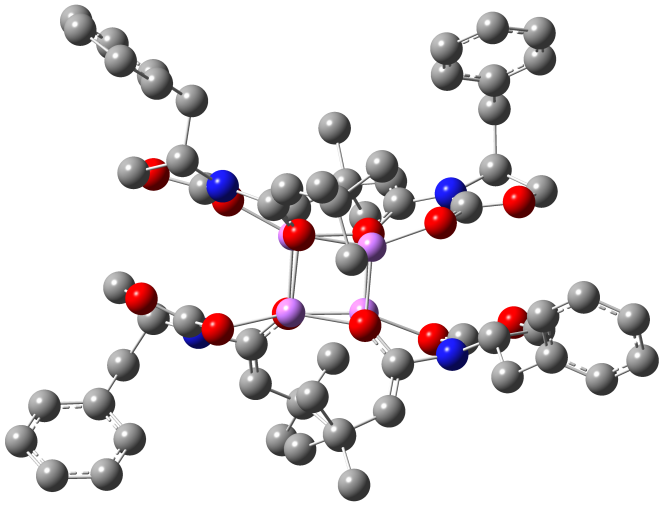
G = -2246.327343 Hartree
G_{MP2} = -1404970.275 kcal/mol
ΔG_{MP2} = 1.815589114 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.96647948	-2.04931723	0.40911467
Li	0.00000000	0.00000000	2.57969880	H	8.98193955	-3.42620388	0.01826326
O	1.44528174	0.00000000	1.29397709	H	8.95788397	-5.85727517	0.54895387
C	2.59287998	-0.33164444	0.77202927	H	6.89474809	-6.89245960	1.47769465
N	2.61747893	-1.68576768	0.18445682	H	4.87900181	-5.51258932	1.86403096
C	1.64894887	-2.09371471	-0.69328142	H	4.52759066	-2.02866746	-0.64866698
O	1.98875288	-3.28018035	-1.25993804	O	0.60285424	-1.53198786	-0.99001839
C	3.20582485	-3.75369367	-0.65758693	C	3.74228942	0.38594298	0.69237504
H	2.95220686	-4.53797203	0.06572678	C	3.96580431	1.79628161	1.22252022
H	3.83714873	-4.17696318	-1.43978157	C	3.73834003	1.85096940	2.74895109
C	3.81668470	-2.52041069	0.03080859	H	2.72971914	1.50680092	2.99323317
C	4.53041324	-2.84004093	1.35462804	H	3.86285200	2.87317480	3.13216489
H	3.82379707	-3.35508557	2.01666938	H	4.45312331	1.20409335	3.27247037
H	4.78727297	-1.88861463	1.83250128	C	5.42429759	2.20358736	0.93152718
C	5.77081573	-3.68480831	1.15026318	H	5.62940506	3.21720348	1.29736121
C	5.77411196	-5.05367717	1.44934882	H	5.63015254	2.18775789	-0.14596393
C	6.91268763	-5.83320784	1.23485581	H	6.13143144	1.52046583	1.41974326
C	8.07011752	-5.25311836	0.71506418	C	3.02217726	2.79946725	0.52005250
C	8.08247252	-3.88879987	0.41602899	H	3.21991994	2.82585982	-0.55766892
C	6.94371607	-3.11365130	0.63351397	H	3.16044645	3.81608103	0.91447042

H	1.97648208	2.50941122	0.65404414
H	4.57258338	-0.05314871	0.14741899
O	-1.44537925	0.00014505	1.29400472
C	-2.59281403	0.33175713	0.77168434
N	-2.61731797	1.68604092	0.18443960
C	-1.64882411	2.09395781	-0.69338285
O	-1.98864311	3.28044840	-1.26000055
C	-3.20540208	3.75413372	-0.65712794
H	-2.95131022	4.53785501	0.06663375
H	-3.83671211	4.17812397	-1.43893620
C	-3.81651689	2.52071538	0.03070792
C	-4.53059214	2.83997737	1.35439800
H	-4.78790001	1.88844713	1.83182390
H	-3.82404594	3.35453579	2.01689362
C	-5.77067427	3.68521417	1.14999719
C	-6.94366744	3.11460133	0.63284657
C	-8.08212687	3.89019370	0.41541087
C	-8.06938134	5.25441519	0.71490500
C	-6.91185846	5.83395710	1.23508623
C	-5.77357307	5.05397973	1.44952376
H	-4.87838075	5.51246857	1.86450558
H	-6.89361233	6.89312018	1.47828653
H	-8.95692810	5.85890690	0.54884365
H	-8.98167841	3.42803254	0.01733472
H	-6.96673135	2.05034807	0.40810075
H	-4.52720507	2.02918415	-0.64915765
O	-0.60274887	1.53221283	-0.99012890
C	-3.74209683	-0.38594842	0.69138053
C	-3.96570751	-1.79636759	1.22126555
C	-3.02168227	-2.79940295	0.51912185
H	-1.97607283	-2.50925333	0.65360926
H	-3.21893947	-2.82573165	-0.55869213
H	-3.16002354	-3.81606790	0.91338703
C	-3.73890152	-1.85119592	2.74778822
H	-3.86363140	-2.87342318	3.13086448
H	-4.45387421	-1.20431590	3.27104241
H	-2.73036625	-1.50709611	2.99253620
C	-5.42404695	-2.20374752	0.92958973
H	-6.13143810	-1.52074567	1.41760003
H	-5.62923827	-3.21743082	1.29518782
H	-5.62943841	-2.18777477	-0.14798751
H	-4.57218609	0.05314393	0.14610950
H	-2.42453728	1.31525938	3.46635404
C	-1.85690065	1.54688012	4.37253612
N	-0.45482651	1.77785410	3.95163354
C	0.43847689	1.97828783	5.09865303
H	0.23980755	2.91667379	5.64247649
H	1.47509096	2.00616131	4.75185785
H	0.32855239	1.14745215	5.80302645
C	-0.33718405	2.90637289	3.01622345
H	-0.57731380	3.87684162	3.48215752
H	-1.00771171	2.74071581	2.16950232
H	0.68713689	2.95686272	2.63779759
C	-2.55676163	2.67262940	5.15011158
H	-2.63052306	3.59766406	4.56815132
H	-3.57730069	2.35853327	5.39645140
H	-2.04853251	2.90621062	6.09172789
H	-1.86012794	0.63805138	4.98590289
N	0.45474454	-1.77696981	3.95151569
C	1.85677738	-1.54572940	4.37242749
C	2.55649385	-2.67091780	5.15091779
H	2.63049186	-3.59634542	4.56961043
H	3.57694957	-2.35659536	5.39732135
H	2.04803939	-2.90390887	6.09256238
H	2.42451647	-1.31473980	3.46614451
H	1.85991194	-0.63644298	4.98512338
C	-0.43876911	-1.97640348	5.09855058
H	-0.24041767	-2.91444804	5.64308045
H	-1.47533470	-2.00426056	4.75160761
H	-0.32873695	-1.14508451	5.80233502
C	0.33718904	-2.90624430	3.01699673
H	0.57760491	-3.87627772	3.48367541
H	1.00756208	-2.74113479	2.17003694
H	-0.68718170	-2.95722949	2.63876089

Table 21. Geometric coordinates and thermally corrected MP2 energies for **7** D_{2d} tetramer





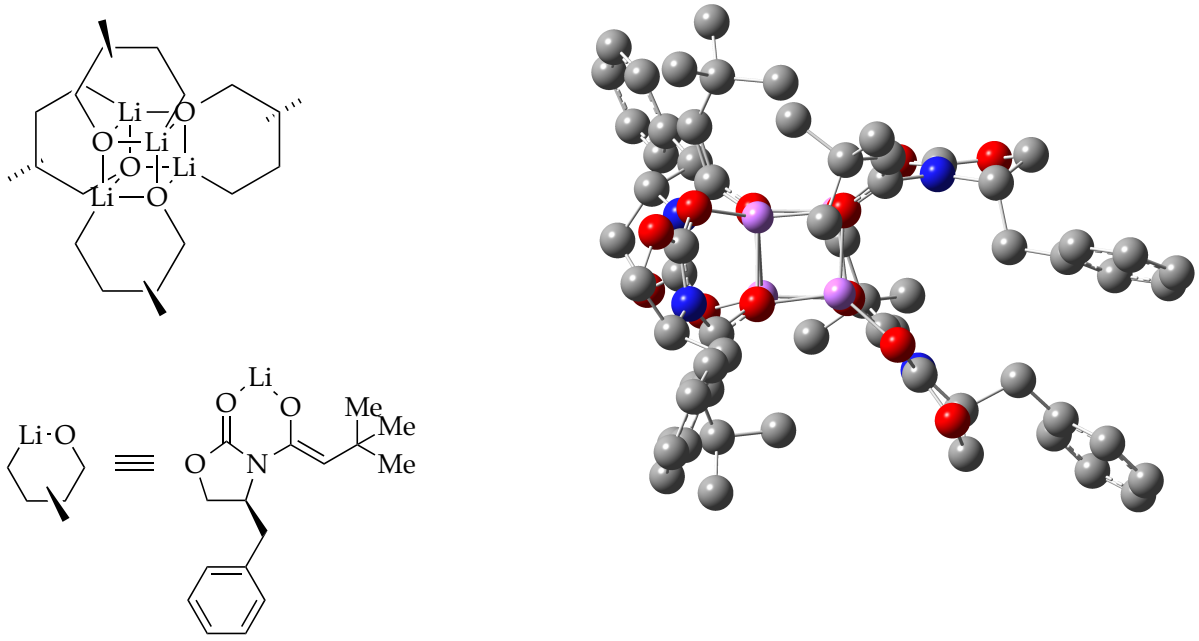
G = -3638.055774 Hartree
G_{MP2} = -2275655.235 kcal/mol
ΔG_{MP2} = -0.291028601 kcal/mol Li vs. **7** dimer with two THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.30166648	3.61231414	-3.84439176
O	0.00000000	0.00000000	1.86336620	N	-0.52030903	2.83830694	-3.02395097
C	1.02009406	0.00000000	2.55043898	C	-1.05568420	2.03403244	-1.92229953
O	0.92543730	-0.30211550	3.86973481	C	-2.22495143	2.46690030	-1.38359735
C	2.25293991	-0.44110657	4.40657425	H	-2.61551485	3.39762875	-1.77314759
H	2.50250927	-1.50643231	4.42894745	C	-3.08214376	1.89521396	-0.25912448
H	2.24992287	-0.03035533	5.41718311	C	-4.47309076	2.56349979	-0.36123268
C	3.13892810	0.33850358	3.42654576	H	-4.39694423	3.65446066	-0.26474142
H	4.07521931	-0.19606696	3.24865730	H	-4.94770169	2.34079201	-1.32468112
N	2.31068419	0.27029547	2.20769910	H	-5.13735938	2.20555907	0.43456820
C	2.83919051	0.38928241	0.84006264	O	-0.33669325	0.97315460	-1.62181582
C	4.12746642	0.80733980	0.74168030	Li	-0.35817973	-0.84297845	-2.50081366
H	4.63047829	1.02561695	1.67462511	O	-0.64366406	-0.58070642	-4.37919917
C	5.09020535	0.96315770	-0.42640312	C	0.33293512	-0.29110568	-5.06891853
C	6.15374457	-0.15886296	-0.32885753	O	0.25980734	0.67741543	-6.01232335
H	6.66469373	-0.13140350	0.64166782	C	1.58260762	0.93286120	-6.53786444
H	5.69290612	-1.14589804	-0.43508662	H	1.91517982	1.89579509	-6.14659119
H	6.91650179	-0.04817421	-1.11151538	H	1.49800531	0.97314128	-7.62520974
O	1.98994545	0.04801005	-0.10714520	C	2.45512124	-0.24523670	-6.04810167
Li	1.66370817	0.69859089	-1.92114367	H	3.36287410	0.11876036	-5.55629874
O	1.71053508	2.11233123	-3.17348716	N	1.57660768	-0.83449543	-5.02476670
C	0.72746097	2.74340151	-3.55662040	C	2.02703343	-1.63889663	-3.88598198
O	0.82270229	3.51099207	-4.67802997	C	2.75324013	-2.74429744	-4.18080714
C	-0.51131616	3.92414005	-5.04967162	H	2.81869962	-2.98908397	-5.23326634
H	-0.91017731	3.19317978	-5.75944674	C	3.46381484	-3.73477584	-3.26442099
H	-0.44908097	4.91036415	-5.51045972	C	4.40144931	-4.59057702	-4.14609397
C	-1.25972710	3.91126081	-3.71646074	H	3.83630008	-5.12732173	-4.91828813

H	5.15105020	-3.96714605	-4.64931635	C	-1.99661115	6.35225470	-3.62649080
H	4.93313762	-5.33547217	-3.54191079	C	-3.39535272	6.33631494	-3.51348861
O	1.66602634	-1.15397823	-2.71271624	C	-4.17523927	7.31332845	-4.13128351
Li	1.64679077	-1.77900884	-0.87721112	C	-3.56877549	8.32886790	-4.87441878
O	1.88456835	-3.06098527	0.56123436	C	-2.17912687	8.36044644	-4.99110408
C	0.93305411	-3.16828188	1.33432382	C	-1.40189536	7.37914193	-4.37189610
O	1.11801112	-3.21797320	2.67807267	H	-0.31796814	7.41694143	-4.45845536
C	-0.16500682	-3.41270132	3.31576311	H	-1.69694472	9.15050042	-5.56082902
H	-0.21206787	-2.76183368	4.18771143	H	-4.17560310	9.09188055	-5.35432384
H	-0.23320305	-4.46168914	3.62598324	H	-5.25683284	7.28458628	-4.02878455
C	-1.20760629	-3.06367000	2.23824685	H	-3.87792211	5.55554783	-2.92895079
H	-1.49201785	-2.00780101	2.31931051	C	3.46918455	1.77900159	3.90893062
N	-0.38474877	-3.23831304	1.02334677	H	4.09831941	1.66760557	4.80193101
C	-0.83815912	-2.94006802	-0.33792647	H	4.08763569	2.26676630	3.15045508
C	-1.62357562	-3.88785925	-0.90135890	C	2.27857037	2.65707063	4.22820078
C	-2.31678111	-3.91436679	-2.25918530	C	1.85425074	2.84782732	5.55031793
C	-3.27370427	-5.12709531	-2.27280816	C	0.75192940	3.65266317	5.84207255
H	-2.72671623	-6.06351858	-2.10681998	C	0.05672370	4.28536866	4.81114907
H	-4.03618828	-5.03901014	-1.48889519	C	0.47603475	4.11450464	3.49013555
H	-3.78934108	-5.20524435	-3.23736370	C	1.57925909	3.31057471	3.20188688
H	-1.74776951	-4.78474580	-0.30230977	H	1.90940602	3.19466992	2.17254154
O	-0.40019369	-1.78874611	-0.81910693	H	-0.05256767	4.61174708	2.68141504
C	-2.46696079	-3.94009622	2.30270660	H	-0.80103008	4.91370908	5.03526724
H	-3.09269982	-3.70288203	1.43595084	H	0.44104259	3.78888214	6.87461248
H	-2.17567302	-4.99339866	2.20855838	H	2.40073921	2.37220925	6.36259073
C	-3.23966546	-3.72240512	3.58870401	C	-2.48139434	2.25526475	1.12034812
C	-3.23709281	-4.68560322	4.60610905	H	-3.13033157	1.90360131	1.93427431
C	-3.93373845	-4.47363347	5.79782615	H	-1.49643884	1.80551461	1.26889260
C	-4.64532956	-3.28949819	5.99068744	H	-2.37469111	3.34226742	1.22133982
C	-4.65903875	-2.32190990	4.98327037	C	-3.29447616	0.37338010	-0.36590815
C	-3.96412148	-2.53833097	3.79388160	H	-3.77745266	0.11873345	-1.31555340
H	-3.98870128	-1.78294244	3.01130470	H	-2.36314267	-0.19445018	-0.31308178
H	-5.21546857	-1.39867406	5.12192074	H	-3.94530413	0.02392269	0.44702613
H	-5.18959269	-3.12262246	6.91635699	C	-3.15809273	-2.64727526	-2.51513098
H	-3.92254165	-5.23632913	6.57219244	H	-3.91590800	-2.51903955	-1.73390458
H	-2.69271085	-5.61616015	4.45948279	H	-2.55056970	-1.73960179	-2.53453641
C	2.88405850	-1.18116598	-7.20736148	H	-3.67090565	-2.71680602	-3.48282815
H	3.54972264	-0.58337128	-7.84430756	C	-1.28838702	-4.09937154	-3.39795940
H	3.50526419	-1.98164313	-6.79483269	H	-1.79308503	-4.13978740	-4.37251042
C	1.76217818	-1.74679681	-8.05471788	H	-0.56396377	-3.28102394	-3.43246508
C	1.57312400	-1.29524514	-9.36885040	H	-0.72736773	-5.03112159	-3.26466874
C	0.54370307	-1.79940820	-10.16574689	C	2.45270265	-4.68396443	-2.58092792
C	-0.31921654	-2.77035716	-9.65801003	H	2.97227516	-5.41105329	-1.94295891
C	-0.14040804	-3.23430076	-8.35322250	H	1.74017834	-4.14313524	-1.95243143
C	0.89047663	-2.73040630	-7.55950983	H	1.87741403	-5.23789124	-3.33142942
H	1.01734941	-3.10714930	-6.54899346	C	4.33545820	-3.03770588	-2.20101313
H	-0.80405282	-3.99427769	-7.94940707	H	5.08194552	-2.39057756	-2.67476709
H	-1.12205477	-3.16601022	-10.27432590	H	3.75150435	-2.41704012	-1.51736903
H	0.42021793	-1.43514574	-11.18238416	H	4.86331454	-3.78087508	-1.59025386
H	2.24894164	-0.54654903	-9.77799816	C	4.44742224	0.93305356	-1.81984741
C	-1.15968616	5.27117410	-2.97605583	H	3.93462949	-0.01075729	-2.02211598
H	-1.46383386	5.12540337	-1.93538848	H	3.74390036	1.76127881	-1.94886390
H	-0.10466862	5.57080397	-2.95754897	H	5.22241839	1.05433667	-2.58792758

C	5.80805714	2.32550808	-0.26475788
H	6.57037521	2.45994461	-1.04283859
H	5.09551756	3.15542127	-0.33856192
H	6.30997808	2.39887826	0.70847080

Table 22. Geometric coordinates and thermally corrected MP2 energies for **7** S_4 tetramer



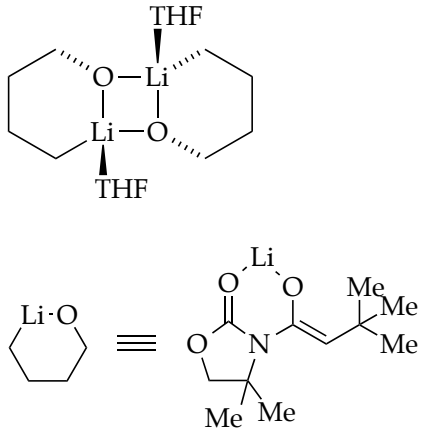
G = -3638.063057 Hartree
G_{MP2} = -2275651.674 kcal/mol
ΔG_{MP2} = 0.599221399 kcal/mol Li vs. **7** dimer with two THF

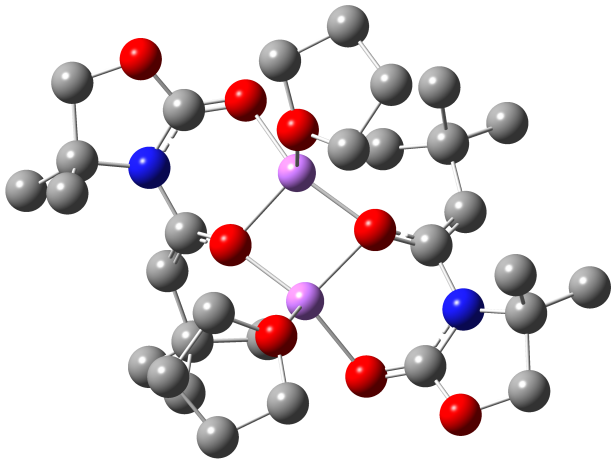
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-1.81186936	-3.49391964	-0.75020971
O	0.00000000	0.00000000	1.87142950	C	-1.96086094	-2.03557271	-0.61761867
C	1.05961540	0.00000000	2.49497578	O	-0.94893622	-1.32772773	-1.08511021
O	1.13549623	0.60388581	3.70668323	Li	-0.54039896	-0.14252202	-2.57461249
C	2.41215309	0.30764109	4.30272648	O	-1.45555498	0.96581420	-3.79584722
H	2.26158478	-0.45953830	5.06942823	C	-0.90461355	2.03398499	-4.05379660
H	2.79222482	1.21604887	4.77284953	O	-0.96998877	2.55768648	-5.30538955
C	3.29095007	-0.19294286	3.14111253	C	-0.43047783	3.89443002	-5.27040700
H	3.83199805	-1.08877814	3.45191951	H	-1.26477534	4.60057199	-5.19404532
N	2.26051768	-0.53271896	2.14514905	H	0.11269034	4.07127669	-6.19952407
C	2.54925687	-1.22444835	0.88167079	C	0.46130506	3.91185787	-4.02021802
O	1.85248896	-0.79473546	-0.15264382	H	0.37635606	4.86803529	-3.50203313
Li	0.91765903	-1.98151615	-1.39717779	N	-0.17202733	2.83687646	-3.23750025
O	0.50147966	-3.75419226	-1.07027294	C	0.07474813	2.60734760	-1.80703802
C	-0.64826299	-4.17316242	-0.95521753	O	0.28030163	1.35014752	-1.46444632
O	-0.88017132	-5.50647444	-1.05257912	Li	1.94379512	0.37586633	-1.69753904
C	-2.24362903	-5.77071012	-0.68137654	O	3.40875714	0.93333521	-2.66189854
H	-2.25674072	-6.12166903	0.35640075	C	3.77550758	0.33968592	-3.67260340
H	-2.63511199	-6.55312939	-1.33298819	O	5.01593497	0.59257833	-4.16787160
C	-2.95655674	-4.42129492	-0.84805289	C	5.29569340	-0.35763355	-5.21105076
H	-3.64668693	-4.26939557	-0.01700266	H	5.86189747	-1.19107479	-4.78051563

H	5.89357493	0.13545412	-5.97841754
C	3.90773088	-0.78393132	-5.69114052
H	3.90430750	-1.84143100	-5.95945755
N	3.12346858	-0.57013821	-4.45809830
C	1.81854191	-1.20757167	-4.20018333
O	1.27355160	-0.91174661	-3.03991775
C	1.35442214	-2.02926244	-5.17701856
H	1.98531071	-2.15946715	-6.04634601
C	0.10821599	-2.90277629	-5.25120596
C	0.43451806	-4.31698775	-4.71109461
H	0.70872865	-4.28179341	-3.65205652
H	-0.42956902	-4.98789547	-4.81971512
H	1.27252721	-4.76299411	-5.26069643
C	3.38224747	0.07809992	-6.86735184
H	2.30891760	-0.10943907	-6.97071342
H	3.50140527	1.13369737	-6.59231893
C	4.09982930	-0.20321262	-8.16961738
C	3.81815854	-1.36704453	-8.90123654
H	3.05260344	-2.05287176	-8.54401562
C	4.49451694	-1.64832688	-10.08779553
H	4.25841842	-2.55307846	-10.64176401
C	5.46638503	-0.76706010	-10.56756522
C	5.75275613	0.39683517	-9.85392969
C	5.07399086	0.67417460	-8.66525589
H	5.29449722	1.59018810	-8.12079567
H	6.50163687	1.09297646	-10.22243656
H	5.99165279	-0.98436155	-11.49361768
C	0.08487682	3.72896949	-1.04829713
H	-0.22135540	4.64122264	-1.55195899
C	0.43630428	3.91053346	0.42153816
C	-0.71498240	3.42965958	1.33427784
H	-0.88728406	2.35571477	1.23310322
H	-0.48582176	3.62812919	2.38987229
H	-1.64817275	3.94822597	1.08567486
C	1.95018044	3.60749753	-4.30082512
H	2.43616556	3.40060098	-3.34168299
H	2.00684078	2.68399230	-4.88982000
C	2.65347677	4.73774386	-5.01986530
C	2.92003732	4.67212493	-6.39431953
H	2.64215832	3.77922286	-6.95101979
C	3.54722657	5.72995731	-7.05642179
H	3.74807667	5.65645826	-8.12213100
C	3.91786760	6.87491566	-6.35096082
C	3.66093408	6.95314094	-4.98003472
C	3.03539954	5.89411504	-4.32298553
H	2.84978265	5.95737234	-3.25263699
H	3.95373458	7.83782643	-4.42067144
H	4.40784741	7.69852905	-6.86317733
C	-3.12317134	-1.61901535	-0.05804058
H	-3.75678189	-2.39997632	0.34806254
C	-3.72882592	-0.23906938	0.15642941
C	-5.24805672	-0.36353442	-0.11849759
H	-5.43953688	-0.63830632	-1.16294210
H	-5.70720187	-1.12681004	0.52356994
H	-5.75834438	0.58710241	0.08071051
C	-3.71744062	-4.26405059	-2.18445213
H	-3.97475612	-3.20480820	-2.28908932
H	-3.03650504	-4.51588137	-3.00576937
C	-4.96251658	-5.12139427	-2.24736915
C	-6.11378232	-4.75671870	-1.53254007
H	-6.11683635	-3.83097878	-0.96069229
C	-7.25633609	-5.55571267	-1.55958970
H	-8.13964328	-5.25299943	-1.00329595
C	-7.26931661	-6.73686363	-2.30549787
C	-6.13406314	-7.10865271	-3.02585532
C	-4.99150213	-6.30610200	-2.99542757
H	-4.11489516	-6.59583834	-3.57122426
H	-6.13684505	-8.02098469	-3.61659096
H	-8.16031964	-7.35843977	-2.32933077
C	3.50823843	-2.17891026	0.96511645
H	3.83467111	-2.41433908	1.97429847
C	4.24817394	-3.00868846	-0.07353987
C	5.74629819	-2.99603522	0.32201281
H	6.15983619	-1.98120270	0.27317859
H	5.88998993	-3.37183591	1.34319260
H	6.33245472	-3.63461950	-0.35094264
C	4.30447007	0.84184003	2.60277747
H	4.69794987	0.44842541	1.65877671
H	3.77236430	1.77071878	2.37030105
C	5.43372814	1.10531487	3.57491729
C	6.45255769	0.15710506	3.75502892
H	6.44360808	-0.75597800	3.16305465
C	7.48250314	0.37731860	4.66886643
H	8.26511340	-0.36719754	4.78971767
C	7.51369824	1.55434036	5.42073987
C	6.51058367	2.50822549	5.24805319
C	5.48017569	2.28330503	4.33248836
H	4.70952269	3.03866611	4.19343633
H	6.53037474	3.43117893	5.82172735
H	8.31759619	1.72818211	6.13091779
C	-3.17784842	0.85339234	-0.77397838
H	-2.12875826	1.08585576	-0.58183062
H	-3.26680165	0.56809276	-1.82748320
H	-3.74409283	1.78211378	-0.62837987
C	-3.53840786	0.18487314	1.63351896
H	-2.47867473	0.27665245	1.88802546
H	-4.02791126	1.14912134	1.82660253
H	-3.98043157	-0.55647688	2.31114032
C	1.74279675	3.17984881	0.79313600
H	1.67267085	2.10484952	0.61092852
H	2.58488597	3.56343864	0.20442116
H	1.97184576	3.33233358	1.85619566
C	0.64939491	5.42056576	0.66883388
H	1.46212051	5.81383053	0.04515211
H	-0.25895697	5.99104634	0.43756960
H	0.90579929	5.61174341	1.71790016

C	-1.11281197	-2.33755801	-4.50493041
H	-0.97329782	-2.35484428	-3.42119468
H	-1.32912686	-1.30962562	-4.81303995
H	-1.99940493	-2.94533556	-4.72817466
C	-0.27453116	-3.02747506	-6.74495290
H	-0.53946707	-2.05057851	-7.16657966
H	0.55469598	-3.43874250	-7.33582899
H	-1.13448855	-3.69646858	-6.87179827
C	4.14242552	-2.47316767	-1.51030921
H	3.13241441	-2.55901020	-1.91658119
H	4.44316697	-1.42164125	-1.56155194
H	4.80324292	-3.05246417	-2.16817593
C	3.74508056	-4.47158112	-0.02934411
H	2.69417634	-4.53320371	-0.32510699
H	4.33445915	-5.10458470	-0.70703559
H	3.84017899	-4.88724660	0.98164402

Table 23. Geometric coordinates and thermally corrected MP2 energies for **18** dimer with two THF



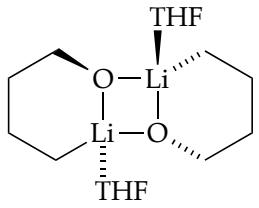


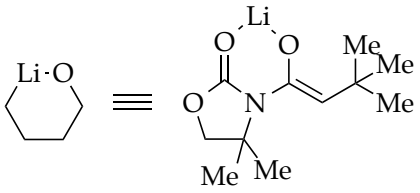
G = -1900.356246 Hartree
G_{MP2} = -1188641.471 kcal/mol
ΔG_{MP2} = 1.153086457 kcal/mol Li vs. 18-Li dimer trans with two THF

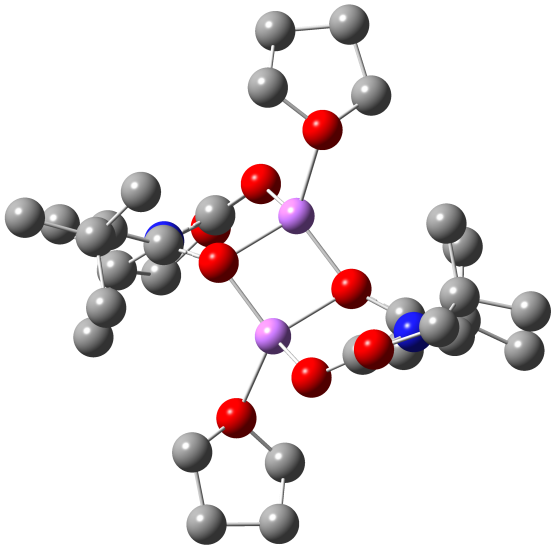
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.69588031	-1.65977763	-5.86991360
O	0.00000000	0.00000000	1.95994010	H	-2.16374140	-2.59482828	-6.19953774
C	1.13192501	0.00000000	2.44079758	H	-1.63919412	-0.96496088	-6.71093966
N	2.19061060	-0.77487976	2.10163807	C	-2.41175525	-1.06860882	-4.63410723
C	3.43361360	-0.25062428	2.72793098	N	-1.56377810	-1.66799866	-3.56930236
C	2.79643034	0.56433655	3.87641068	C	-1.71625417	-1.39340117	-2.12348323
H	2.72927239	-0.02253361	4.79995778	C	-2.80465930	-1.95843024	-1.54419069
H	3.31448903	1.50439393	4.07942744	C	-3.27934885	-1.81607666	-0.10379532
O	1.46217834	0.87002950	3.43608724	C	-2.31074096	-2.52818328	0.86898495
C	4.18948124	0.65062360	1.73657005	H	-1.30545865	-2.10155549	0.82617710
H	5.09171268	1.06281432	2.20376825	H	-2.66420615	-2.44516292	1.90564940
H	4.49139333	0.07367009	0.85720927	H	-2.23215282	-3.59271164	0.61939530
H	3.55956075	1.48219588	1.40284625	C	-3.43511672	-0.33284723	0.29970122
C	4.35593392	-1.33996946	3.27849208	H	-4.18336243	0.16102631	-0.33319185
H	3.81498877	-2.01074574	3.95341213	H	-3.76050721	-0.24532044	1.34439894
H	4.78032156	-1.93565680	2.46717874	H	-2.49546936	0.21553661	0.19375177
H	5.17886292	-0.87666295	3.83625931	C	-4.66307453	-2.49017918	0.01282838
C	2.15392330	-1.58749237	0.86577211	H	-5.39386172	-2.01458735	-0.65378767
O	1.71024891	-0.95035176	-0.18456591	H	-4.60664222	-3.55278437	-0.25453342
Li	1.08138965	-1.14977045	-1.97225976	H	-5.04712960	-2.42224907	1.03803870
O	0.65993630	-2.34870740	-3.46432792	H	-3.37961375	-2.63367124	-2.16871521
C	-0.35610424	-2.01908503	-4.07382737	O	-0.78155709	-0.63376880	-1.61820198
O	-0.35696259	-1.95218007	-5.43476173	C	-2.31134759	0.46587187	-4.59328425

H	-2.91211249	0.91119482	-5.39513676
H	-2.68361712	0.84273385	-3.63584386
H	-1.27343826	0.79485062	-4.71245051
C	-3.87409736	-1.51540411	-4.58519644
H	-3.95273134	-2.60706695	-4.57231774
H	-4.37006909	-1.12330378	-3.69443880
H	-4.40223456	-1.14018053	-5.47021027
O	2.27646772	0.14027913	-3.02019889
C	2.81468574	-0.09304498	-4.33140283
C	4.30601165	-0.35661744	-4.09174958
C	4.62600294	0.49689680	-2.83477561
C	3.23880926	0.95671294	-2.32932642
H	3.05510863	2.01184179	-2.57930017
H	3.07051360	0.79886711	-1.26419268
H	5.26124674	1.35625583	-3.07171618
H	5.14588875	-0.09951785	-2.07972329
H	4.91805678	-0.08617155	-4.95768212
H	4.46582708	-1.41890407	-3.88449412
H	2.26819154	-0.93099386	-4.76355037
H	2.66166813	0.80498331	-4.95027630
C	2.59549773	-2.86234158	1.00446704
H	2.82124613	-3.18039063	2.01661159
C	2.74688554	-3.92427464	-0.07706658
C	3.60308929	-3.41519001	-1.25807740
H	4.61465304	-3.16010600	-0.91747735
H	3.68897935	-4.18391540	-2.03693358
H	3.17049956	-2.52132374	-1.71497499
C	1.36429088	-4.38970336	-0.59030026
H	0.79808781	-3.56738653	-1.03487309
H	1.47206906	-5.17152564	-1.35426570
H	0.76796822	-4.79787690	0.23400929
C	3.46595296	-5.14074483	0.54410471
H	4.46062167	-4.86577678	0.91778803
H	2.89237687	-5.54913795	1.38554685
H	3.59252769	-5.94099950	-0.19531330
O	-0.02729306	2.03182316	-0.24836017
C	-0.50209103	2.60289994	-1.48059370
C	-1.76530084	3.41535872	-1.11261478
C	-1.70696241	3.52371031	0.43520185
C	-0.30769347	2.99808033	0.77687268
H	-0.23574558	2.48569630	1.73596073
H	0.44363053	3.80202107	0.73144863
H	-2.46570328	2.88218339	0.89313632
H	-1.86505899	4.54424405	0.79727511
H	-2.67548254	2.90123353	-1.43407751
H	-1.75329479	4.39803733	-1.59466259
H	0.28108445	3.25356593	-1.89628731
H	-0.68241243	1.76902617	-2.15874284

Table 24. Geometric coordinates and thermally corrected MP2 energies for **18** dimer trans with two THF







G = -1900.363388 Hartree
G_{MP2} = -1188643.777 kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. 18-Li dimer trans with two THF

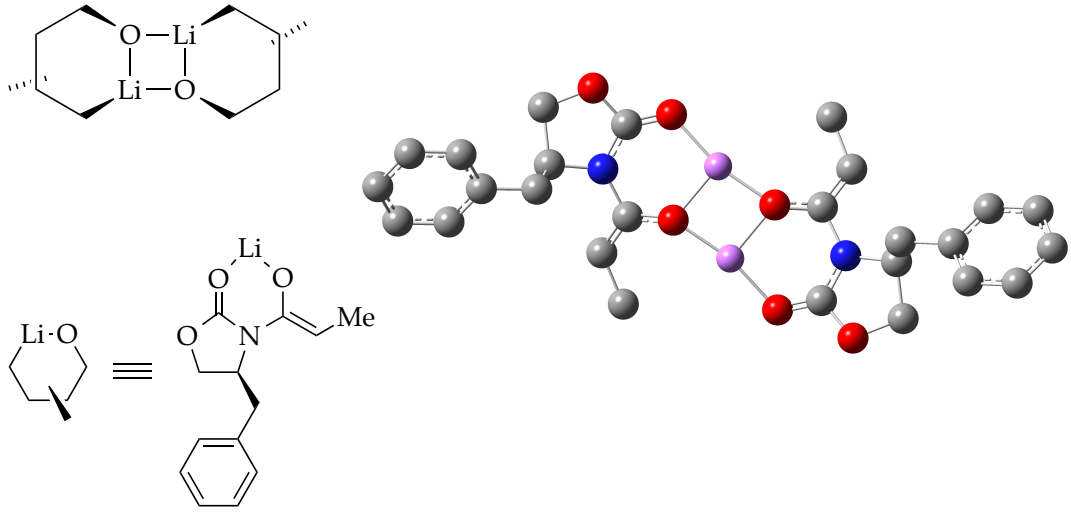
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.34235453	-0.92202317	-3.79550398
O	0.00000000	0.00000000	1.88548830	H	-4.64548477	-2.21618408	-2.61844424
C	0.84877770	0.00000000	2.87446071	H	-5.85970008	-0.94727391	-2.86964671
N	1.64306499	-1.23695890	2.97597335	C	-1.88723680	-2.57788055	-2.19713438
C	3.11947066	-1.36248601	3.10853301	C	-1.27252165	-3.95527353	-1.97026611
C	3.29092324	-2.78524037	2.52606047	C	0.25009777	-3.86435290	-1.72426518
H	3.52163666	-2.76114194	1.45438242	H	0.75978089	-3.44001596	-2.59806340
H	4.04384718	-3.37828455	3.04941653	H	0.46059829	-3.22993527	-0.85886074
O	2.01511270	-3.42591744	2.69977751	H	0.67624673	-4.85903782	-1.53634519
C	1.06762201	-2.45414175	2.80071546	C	-1.51961191	-4.81072607	-3.22925973
O	-0.12865726	-2.73183954	2.74265517	H	-1.09544185	-5.81535267	-3.11093901
Li	-1.24916095	-1.46735698	1.71853486	H	-2.59320830	-4.92058946	-3.42906718
O	-1.27979578	-1.45607352	-0.16536285	H	-1.05970736	-4.35249707	-4.11399558
C	-1.88392361	-1.54629572	-1.31652437	C	-1.93302692	-4.65485791	-0.75982053
N	-2.66295158	-0.35071685	-1.70249855	H	-3.01277477	-4.76796285	-0.91737976
C	-4.15048767	-0.30080682	-1.71577933	H	-1.50611462	-5.65460506	-0.60318803
C	-4.33717937	1.20599155	-2.00846845	H	-1.77713256	-4.07391135	0.15398791
H	-4.46014120	1.39824565	-3.08099440	H	-2.38419522	-2.41373060	-3.14745669
H	-5.17106527	1.65154875	-1.46145248	O	-2.92992609	-1.65782462	2.79650534
O	-3.12283297	1.83855710	-1.57182279	C	-3.50076379	-2.99083136	2.79325887
C	-2.15603011	0.88943616	-1.47241254	C	-3.91581641	-3.27918211	4.23904324
O	-0.99520474	1.19813793	-1.20958222	C	-2.91195436	-2.43287809	5.03694989
C	-4.70838867	-0.69272097	-0.33815974	C	-2.78363664	-1.18849852	4.16090959
H	-5.80290441	-0.62507863	-0.33565013	H	-1.81700573	-0.68701163	4.24219587
H	-4.42549568	-1.72224917	-0.10011830	H	-3.58027837	-0.46112556	4.36679414
H	-4.31413536	-0.04290692	0.44940579	H	-1.94672084	-2.94624081	5.10008303
C	-4.78312406	-1.15120769	-2.81978943	H	-3.25120311	-2.19847344	6.05066241

H	-3.86864243	-4.34610893	4.47638650
H	-4.94039056	-2.93420283	4.42347888
H	-4.33771105	-3.00388611	2.08844844
H	-2.73304140	-3.69239229	2.44775990
C	3.56859311	-1.33693068	4.58121329
H	4.63947957	-1.56405340	4.64771529
H	3.40562806	-0.35610794	5.03357103
H	3.02171652	-2.08427794	5.16638719
C	3.86829858	-0.31992985	2.27662807
H	3.52266584	-0.33581112	1.23799337
H	3.70583723	0.68293417	2.67992592
H	4.94408034	-0.53157560	2.29628734
C	1.07775116	0.98064024	3.78252086
H	1.76181495	0.76552067	4.59568620
C	0.45073013	2.37167260	3.76984099
C	0.77711907	3.11658744	2.45530100
H	1.86171292	3.21951153	2.32542636
H	0.37686258	2.57442312	1.59385147
H	0.33991217	4.12426622	2.45648036
C	1.03457975	3.17595030	4.94883316
H	0.61135046	4.18732245	4.98250081
H	0.81581414	2.68731372	5.90681154
H	2.12462611	3.27024099	4.86177281
C	-1.08463227	2.29782332	3.93154504
H	-1.35241667	1.83001587	4.88703528
H	-1.53050468	3.30160594	3.91129840
H	-1.52514194	1.70793466	3.12270864
O	1.81342185	0.21692120	-0.87830021
C	2.25595091	1.59925882	-0.92990658
C	2.92549204	1.77236160	-2.29458836
C	2.13787674	0.77946132	-3.16322541
C	1.91555255	-0.38207351	-2.19504671
H	2.76451668	-1.07864687	-2.19382042
H	0.99856379	-0.94480020	-2.38591523
H	2.67210781	0.47315233	-4.06783476
H	1.17576825	1.21299711	-3.45668840
H	3.98338147	1.48663876	-2.24708684
H	2.86739149	2.80355221	-2.65545910
H	1.37770987	2.24588682	-0.82882421
H	2.92499791	1.77087022	-0.08228179

Part 6: 5 Ground State Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 25. Geometric coordinates and thermally corrected MP2 energies for **5** dimer with no THF

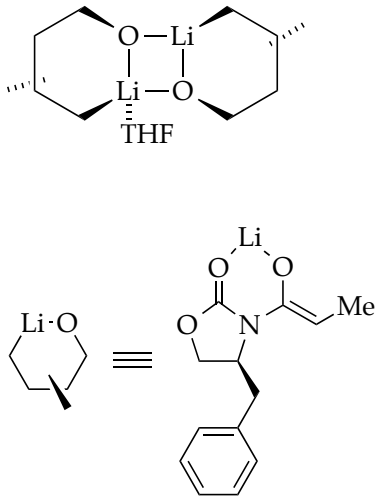


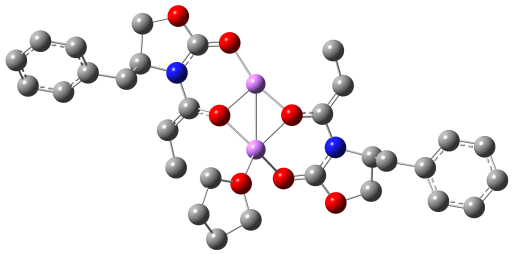
G = -1583.317665 Hartree
G_{MP2} = -990442.4092 kcal/mol
ΔG_{MP2} = 11.86946681 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	-3.35681888	-1.08332939	-1.21379716
H	0.00000000	0.00000000	1.09526210	C	-3.61177195	-2.32077403	-0.72862192
H	1.02899631	0.00000000	-0.36225780	H	-2.95504671	-2.75082201	0.01983975
C	-0.85702190	-1.13646353	-0.58266107	C	-4.82282491	-3.10940012	-1.14523176
H	-0.99038974	-1.92721011	0.15903753	H	-5.04259565	-2.98170680	-2.21407411
N	-2.12240573	-0.42206300	-0.80508951	H	-4.67538249	-4.18138533	-0.97146182
C	-1.91968504	0.92375563	-0.80075752	H	-5.73231671	-2.81971773	-0.59542900
O	-0.64127993	1.20995803	-0.45051122	Li	-5.72623165	-0.34153080	-2.89357968
O	-2.70781346	1.83520023	-1.05740748	O	-7.36822503	-0.71475098	-3.69972598
Li	-4.24245239	1.46201826	-2.05312492	C	-7.99209005	0.19636745	-4.24600137
O	-4.09426731	-0.40706552	-2.05249161	O	-8.94825695	-0.09045763	-5.16381626

C	-9.66310551	1.11950671	-5.48501566
H	-10.60352260	1.12074998	-4.92357440
H	-9.87953011	1.11826923	-6.55423111
C	-8.72287810	2.25598912	-5.04923188
H	-9.29094195	3.04765754	-4.55552336
N	-7.88372592	1.54232380	-4.07577832
C	-6.89960064	2.20410138	-3.22625667
C	-7.18490120	3.44223961	-2.76009239
C	-6.20600167	4.23159381	-1.93498928
H	-6.21316690	3.94464151	-0.87151478
H	-5.17552454	4.10149629	-2.29301723
H	-6.42923260	5.30380910	-1.97542014
H	-8.16404042	3.87245755	-2.94072910
O	-5.80174629	1.52756235	-3.02236533
C	-7.87984289	2.86530181	-6.19291680
H	-7.10255850	3.48038761	-5.72607410
H	-7.37526489	2.05105770	-6.72733424
C	-8.70829404	3.69366071	-7.15009031
C	-9.07423883	3.19994757	-8.40949732
C	-9.86543844	3.95785561	-9.27555646
C	-10.30441146	5.22554737	-8.89309843
C	-9.94335135	5.73210420	-7.64221603
C	-9.15238871	4.97251895	-6.78088857
H	-8.86460102	5.37893651	-5.81336935
H	-10.27311345	6.72259855	-7.33979868
H	-10.91820132	5.81801641	-9.56611471
H	-10.13360222	3.55828069	-10.25005974
H	-8.72442926	2.21777006	-8.72075632
C	-0.30750261	-1.74767696	-1.89205730
H	-1.10725555	-2.36250920	-2.31962675
H	-0.10644914	-0.93434971	-2.60006329
C	0.93819097	-2.57697949	-1.67025618
C	0.84735688	-3.85519280	-1.09844242
C	1.99151981	-4.61569103	-0.85975316
C	3.25124710	-4.11072547	-1.19110610
C	3.35607269	-2.84371560	-1.76529415
C	2.20770439	-2.08487113	-2.00176411
H	2.29675007	-1.10324597	-2.46263370
H	4.33074749	-2.44540930	-2.03471126
H	4.14308647	-4.70393532	-1.00824888
H	1.89981034	-5.60566691	-0.42064307
H	-0.13140620	-4.26032064	-0.84948387

Table 26. Geometric coordinates and thermally corrected MP2 energies for **5** dimer with one THF *cis* to the benzyl groups



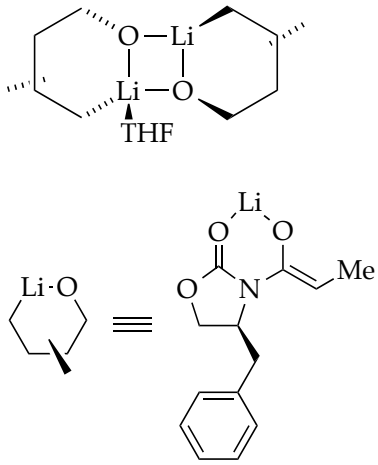


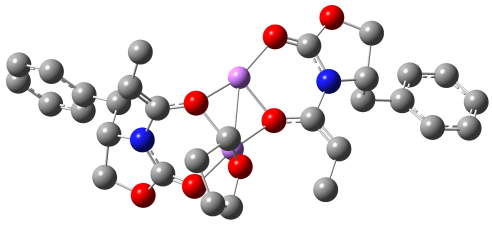
G = -1815.672391 Hartree
G_{MP2} = -1135764.368 kcal/mol
ΔG_{MP2} = 7.035258123 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.94021121	-4.80306340	-4.80782931
O	0.00000000	0.00000000	1.93357650	H	-1.64265338	-3.64059808	-6.12792758
C	1.06785916	0.00000000	2.54046381	C	-2.31683438	-2.71344770	-4.23508366
O	1.14031622	0.53620196	3.79081529	H	-3.27122891	-3.09822764	-3.86895147
C	2.42558891	0.22036312	4.35780345	N	-1.37220089	-2.53604257	-3.12362161
H	2.30548888	-0.63783752	5.02822747	C	-1.65677676	-1.71893832	-1.93939904
H	2.77155605	1.08157984	4.93179048	C	-2.94190761	-1.68101848	-1.50636626
C	3.31421656	-0.10942316	3.14774756	C	-3.39632374	-0.86324091	-0.33045646
H	3.94864024	-0.97025231	3.37054089	H	-2.67008705	-0.08304153	-0.08072016
N	2.28897827	-0.46772259	2.15853178	H	-4.35844492	-0.37099204	-0.53055524
C	2.59731490	-1.04014127	0.85273322	H	-3.53707388	-1.47155850	0.57610127
C	3.68615760	-1.84296096	0.75315556	H	-3.68002492	-2.32022835	-1.97991279
H	4.23255187	-2.12494474	1.64662496	O	-0.63002636	-1.08903169	-1.44845058
C	4.15058521	-2.41053853	-0.56014145	C	-2.55683278	-1.39032428	-4.99861332
H	3.91074172	-1.73556956	-1.39204520	H	-2.85466827	-0.64292483	-4.25480078
H	5.23760599	-2.55936222	-0.56503716	H	-1.60540748	-1.06012451	-5.43340488
H	3.70031031	-3.38805008	-0.79689748	C	-3.61370293	-1.51766583	-6.07330490
O	1.79646928	-0.68804849	-0.11335938	C	-3.26776199	-1.59083764	-7.42922989
Li	1.10694096	-1.73254946	-1.46555739	C	-4.24777352	-1.73754047	-8.41347166
O	0.90886146	-3.00199231	-2.82629674	C	-5.59366635	-1.81474761	-8.05463805
C	-0.15322447	-3.04833595	-3.44715221	C	-5.95328681	-1.73981841	-6.70678578
O	-0.20947102	-3.68910609	-4.64356418	C	-4.97178875	-1.59191555	-5.72742046
C	-1.58709118	-3.79456134	-5.04916143	H	-5.26039395	-1.52274413	-4.68049452

H	-7.00007050	-1.79090077	-6.41868628
H	-6.35800249	-1.92719778	-8.81877522
H	-3.95812825	-1.78735647	-9.45984238
H	-2.22113523	-1.51973219	-7.71796871
C	4.19353608	1.06420232	2.65746942
H	4.57820872	0.78358517	1.67081469
H	3.55461664	1.94552024	2.52101682
C	5.33287326	1.37873112	3.60113176
C	6.46064892	0.54520906	3.65501910
C	7.50506968	0.80919851	4.54040638
C	7.44171454	1.91615595	5.39030279
C	6.32873228	2.75599552	5.34469340
C	5.28440628	2.48714819	4.45720848
H	4.42612310	3.15487816	4.41855087
H	6.27305520	3.62422601	5.99620593
H	8.25660933	2.12447338	6.07831447
H	8.37211135	0.15413608	4.56286109
H	6.52318344	-0.31160126	2.98717438
O	-0.55971357	1.86686424	-0.42078710
C	-1.15429262	2.22995678	-1.69035909
C	-1.98617267	3.50109617	-1.43064307
C	-2.15705416	3.50237350	0.09914170
C	-0.83787199	2.88609277	0.55625149
H	-0.87227039	2.39704207	1.53142524
H	-0.02743076	3.63059247	0.55406202
H	-2.99301540	2.85930396	0.39708774
H	-2.32606012	4.50142268	0.51245939
H	-2.93894089	3.48734944	-1.96795129
H	-1.43593546	4.39348528	-1.74999175
H	-0.35580594	2.39161281	-2.42293611
H	-1.76062957	1.38109826	-2.01729331

Table 27. Geometric coordinates and thermally corrected MP2 energies for **5** dimer with one THF *trans* to the benzyl groups



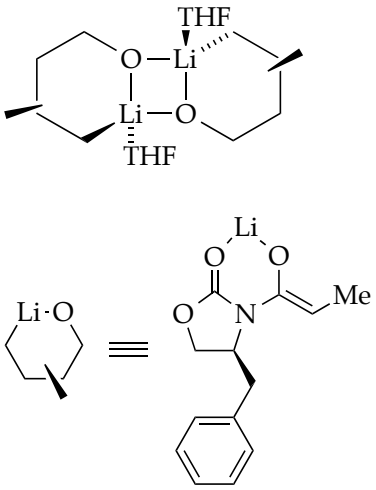


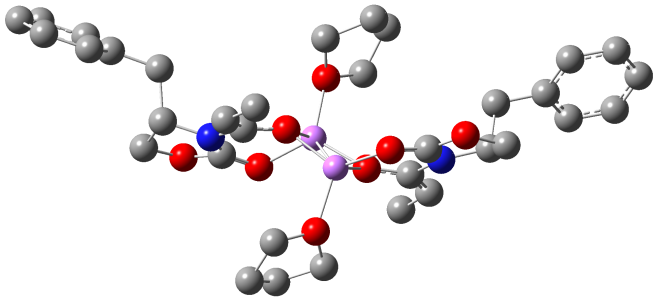
G = -1815.672721 Hartree
G_{MP2} = -1135764.755 kcal/mol
ΔG_{MP2} = 6.841829302 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.53586973	0.67139525	-2.61273510
O	0.00000000	0.00000000	1.90896360	C	-4.85321076	1.33673694	-0.57275298
C	0.81665696	0.00000000	2.92153925	H	-4.93037094	0.32521016	-0.15744890
N	0.24137884	-0.46162947	4.18797770	H	-4.31689468	1.95060194	0.16114646
C	0.71374889	0.00062137	5.50238950	C	-6.23060855	1.90500969	-0.83406205
C	-0.05279430	-0.95875597	6.42452782	C	-6.54285143	3.23093000	-0.50491493
H	0.53784533	-1.84388041	6.68546541	C	-7.80585027	3.76050080	-0.77815660
H	-0.42153353	-0.48692321	7.33653694	C	-8.77957479	2.96863488	-1.38724598
O	-1.18365255	-1.38423315	5.64137087	C	-8.48376995	1.64369652	-1.71654584
C	-0.90719070	-1.17986241	4.32716715	C	-7.22156170	1.11855066	-1.44112596
O	-1.66927019	-1.63097595	3.47020022	H	-7.00302735	0.08187565	-1.68957013
Li	-1.54650884	-0.98744546	1.72773394	H	-9.23921978	1.01657534	-2.18278949
O	-1.74602642	-0.89550125	-0.07519385	H	-9.76394453	3.37751072	-1.59848970
C	-2.53012957	-0.75622224	-1.10917821	H	-8.02877168	4.78985557	-0.50978732
N	-2.68736358	0.61949465	-1.58390494	H	-5.79330100	3.85080943	-0.01740325
C	-3.99104066	1.23812725	-1.85352457	C	-3.22275476	-1.71629292	-1.76562525
C	-3.53144105	2.59357554	-2.41772005	C	-3.24674804	-3.15729974	-1.34387201
H	-3.47005623	2.58409103	-3.51168333	H	-4.27103172	-3.51845937	-1.17116698
H	-4.14968632	3.43339224	-2.09718433	H	-2.80837627	-3.81941186	-2.10541936
O	-2.20298511	2.77766871	-1.89061538	H	-2.68217764	-3.29925302	-0.41716773
C	-1.71145093	1.56639763	-1.51373904	H	-3.78890410	-1.43803258	-2.65036041
O	-0.53507843	1.44250802	-1.18381423	H	1.78896077	-0.16280062	5.60023872

C	0.39242251	1.49607210	5.73066529
H	0.79318912	2.04438810	4.87133951
H	-0.69718358	1.62297035	5.72151594
C	0.97509924	2.02941430	7.02058910
C	2.35048381	2.28874831	7.12365871
C	2.90462969	2.75412644	8.31553540
C	2.09058383	2.97109008	9.42994711
C	0.72083833	2.72219126	9.34071068
C	0.17012169	2.25494803	8.14527469
H	-0.90123472	2.07630485	8.08002435
H	0.07756023	2.89537354	10.19952317
H	2.52083115	3.33682151	10.35836003
H	3.97150977	2.95374214	8.37305955
H	2.98884305	2.13535388	6.25588457
C	2.10873114	0.41155445	2.92821340
H	2.70805435	0.30058527	3.82472766
C	2.77791178	0.98362104	1.70929623
H	2.06391037	1.53708115	1.08647050
H	3.57704567	1.68083790	1.99037881
H	3.23412778	0.21323194	1.06831542
O	1.37107339	-1.03521314	-1.00907529
C	2.09473682	-0.43428125	-2.11187503
C	2.26963215	-1.54111709	-3.16189989
C	1.10791815	-2.49600810	-2.84136235
C	1.04657300	-2.40888151	-1.31806191
H	1.78783072	-3.06833425	-0.84512824
H	0.05895882	-2.61097051	-0.89799228
H	1.27597246	-3.51644612	-3.19913604
H	0.17083692	-2.12778631	-3.27430092
H	3.22938072	-2.05340257	-3.02624118
H	2.23913294	-1.14983133	-4.18321202
H	1.49573543	0.40307725	-2.48423052
H	3.04620046	-0.04678309	-1.73322537

Table 28. Geometric coordinates and thermally corrected MP2 energies for **5** dimer trans solvated with two THF



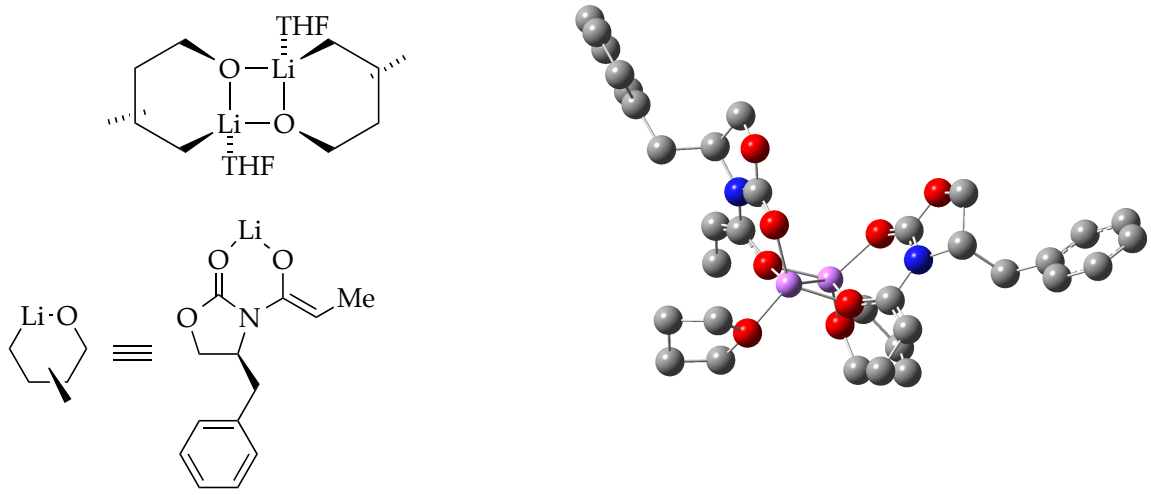


G = - 2048.024941 Hartree
G_{MP2} = - 1281086.884 kcal/mol
ΔG_{MP2} = 1.922583795 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.36484468	-2.59957887	-4.95850904
O	0.00000000	0.00000000	1.93578920	C	-1.65780678	-2.33987376	-5.52823069
C	1.08678450	0.00000000	2.50476227	H	-2.20476629	-3.28721778	-5.59678719
O	1.20230383	0.54929065	3.74732190	H	-1.52054692	-1.92913305	-6.52986341
C	2.50484656	0.24290609	4.27363638	C	-2.32005730	-1.36042042	-4.54857758
H	2.41296575	-0.61313565	4.95198378	H	-3.37587456	-1.61039517	-4.42082399
H	2.86606427	1.10831307	4.83156527	N	-1.56880282	-1.66066167	-3.32287020
C	3.35201800	-0.08743253	3.03642258	C	-1.94700378	-1.17025654	-1.99577312
H	4.01243076	-0.93147893	3.24725131	C	-3.23672387	-0.78393388	-1.80311470
N	2.29804087	-0.48165960	2.09179088	C	-3.74838035	-0.27728512	-0.48351928
C	2.56319996	-1.12117928	0.80163657	H	-2.95214490	-0.26584082	0.26698436
C	3.74355776	-1.78089211	0.65112989	H	-4.15703963	0.74260583	-0.55313244
H	4.42114941	-1.88310167	1.49163814	H	-4.56044882	-0.90733937	-0.09058129
C	4.16287121	-2.39636826	-0.65524289	H	-3.95891109	-0.88600337	-2.60566379
H	3.54772505	-2.01891121	-1.47842416	O	-0.98706136	-1.15122243	-1.12187341
H	5.21217164	-2.16764481	-0.88855356	C	-2.18481566	0.12617879	-4.95723288
H	4.07634693	-3.49480511	-0.66202073	H	-2.46932801	0.72559796	-4.08558015
O	1.63530001	-0.97411660	-0.09505670	H	-1.12732624	0.33054867	-5.16665986
Li	0.56086988	-2.26621111	-1.02058606	C	-3.03801190	0.49114963	-6.15168946
O	0.52539969	-2.65270600	-2.90362557	C	-2.47441019	0.66462120	-7.42297910
C	-0.40554532	-2.31620407	-3.62459511	C	-3.27228228	0.97338753	-8.52684673

C	-4.65201188	1.11333297	-8.37558089	C	5.35277074	1.45253861	3.39407166
C	-5.22727953	0.94678224	-7.11348430	C	6.49994693	0.64442482	3.41523745
C	-4.42675284	0.63963121	-6.01381177	C	7.57019095	0.94143702	4.25837969
H	-4.88172863	0.52278377	-5.03222315	C	7.51384381	2.05698838	5.09747678
H	-6.30039164	1.06165412	-6.98455166	C	6.38212930	2.87250306	5.08320352
H	-5.27475672	1.35520278	-9.23258618	C	5.31205159	2.57062921	4.23804063
H	-2.81370420	1.10780128	-9.50304123	H	4.43803341	3.21854003	4.22349228
H	-1.39779031	0.56813770	-7.54731179	H	6.33151429	3.74723357	5.72636282
O	0.15761249	-3.89248321	0.07468157	H	8.34863637	2.29087789	5.75264543
C	1.10903767	-4.56145187	0.93551575	H	8.45166313	0.30549861	4.25627186
H	1.38860488	-5.51958183	0.48094080	H	6.55686248	-0.21878660	2.75517166
H	1.99466161	-3.92245936	0.99448941	O	0.22538789	1.85375082	-0.71656613
C	0.41074953	-4.74931100	2.30195498	C	1.40603272	2.05756213	-1.52543431
H	0.14261046	-5.80056819	2.45569555	H	2.00408817	2.87125706	-1.09022145
H	1.05199318	-4.44698447	3.13527221	H	1.98112859	1.12973345	-1.49416496
C	-0.85803979	-3.88229209	2.18309954	C	0.87578380	2.43656240	-2.90558100
C	-1.14556781	-3.94668562	0.68590853	C	-0.36082055	3.27610814	-2.54466394
H	-1.71506980	-3.10161511	0.29591106	C	-0.89904299	2.56363857	-1.29394317
H	-1.64353343	-4.88845831	0.40907479	H	-1.67036999	1.82533659	-1.53956049
H	-1.68793238	-4.25454653	2.79194999	H	-1.29674132	3.25618514	-0.54468085
H	-0.65595798	-2.84496371	2.47071216	H	-1.10347315	3.32040216	-3.34694748
C	4.18477452	1.10129545	2.49962854	H	-0.06310816	4.30366778	-2.30538331
H	4.53527615	0.81984970	1.50080244	H	1.60987981	2.98345069	-3.50521363
H	3.51917185	1.96551400	2.38244968	H	0.58394021	1.53424309	-3.4550600

Table 29. Geometric coordinates and thermally corrected MP2 energies for **5** dimer cis solvated with two THF

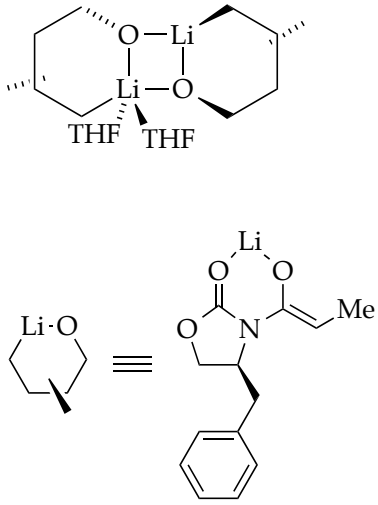


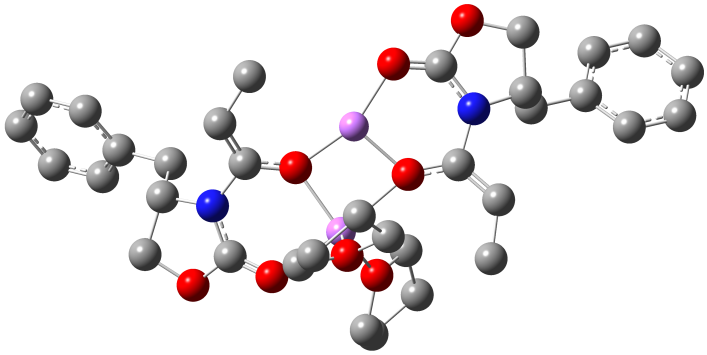
G = - 2048.024728 Hartree
G_{MP2} = - 1281084.394 kcal/mol
ΔG_{MP2} = 3.167104249 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.04815982	-3.36700301	-4.06778651
O	0.00000000	0.00000000	1.90200070	H	-1.99043607	-2.81314426	-4.00861762
C	0.99187449	0.00000000	2.74386037	H	-0.29097343	-2.67180236	-4.45138401
N	1.34693117	-1.31838930	3.27071766	C	-1.18398256	-4.55308462	-4.99775901
C	2.53776229	-1.59367919	4.08486436	C	-0.21032866	-4.83014535	-5.96691458
C	2.69164624	-3.09655581	3.82874163	C	-0.32635474	-5.94011683	-6.80653679
H	3.31699491	-3.30600885	2.95344676	C	-1.42254667	-6.79474542	-6.68865263
H	3.06491054	-3.65388994	4.68918100	C	-2.40249926	-6.52976166	-5.72902572
O	1.34822199	-3.53626822	3.54966789	C	-2.28311530	-5.41953874	-4.89372581
C	0.62787231	-2.46752176	3.10090252	H	-3.05733099	-5.21662941	-4.15650405
O	-0.50394777	-2.64110264	2.65842568	H	-3.26374296	-7.18600271	-5.63424626
Li	-1.42706792	-1.23867134	1.70945960	H	-1.51621787	-7.65817385	-7.34176312
O	-1.52405631	-1.12494563	-0.18314050	H	0.43855585	-6.13322318	-7.55421105
C	-1.78526632	-2.04734377	-1.06134669	H	0.64235196	-4.16252977	-6.07228445
N	-0.60890459	-2.61834602	-1.71840540	C	-3.00995132	-2.53352211	-1.39309563
C	-0.64354215	-3.77195237	-2.62680855	C	-4.27424996	-2.04444339	-0.74439239
C	0.81316854	-4.23597934	-2.52262135	H	-4.96729061	-1.59350414	-1.47168281
H	0.96062995	-4.96064195	-1.71377919	H	-4.82832412	-2.85924449	-0.25381951
H	1.21463412	-4.63815507	-3.45393256	H	-4.05032893	-1.28976655	0.01514627
O	1.53487497	-3.03220780	-2.19833358	H	-3.10807312	-3.31010324	-2.14251351
C	0.67181915	-2.15567793	-1.60797430	O	-3.03777167	-0.74890728	2.78748456
O	1.10588051	-1.12072148	-1.11031076	C	-3.66888061	-1.74321119	3.63153705
H	-1.33092017	-4.52621690	-2.23689950	C	-3.92815669	-1.06002938	4.98561563

C	-2.93084683	0.11078871	4.97476651
C	-2.92939917	0.50267020	3.49945661
H	-2.01145401	0.98643481	3.15872288
H	-3.79344524	1.13644238	3.25204624
H	-1.93177364	-0.22781263	5.27217767
H	-3.22536721	0.93432520	5.63255993
H	-3.78231998	-1.74365712	5.82724878
H	-4.95555197	-0.68093991	5.03562593
H	-4.58811391	-2.08541557	3.14432758
H	-2.97711744	-2.58759160	3.71663425
H	3.38850942	-1.03176473	3.69260681
C	2.31180689	-1.25632124	5.58146606
H	1.94649500	-0.22633495	5.64235538
H	1.51048017	-1.90359642	5.95927546
C	3.55953311	-1.42923542	6.42004300
C	4.60925261	-0.50143471	6.33633306
C	5.77370014	-0.66664405	7.08547635
C	5.91055499	-1.76577044	7.93671882
C	4.87391790	-2.69417265	8.03345370
C	3.70992743	-2.52521752	7.28040767
H	2.90154768	-3.24800134	7.36996157
H	4.96720590	-3.54937434	8.69778001
H	6.81651893	-1.89384097	8.52294687
H	6.57305024	0.06581340	7.00859176
H	4.50886152	0.36366354	5.68394238
C	1.72341216	1.07280222	3.14274125
H	2.52875001	0.95078396	3.85755795
C	1.47521831	2.46028290	2.62160036
H	0.70788367	2.44894715	1.84227639
H	1.14057567	3.15001355	3.41252511
H	2.38411398	2.90326313	2.18824475
O	-0.21242423	1.75245228	-0.93129671
C	-1.59711635	2.15025839	-1.11365706
C	-1.72589728	2.61563483	-2.57555827
C	-0.50240284	1.97466914	-3.25319681
C	0.53369890	2.02413399	-2.13292031
H	0.99810320	3.01832408	-2.05879654
H	1.31634829	1.26589078	-2.20854862
H	-0.18062054	2.50667463	-4.15393252
H	-0.71184049	0.93308191	-3.52258910
H	-1.66493478	3.70815110	-2.64056151
H	-2.67445676	2.30576635	-3.02357111
H	-2.21222273	1.27285443	-0.89316831
H	-1.83077959	2.94418513	-0.39597240

Table 30. Geometric coordinates and thermally corrected MP2 energies for **5** dimer unsymmetrically solvated with two THF



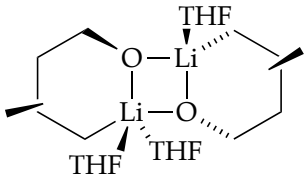


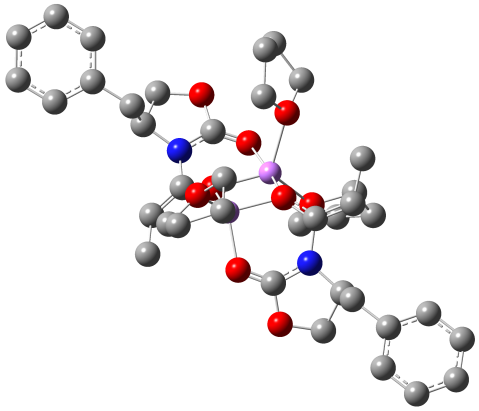
G = -2048.015294 Hartree
G_{MP2} = -1281081.588 kcal/mol
ΔG_{MP2} = 4.570565321 kcal/mol Li vs. **5** spirocyclic dimer with three THF

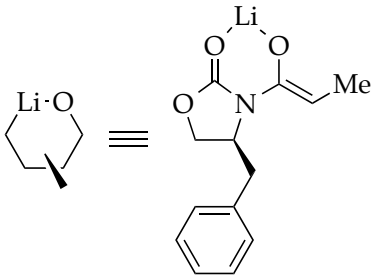
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.47959596	-0.01309133	-3.06636142
O	0.00000000	0.00000000	2.22537890	C	-4.36746300	1.94692962	-2.14734873
C	0.64493755	0.00000000	3.34809936	H	-4.68223003	1.61117865	-1.15273920
N	-0.19194029	0.09417793	4.56135318	H	-3.60478437	2.72206735	-2.00380412
C	0.26747311	0.69499075	5.82331098	C	-5.54741936	2.49790742	-2.91648702
C	-0.88425383	0.29757094	6.75819034	C	-5.44639181	3.68436776	-3.65530391
H	-0.67593053	-0.63176827	7.30008399	C	-6.53173716	4.16908462	-4.38858735
H	-1.15803700	1.07791841	7.47013805	C	-7.73945067	3.47092936	-4.39500888
O	-1.99975958	0.06956666	5.87885369	C	-7.85591239	2.28876482	-3.65975136
C	-1.52770118	-0.16327467	4.62487819	C	-6.77023553	1.80927004	-2.92786767
O	-2.30178717	-0.54920072	3.74894905	H	-6.87262788	0.89447409	-2.34749660
Li	-1.77561316	-0.34198191	1.96818121	H	-8.79579133	1.74285872	-3.65153736
O	-1.97146768	-0.12078010	0.17699740	H	-8.58595801	3.84691740	-4.96326537
C	-2.84751123	-0.44821569	-0.72850055	H	-6.43300178	5.09410394	-4.95074275
N	-2.63826976	0.14817508	-2.04081012	H	-4.51146635	4.24092984	-3.64609348
C	-3.71171374	0.73406762	-2.84871033	C	-3.93229051	-1.24415057	-0.56311205
C	-2.92800746	1.08402435	-4.12690999	C	-4.28131941	-1.84291063	0.77303748
H	-3.01122363	0.29922202	-4.88720801	H	-5.22448373	-2.39728013	0.72127737
H	-3.21594802	2.04130892	-4.56476010	H	-3.51650575	-2.54841220	1.13576730
O	-1.55334645	1.16687873	-3.70723773	H	-4.40108752	-1.08185498	1.55915721
C	-1.41390058	0.49271753	-2.52703385	H	-4.55744238	-1.48163642	-1.41743698
O	-0.30692146	0.26599332	-2.05841647	H	1.19671848	0.22763831	6.15504420

C	0.47712085	2.22130528	5.68726925
H	1.14343503	2.37606361	4.83177589
H	-0.48630568	2.68492668	5.44161072
C	1.06189210	2.84834562	6.93338477
C	2.41336255	2.65409625	7.25809969
C	2.95805542	3.20437810	8.41771328
C	2.15916743	3.96367084	9.27625311
C	0.81527757	4.16925056	8.96372242
C	0.27332419	3.61479981	7.80202919
H	-0.77289859	3.78964419	7.55964208
H	0.18688871	4.76453078	9.62109059
H	2.58339391	4.39565993	10.17859986
H	4.00826475	3.04584330	8.64869036
H	3.04552362	2.07519284	6.58776169
C	1.99053276	-0.05349894	3.54830293
H	2.37344179	-0.11620824	4.56123309
C	3.00656463	-0.08785639	2.44120402
H	2.54771764	0.13694825	1.47503161
H	3.80797720	0.64693528	2.60994552
H	3.50334915	-1.06718109	2.35599308
O	0.78800255	-1.89219978	-0.27612789
C	1.20700077	-2.73826835	0.81646208
C	0.49554640	-4.07038161	0.58940786
C	0.50547438	-4.16383135	-0.94416388
C	0.27677863	-2.70543289	-1.36063460
H	-0.78847957	-2.48192749	-1.48058801
H	0.79752703	-2.42652071	-2.28097341
H	-0.26082326	-4.83403103	-1.34573129
H	1.48227174	-4.51853654	-1.29479660
H	-0.53404277	-4.02199525	0.96433112
H	1.00061891	-4.90802433	1.08055537
H	2.29870186	-2.86196332	0.77646111
H	0.94191070	-2.22963726	1.74358814
O	1.22964021	1.65762614	-0.01398323
C	1.10184933	2.72472878	0.95376961
C	2.00148244	3.86208334	0.45118996
C	2.04846602	3.60556069	-1.06296658
C	2.06104817	2.07846735	-1.11433411
H	3.07834082	1.68668882	-0.96673455
H	1.63808750	1.65117780	-2.02405920
H	2.91923940	4.05230202	-1.55312048
H	1.14509430	3.99387533	-1.54867972
H	3.00680764	3.77390566	0.88015480
H	1.60951742	4.84955031	0.71427227
H	0.04738290	3.02443256	0.99109229
H	1.38922488	2.34124997	1.93557275

Table 31. Geometric coordinates and thermally corrected MP2 energies for **5** dimer with three THF





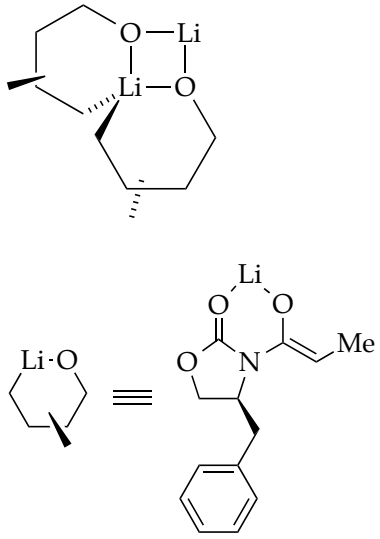


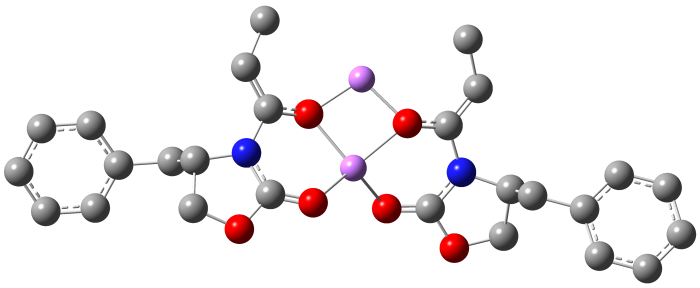
G = - 2280.364885 Hartree
G_{MP2} = - 1426402.09 kcal/mol
ΔG_{MP2} = 0.464733826 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.01503670	-1.91847151	-3.09335609
O	0.00000000	0.00000000	2.09165270	C	-4.63738511	-0.24444646	-1.86884380
C	0.99342614	0.00000000	2.92031074	H	-4.65688413	-0.80630148	-0.92799016
N	1.35790556	-1.31744840	3.45956960	H	-4.26822896	0.76228810	-1.63740089
C	2.56016196	-1.59371484	4.25589949	C	-6.02304792	-0.17499475	-2.47070542
C	2.69389166	-3.10082569	4.01566581	C	-6.52422398	1.01688896	-3.01127189
H	3.28970852	-3.32774722	3.12388995	C	-7.79327332	1.06592495	-3.59233283
H	3.08959768	-3.65072230	4.87091330	C	-8.58428306	-0.08200330	-3.64294606
O	1.33842747	-3.52980655	3.78567089	C	-8.09927586	-1.27666425	-3.10502875
C	0.61810509	-2.45833344	3.33951555	C	-6.83209370	-1.32052062	-2.52466066
O	-0.53172776	-2.62126051	2.94395121	H	-6.46623006	-2.25219015	-2.09776763
Li	-1.40648311	-1.23455606	1.90689905	H	-8.71140586	-2.17448575	-3.13269963
O	-1.51931076	-1.21005511	0.04284567	H	-9.57282570	-0.04630622	-4.09284627
C	-2.10322095	-1.87011204	-0.91261454	H	-8.16372082	2.00248014	-4.00121262
N	-2.31124588	-1.10492024	-2.14788611	H	-5.91847749	1.91974592	-2.96570610
C	-3.61455113	-0.94601960	-2.79377029	C	-2.57268915	-3.14171282	-0.92038581
C	-3.20408559	-0.12653378	-4.03156278	C	-2.51463799	-4.07748817	0.25310929
H	-3.02663598	-0.76560011	-4.90400252	H	-3.49784619	-4.22365210	0.73022749
H	-3.92124598	0.65268466	-4.29624722	H	-2.17053731	-5.07515484	-0.05321954
O	-1.96007706	0.49962652	-3.66444034	H	-1.82373156	-3.72053407	1.02269769
C	-1.41327035	-0.20250651	-2.61866675	H	-2.99976656	-3.52264780	-1.84452985
O	-0.27332877	0.01906335	-2.23413517	O	-3.05684484	-0.79601339	2.99063715

C	-3.73293446	-1.88287944	3.67130715	H	0.88934411	2.44509583	1.90195053
C	-3.99883526	-1.39581749	5.10465580	H	0.95726403	3.08984048	3.55268320
C	-2.93348887	-0.30328514	5.29270751	H	2.42908239	2.98822003	2.59189110
C	-2.87332658	0.31272248	3.89679561	O	1.95039740	-0.53940289	-0.30104156
H	-1.91739946	0.77793082	3.64597446	C	3.01066083	0.43326776	-0.18837346
H	-3.68448258	1.04034412	3.74672057	C	4.23159562	-0.21769199	-0.84052911
H	-1.96551540	-0.74898021	5.54843321	C	3.58024837	-1.06066299	-1.94818025
H	-3.19328189	0.42576568	6.06651105	C	2.30254031	-1.55757141	-1.26565303
H	-3.92101197	-2.20547658	5.83636819	H	2.47149455	-2.49894500	-0.72635721
H	-5.00327860	-0.96382360	5.18649221	H	1.45970583	-1.67968865	-1.94808768
H	-4.65036860	-2.12158338	3.12323247	H	4.21286758	-1.88111916	-2.30110089
H	-3.06775763	-2.75178563	3.64851321	H	3.33038284	-0.42837161	-2.80817736
H	3.40864007	-1.04259418	3.84399633	H	4.75128748	-0.86379840	-0.12224776
C	2.36379984	-1.24336279	5.75441647	H	4.94893926	0.51806875	-1.21742955
H	2.00086572	-0.21276789	5.81525278	H	2.71711376	1.34649492	-0.72500813
H	1.56911011	-1.88679566	6.15219384	H	3.13145610	0.67037836	0.87190492
C	3.62684159	-1.41173845	6.57053396	O	-0.43464958	2.06821086	-0.12169904
C	4.67443452	-0.48389166	6.46263395	C	-1.68392735	2.44700904	0.50030975
C	5.85297833	-0.64472326	7.19041397	C	-2.13374394	3.73997457	-0.19545659
C	6.00683617	-1.73937737	8.04448791	C	-1.43959934	3.64357360	-1.56382563
C	4.97270022	-2.66777565	8.16531966	C	-0.11539018	2.97785463	-1.19151905
C	3.79460207	-2.50323371	7.43345004	H	0.61523850	3.71715369	-0.83065384
H	2.98877931	-3.22628726	7.54177627	H	0.32366584	2.39097183	-1.99983444
H	5.07891459	-3.51973402	8.83186893	H	-1.30279422	4.61487808	-2.04978348
H	6.92375559	-1.86384556	8.61423792	H	-2.00155405	2.99444720	-2.24494312
H	6.65006320	0.08813656	7.09520311	H	-1.77084626	4.61814051	0.35196101
H	4.56091358	0.37828175	5.80852951	H	-3.22355182	3.81623910	-0.26445268
C	1.74204533	1.06830151	3.31586929	H	-2.39499499	1.62595679	0.35177415
H	2.53273475	0.94198701	4.04598933	H	-1.51338682	2.56604152	1.57390323
C	1.48882385	2.46406972	2.81625263				

Table 32. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with no THF



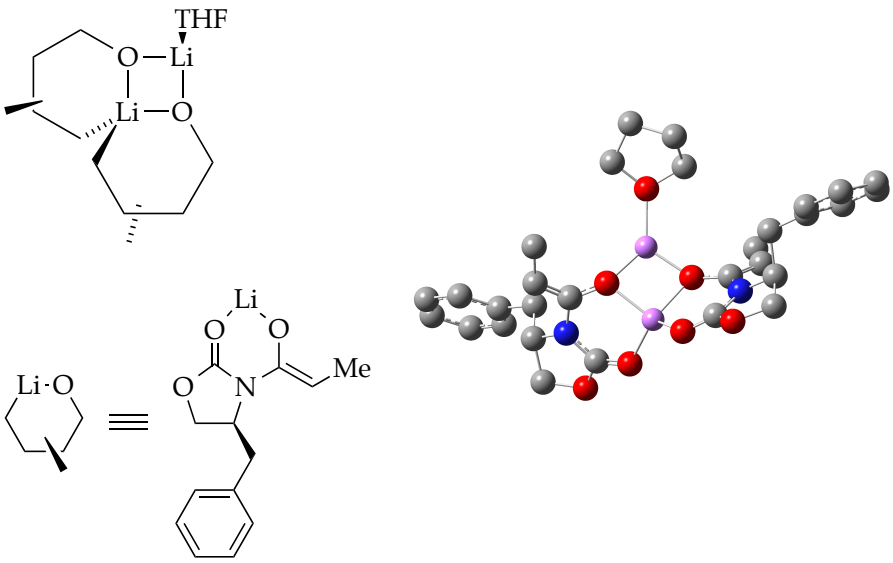


G = -1583.305352 Hartree
G_{MP2} = -990435.4088 kcal/mol
ΔG_{MP2} = 15.36966258 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.73147795	1.92380878	-2.72442778
O	0.00000000	0.00000000	1.92708970	H	-3.45904995	2.56678854	-3.56853142
C	1.04944315	0.00000000	2.55894929	H	-4.76550360	2.12233605	-2.43812441
O	1.11406590	0.56476070	3.79370448	O	-2.87936755	2.25174154	-1.61172131
C	2.38134588	0.24097393	4.39445023	C	-1.88238629	1.33150252	-1.52815768
H	2.22863714	-0.58540015	5.09724962	O	-0.94175791	1.49876413	-0.76148061
H	2.73957410	1.11632827	4.93853580	H	-3.38627414	0.26964203	-4.08984916
C	3.28581298	-0.15934871	3.21571544	C	-4.47900764	-0.53958669	-2.39813178
H	3.88314255	-1.03541517	3.48046287	H	-4.04637698	-1.54435381	-2.46254555
N	2.27053562	-0.51103240	2.21576393	H	-4.59397074	-0.30217616	-1.33355181
C	2.57243187	-1.14400142	0.94919550	C	-5.81924367	-0.49529785	-3.09841417
C	3.61556208	-2.00832709	0.88212467	C	-6.92185762	0.14745774	-2.51985652
H	4.15093798	-2.28670640	1.78278751	C	-8.14833929	0.20748311	-3.18522863
C	4.04048615	-2.64014956	-0.41492612	C	-8.29077523	-0.37583221	-4.44440423
H	3.88678961	-1.95413791	-1.26064324	C	-7.20086051	-1.02303801	-5.03165259
H	5.10566874	-2.90000235	-0.40390143	C	-5.97854606	-1.08176255	-4.36327792
H	3.50158787	-3.57674757	-0.64512859	H	-5.13793982	-1.59940268	-4.82120289
O	1.80317809	-0.79368288	-0.04749626	H	-7.30511400	-1.48804070	-6.00854056
Li	1.11586364	-1.77063797	-1.37843047	H	-9.24477801	-0.33225780	-4.96281143
O	-0.56555330	-1.16952498	-1.48146004	H	-8.99237869	0.70632829	-2.71617617
C	-1.29469158	-0.87735140	-2.52589866	H	-6.82261805	0.59342601	-1.53241074
N	-2.12899045	0.29785386	-2.38886017	C	-1.34633285	-1.58515348	-3.68179063
C	-3.45046155	0.43856894	-3.01201603	C	-0.57194807	-2.86133317	-3.86581301

H	0.45716462	-2.70198583	-4.23491923	C	7.45900599	0.64585027	4.70532255
H	-0.50147736	-3.42330925	-2.92311253	C	7.42091373	1.78969725	5.50645374
H	-1.05522077	-3.52137394	-4.59589847	C	6.34927851	2.67537643	5.39139093
H	-1.93285311	-1.22109405	-4.51769661	C	5.32007038	2.41581968	4.48368056
C	4.21862880	0.96639156	2.71161569	H	4.49442273	3.11826069	4.39056826
H	4.62046707	0.64304169	1.74473680	H	6.31423692	3.57226640	6.00426825
H	3.61530068	1.86407214	2.52973738	H	8.22385104	1.99091685	6.21042009
C	5.34342683	1.27067494	3.67638215	H	8.29445203	-0.04522102	4.78184228
C	6.43002622	0.39126869	3.79944530	H	6.47350935	-0.49479237	3.16915224

Table 33. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with one THF

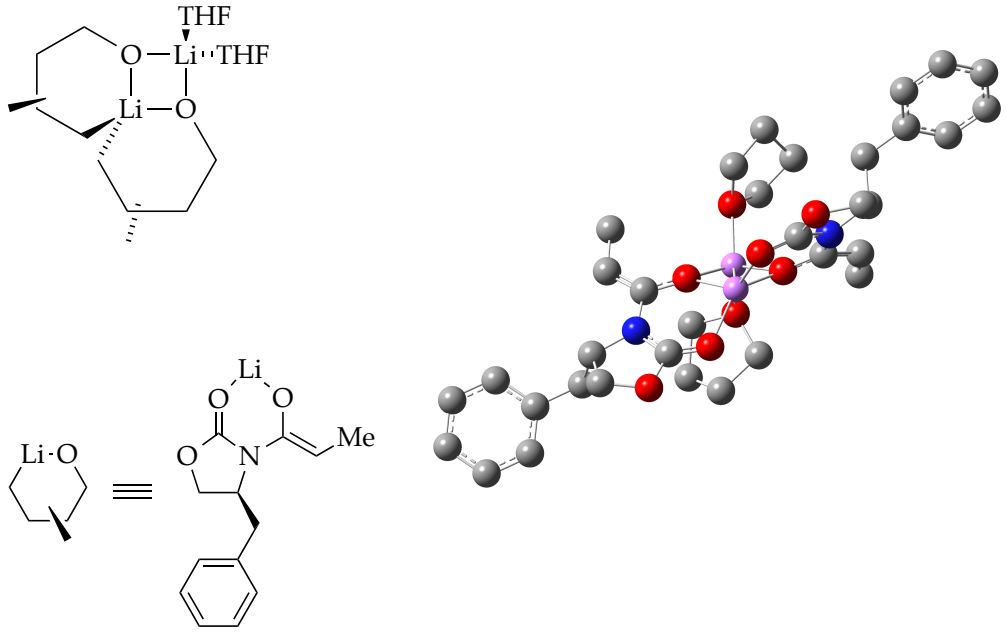


G = -1815.66899 Hartree
G_{MP2} = -1135761.455 kcal/mol
ΔG_{MP2} = 8.491542879 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-1.92920023	0.38526192	-2.51071411
O	0.00000000	0.00000000	1.91958140	C	-2.54047708	0.31006307	-3.84085663
C	1.02376138	0.00000000	2.59020437	C	-3.07901205	-1.13166002	-3.81187915
O	0.95718669	0.15975008	3.94210213	H	-4.13191670	-1.17025041	-3.51128148
C	2.24588609	-0.12741943	4.50960344	H	-2.95396252	-1.66260355	-4.75715795
H	2.23392431	-1.15208681	4.89760098	O	-2.29507341	-1.79850199	-2.80643434
H	2.42666399	0.56744737	5.33148345	C	-1.74006572	-0.86091330	-1.98876083
C	3.23226250	0.03669571	3.34177954	O	-1.17955338	-1.19002627	-0.95040952
H	3.98387738	-0.75603344	3.36989080	H	-3.36642407	1.02094293	-3.92599638
N	2.32721961	-0.14831192	2.20198717	C	-1.51177193	0.58644347	-4.96269285
C	2.77543422	-0.27179532	0.81699291	H	-1.04045763	1.54969064	-4.73534352
C	4.00209832	-0.80844440	0.59092111	H	-0.72922298	-0.18072811	-4.91431856
H	4.58353872	-1.18259164	1.42726950	C	-2.13664973	0.61845676	-6.33986175
C	4.56485372	-1.02007805	-0.78617512	C	-1.98515554	-0.45144611	-7.23212350
H	5.50883096	-0.47708373	-0.94943780	C	-2.58932594	-0.42819388	-8.49108078
H	4.78306094	-2.08138081	-0.97408183	C	-3.35789449	0.66975928	-8.87827834
H	3.85216697	-0.69494235	-1.55034083	C	-3.51466635	1.74509481	-8.00041756
O	1.93352029	0.16924144	-0.07221772	C	-2.90861845	1.71824557	-6.74478143
Li	1.58038888	1.47203773	-1.29563954	H	-3.02647564	2.56481800	-6.07121726
O	-0.22977177	1.43659559	-1.30957587	H	-4.10536204	2.60820018	-8.29638757
C	-1.35729175	1.60431192	-1.94419861	H	-3.82753277	0.69086810	-9.85797867

H	-2.45522636	-1.26702713	-9.16910129	H	3.67949204	4.25644117	0.23230131
H	-1.37807387	-1.30655517	-6.94221223	H	4.20462367	1.98277233	-0.53304155
C	-2.03198491	2.76215984	-2.13948505	H	4.96753121	2.61238587	-2.01868524
C	-1.54767608	4.09010589	-1.63338483	C	3.93732913	1.41322670	3.29766395
H	-2.31824603	4.60113694	-1.03927167	H	4.41793516	1.49477482	2.31617592
H	-0.67271256	3.95656833	-0.98916082	H	3.17100978	2.19600469	3.35597823
H	-1.27242035	4.78233146	-2.44538301	C	4.95762734	1.59051286	4.40008454
H	-2.99325064	2.73497098	-2.64396958	C	6.18759850	0.91681426	4.34506420
O	2.88895999	2.74404008	-1.91709897	C	7.12401955	1.04985150	5.36972204
C	4.18168322	2.78784547	-1.27087919	C	6.84801060	1.86346108	6.47127954
C	4.26018559	4.19777655	-0.69543168	C	5.63165098	2.54323507	6.53707100
C	3.59977147	5.03192308	-1.80925184	C	4.69585101	2.40576917	5.50938987
C	2.55511703	4.06881184	-2.40989920	H	3.75362319	2.94712711	5.56375963
H	2.57865600	4.05507571	-3.50478526	H	5.40948678	3.18386707	7.38649784
H	1.53425240	4.28613550	-2.08406709	H	7.57801142	1.96939116	7.26917541
H	4.34216537	5.31133531	-2.56468386	H	8.07210507	0.52209463	5.30636236
H	3.14273224	5.95253582	-1.43599771	H	6.41568571	0.28977998	3.48537626
H	5.28575752	4.51076019	-0.47864388				

Table 34. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with two THF

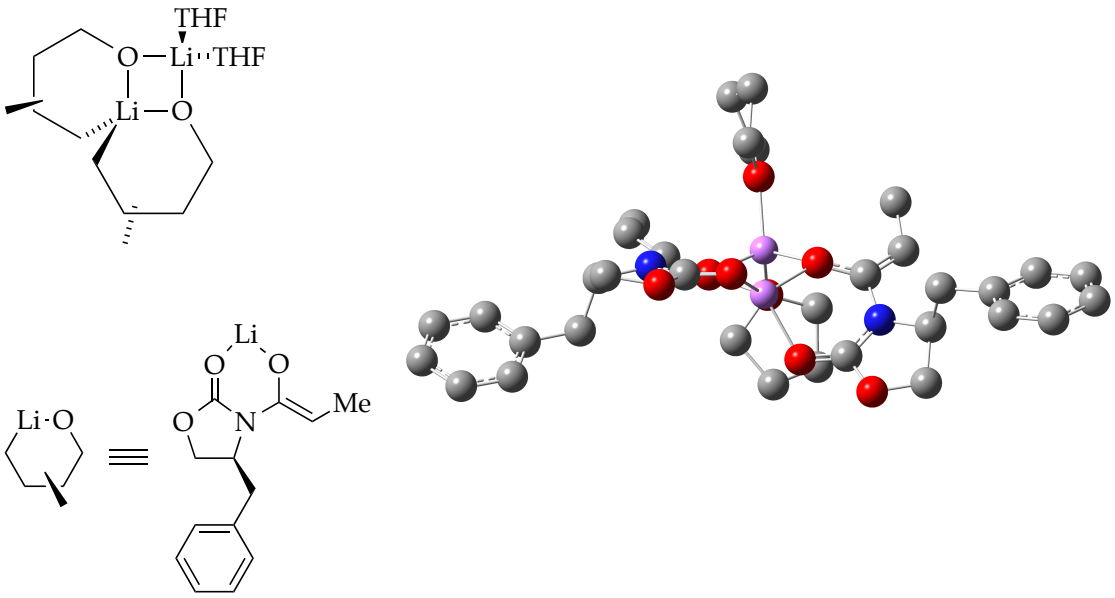


G = - 2048.021479 Hartree
G_{MP2} = - 1281086.85 kcal/mol
ΔG_{MP2} = 1.939384828 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	1.33472490	1.58354811	-1.49517439
O	0.00000000	0.00000000	1.90774580	O	-0.52321012	1.31183697	-1.28183373
C	1.03245062	0.00000000	2.56391855	C	-1.67164774	1.45498192	-1.86897011
O	0.96991935	-0.11135469	3.92185282	N	-2.48853439	0.24095840	-1.93680571
C	2.29454408	-0.33645201	4.42980940	C	-3.72162893	0.12411960	-2.72634322
H	2.43170686	-1.41309204	4.58252638	C	-4.30850400	-1.16247067	-2.13298729
H	2.39360474	0.18072815	5.38553090	H	-4.99382699	-0.95935895	-1.30219134
C	3.21831636	0.21460404	3.33618190	H	-4.80738773	-1.79499268	-2.86889033
H	4.09223315	-0.42985287	3.21748330	O	-3.16603839	-1.86871141	-1.62111998
N	2.33913008	0.10452420	2.16396745	C	-2.16471351	-0.97182147	-1.38788864
C	2.80454053	0.22376953	0.78034585	O	-1.16585907	-1.32307447	-0.77247814
C	4.14668676	0.16394247	0.55912364	H	-4.37942607	0.97278493	-2.52531751
H	4.82361070	-0.02568103	1.38377921	C	-3.43102342	0.02883607	-4.24512886
C	4.76038824	0.22754098	-0.81134746	H	-2.79697599	0.88173137	-4.50924468
H	5.64576009	0.87929364	-0.83205815	H	-2.84659659	-0.88218291	-4.42511320
H	5.09563481	-0.75983702	-1.16785550	C	-4.68760292	0.01969144	-5.08714226
H	4.04878255	0.60931214	-1.54848042	C	-5.15949117	-1.16102596	-5.67656504
O	1.87045233	0.38172643	-0.10834849	C	-6.33582050	-1.16869455	-6.42934977

C	-7.06203789	0.00945234	-6.60446280
C	-6.60183592	1.19482322	-6.02601731
C	-5.42600491	1.19809667	-5.27646312
H	-5.06939578	2.12861752	-4.83946131
H	-7.15692231	2.11920120	-6.16317627
H	-7.97687858	0.00647356	-7.19085467
H	-6.68124645	-2.09513607	-6.88070949
H	-4.59307839	-2.08191667	-5.55370777
C	-2.18050413	2.59502334	-2.41107371
C	-1.46801369	3.91786363	-2.36027587
H	-1.91978597	4.60616834	-1.62755064
H	-0.41681692	3.79484979	-2.08459365
H	-1.50117366	4.43488899	-3.33032654
H	-3.17633525	2.59690642	-2.83856240
C	3.67076127	1.67469418	3.58303805
H	4.11117786	2.03906475	2.64893919
H	2.77778284	2.27985191	3.78371731
C	4.65811849	1.80458959	4.72152027
C	5.98837301	1.38659537	4.56221670
C	6.89881601	1.47597929	5.61467832
C	6.49550376	1.98902606	6.84988167
C	5.17784693	2.41366357	7.02134930
C	4.26905815	2.32085190	5.96499159
H	3.24596904	2.66419748	6.10371578
H	4.85530138	2.82088654	7.97604012
H	7.20496528	2.06125359	7.66977715
H	7.92540699	1.14977447	5.46937596
H	6.31507605	0.99688116	3.60013571
C	1.14175316	1.45370681	-4.43570359
O	1.93658918	0.97950210	-3.31566845
C	2.11803990	-0.45435861	-3.41827013
C	0.96469438	-0.93517015	-4.29279961
C	0.83174239	0.22066925	-5.29786054
H	1.57121971	0.11304764	-6.10013791
H	-0.15837912	0.28116061	-5.75928906
H	1.17007730	-1.89925229	-4.76809266
H	0.05690268	-1.03268124	-3.68777948
H	3.09123731	-0.65818442	-3.88690814
H	2.11779636	-0.85349621	-2.40218681
H	0.23149695	1.90794444	-4.03120215
H	1.71591346	2.21701138	-4.97188621
C	3.33690469	3.84742829	-1.63469747
O	2.02129225	3.43205460	-1.21381021
C	1.73963404	3.95739229	0.11175529
C	2.98495760	4.75387242	0.52955013
C	4.09188749	4.13353731	-0.33941457
H	4.94985199	4.79693988	-0.48579188
H	4.44255409	3.19300630	0.10002037
H	2.86266578	5.81661990	0.28976768
H	3.18472499	4.67299703	1.60206695
H	0.83289920	4.56704427	0.05731129
H	1.55027018	3.10248872	0.76833571
H	3.76040022	3.03947385	-2.23603430
H	3.24969793	4.74879272	-2.25838352

Table 35. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with two THF isomer

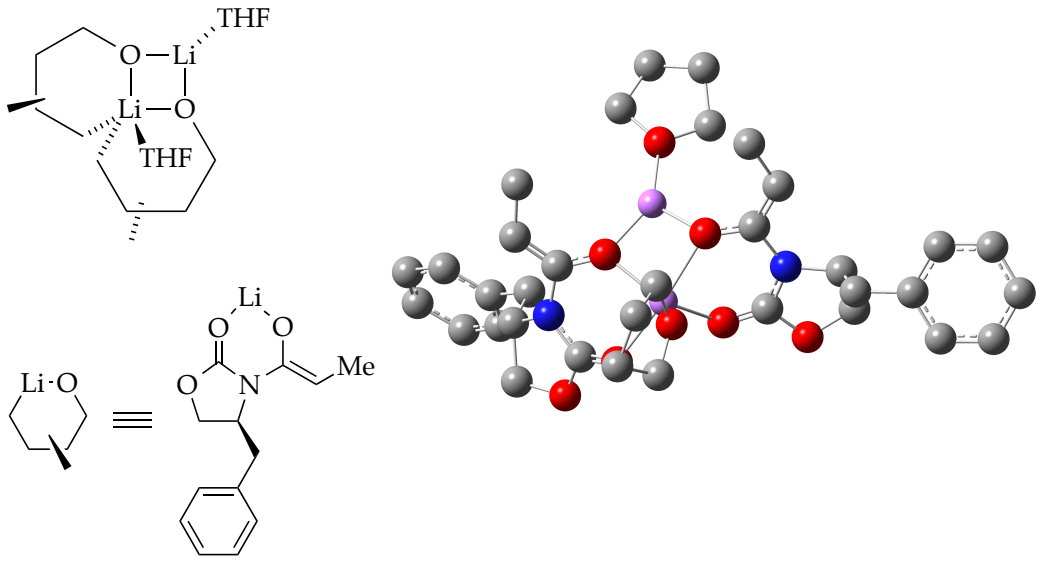


G = -2048.023225 Hartree
G_{MP2} = -1281086.402 kcal/mol
ΔG_{MP2} = 2.163553926 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.02343338	-0.76505956	-1.91714880
O	0.00000000	0.00000000	1.91862420	N	-2.50701820	0.60600477	-1.73338174
C	1.09275453	0.00000000	2.47370464	C	-3.91524618	1.00154200	-1.86962360
O	1.24927809	0.60988408	3.68155922	C	-3.77759626	2.53123740	-1.82392320
C	2.55467968	0.29585299	4.19663437	H	-3.71433802	2.97000525	-2.82633070
H	2.45307460	-0.51327012	4.92884815	H	-4.57429000	3.02391678	-1.26411179
H	2.95482555	1.18247805	4.69129861	O	-2.53108401	2.76405919	-1.14560711
C	3.36469494	-0.13845082	2.96484984	C	-1.77318164	1.63385729	-1.21183939
H	3.99855516	-0.99187895	3.21494558	O	-0.60832682	1.64958300	-0.82690270
N	2.27685043	-0.54400070	2.06449559	H	-4.31123963	0.69030390	-2.83878969
C	2.49787380	-1.21262757	0.77990720	C	-4.78742697	0.40456475	-0.73993411
C	3.54832363	-2.07437749	0.71685953	H	-4.61316015	-0.67699926	-0.73825356
H	4.10432095	-2.29589344	1.62214764	H	-4.42785385	0.79398038	0.22029794
C	4.00954006	-2.74858459	-0.54325132	C	-6.25911977	0.70548535	-0.91571029
H	3.46785124	-2.37210704	-1.41555548	C	-6.89977525	1.68168319	-0.14073173
H	3.86855884	-3.84086042	-0.51555301	C	-8.25216475	1.97547532	-0.32891985
H	5.08259451	-2.58318594	-0.72218690	C	-8.98763681	1.29520517	-1.29971445
O	1.67891324	-0.88018089	-0.17346067	C	-8.36333256	0.31632918	-2.07667222
Li	0.75702020	-1.81591107	-1.58566120	C	-7.01321997	0.02522671	-1.88439010
O	-0.96920526	-1.07835612	-1.22862586	H	-6.53760144	-0.74782886	-2.48472287

H	-8.93058508	-0.22552940	-2.82913270	C	1.69345103	1.04651074	-3.90084941
H	-10.04048024	1.52065893	-1.44671034	C	0.96481420	0.34273916	-5.05979039
H	-8.73018113	2.73284919	0.28692778	C	0.67018805	-1.05922381	-4.49164349
H	-6.33661190	2.20745733	0.62751333	H	0.88017786	-1.85581753	-5.21485257
C	-2.72944196	-1.56186219	-2.76490574	H	-0.36060868	-1.15781193	-4.13908281
C	-2.42272993	-3.01693719	-2.98145308	H	1.62052167	0.27450863	-5.93558730
H	-1.58323183	-3.33660275	-2.35735518	H	0.05085176	0.85959519	-5.36701774
H	-3.28445083	-3.65762801	-2.73885439	H	2.35509987	1.85062007	-4.23807066
H	-2.16120815	-3.23852407	-4.02837325	H	0.98064391	1.46227084	-3.18061717
H	-3.56795188	-1.14810195	-3.31497264	H	2.69051379	0.02821123	-2.20687759
O	0.76784189	-3.78433097	-1.38566858	H	3.36977307	-0.35109497	-3.82189007
C	0.40236445	-4.27043885	-0.07049658	C	4.23302618	0.97989405	2.34248417
C	0.33599840	-5.79057382	-0.21361131	H	4.56060487	0.61985566	1.36090051
C	1.43432942	-6.05936791	-1.25512418	H	3.60044362	1.85984023	2.17359880
C	1.29523927	-4.85567164	-2.19397338	C	5.42582204	1.34204183	3.19911028
H	0.58698076	-5.05541755	-3.00842535	C	6.53346067	0.48351260	3.27478081
H	2.24613941	-4.52989226	-2.62602730	C	7.62565335	0.79241661	4.08482060
H	1.31379244	-7.01227672	-1.77928307	C	7.63141238	1.97042389	4.83581779
H	2.42009556	-6.05696244	-0.77557950	C	6.53942215	2.83580825	4.76671366
H	-0.64294892	-6.09703361	-0.60071622	C	5.44701545	2.52186140	3.95511797
H	0.50537739	-6.30760374	0.73563940	H	4.60445745	3.20779899	3.89734341
H	1.17443247	-3.95636940	0.64246900	H	6.53705101	3.75871513	5.34084076
H	-0.54734211	-3.80219567	0.20000689	H	8.48330751	2.21332857	5.46524022
O	1.54093430	-1.23135114	-3.34180368	H	8.47581030	0.11631285	4.12586915
C	2.45317306	-0.11149046	-3.26265637	H	6.54151720	-0.43012825	2.68364610

Table 36. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer trans with two THF

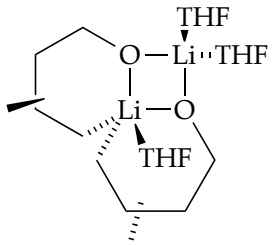


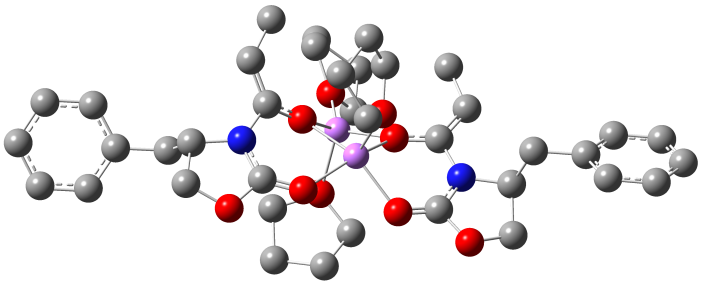
G = -2048.016706 Hartree
G_{MP2} = -1281080.017 kcal/mol
ΔG_{MP2} = 5.355753957 kcal/mol Li vs. **5** spirocyclic dimer with three THF

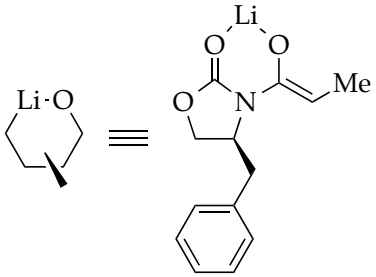
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.09763975	2.16355520	-2.90543720
Li	0.00000000	0.00000000	2.63048850	H	8.40275767	2.97837866	-3.28012117
O	1.43067082	0.00000000	1.52819888	H	10.09629211	2.81461334	-1.46423555
C	2.63862969	0.46689047	1.53439309	H	9.45700041	1.82170722	0.72635727
N	2.89013112	1.53213980	0.57511335	H	7.15210701	1.00881891	1.09674796
C	1.94999408	2.07618534	-0.26528132	C	3.66133730	0.06607244	2.34322836
O	0.77753636	1.78617716	-0.43764247	H	4.63126677	0.54565609	2.27988423
O	2.51856100	3.08900067	-0.98819034	C	3.52061909	-1.06955598	3.31889441
C	3.83030671	3.35488389	-0.46793255	H	4.32615936	-1.80945023	3.20285409
H	3.77083994	4.20799893	0.21861877	H	3.55448814	-0.74540140	4.37252400
H	4.49014384	3.60602027	-1.30011436	H	2.56959561	-1.59071895	3.16705641
C	4.22068675	2.05916429	0.25531595	O	-1.31549075	-0.42814885	1.47565498
H	4.77147415	2.28345484	1.17220736	C	-2.57108934	-0.75350046	1.38850354
C	5.03444777	1.07613349	-0.62321645	N	-3.30942195	-0.08179707	0.32398879
H	5.03113916	0.10606192	-0.11518506	C	-4.64410456	0.49546492	0.49490984
H	4.50224919	0.94620717	-1.57339851	C	-4.94262730	0.92155303	-0.95405729
C	6.45142087	1.54257429	-0.87248881	H	-5.52233108	0.16255254	-1.49191697
C	7.41984682	1.45145158	0.13933117	H	-5.45343251	1.88338700	-1.02860330
C	8.72138614	1.90642615	-0.06945847	O	-3.65321215	1.03890780	-1.57871324
C	9.08158641	2.46232842	-1.29936863	C	-2.74127345	0.33375812	-0.84552081
C	8.13136799	2.55496718	-2.31651809	O	-1.60952594	0.14184257	-1.26232091
C	6.82890308	2.09865112	-2.10246626	H	-5.35718122	-0.26666019	0.82042744

C	-4.64154656	1.65677415	1.51728025
H	-4.18894088	1.26876953	2.43728483
H	-3.98670890	2.45185509	1.14084183
C	-6.02611276	2.19506484	1.80062006
C	-6.45843709	3.41527090	1.26376439
C	-7.74899418	3.89053278	1.50746933
C	-8.63101422	3.14977098	2.29460732
C	-8.21263176	1.93317415	2.83919831
C	-6.92291713	1.46309123	2.59433598
H	-6.60101038	0.51954411	3.03082226
H	-8.89034828	1.35246127	3.45976793
H	-9.63501719	3.51848487	2.48681473
H	-8.06205228	4.84157957	1.08445176
H	-5.77300493	4.00458234	0.65826759
C	-3.26739678	-1.61645675	2.17144835
C	-2.66739336	-2.35535561	3.33283132
H	-2.87153962	-3.43409610	3.27634588
H	-1.57856086	-2.23359333	3.35398658
H	-3.05919341	-2.01827671	4.30657071
H	-4.30632242	-1.82183982	1.93101271
O	0.03555860	0.77747213	4.39387688
C	-0.90619139	0.64513357	5.48686300
C	-0.33138059	1.47367515	6.64833113
C	1.15973581	1.59009626	6.28667510
C	1.10213228	1.68155001	4.76544921
H	2.00599121	1.35596886	4.24479793
H	0.84404541	2.69806492	4.43548583
H	1.70592134	0.68947351	6.59014993
H	1.64528737	2.45743817	6.74369143
H	-0.50426581	0.99835005	7.61810730
H	-0.79222292	2.46750647	6.67522367
H	-1.88762005	0.99740455	5.15330248
H	-0.98200686	-0.41958840	5.73110420
O	0.90614935	-1.51861945	-1.04563279
C	1.17152339	-2.70447016	-0.25896934
C	1.06501395	-3.88916165	-1.22821216
C	0.10280466	-3.35140627	-2.29934351
C	0.53006278	-1.88682286	-2.38814124
H	-0.26147899	-1.20641562	-2.70544159
H	1.40029565	-1.76756620	-3.05018547
H	-0.93515124	-3.42128337	-1.95291368
H	0.18161069	-3.87461523	-3.25766260
H	0.70437456	-4.79737229	-0.73535141
H	2.04169230	-4.11266913	-1.67455701
H	2.15670208	-2.60120836	0.20414874
H	0.41820269	-2.75848496	0.53550613

Table 37. Geometric coordinates and thermally corrected MP2 energies for **5** spirocyclic dimer with three THF





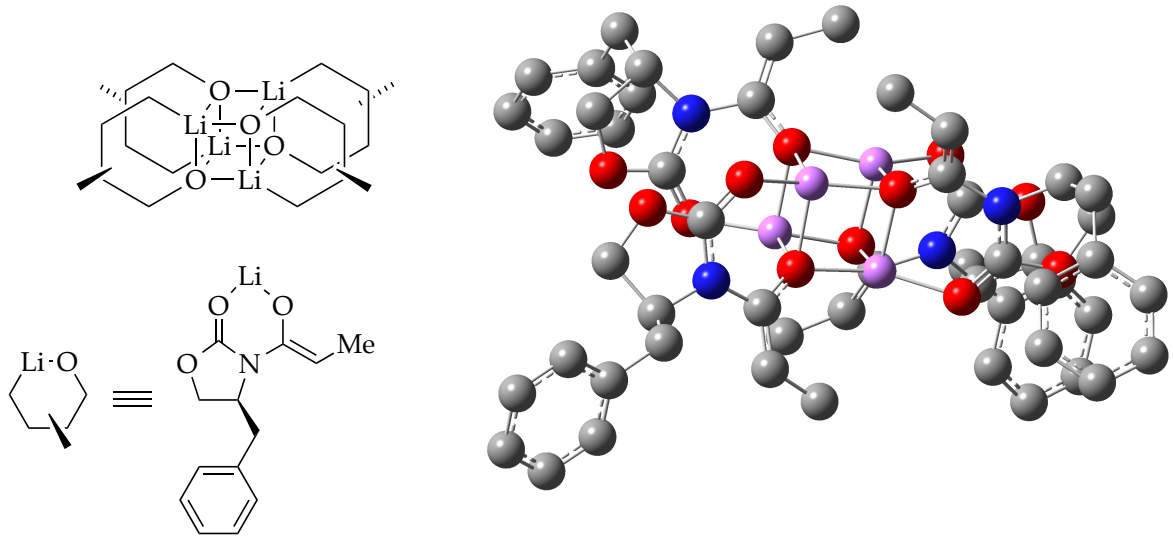


G = - 2280.364091 Hartree
G_{MP2} = - 1426403.019 kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	10.20173676	-0.42171454	5.18406992
Li	0.00000000	0.00000000	2.64675340	H	9.57085847	0.21525196	2.86257466
O	1.42158727	0.00000000	1.22252404	H	7.19038623	0.45962248	2.24437674
C	2.70017616	-0.07916138	1.40962945	C	3.68347372	0.54005379	0.69736431
N	3.10345919	-0.95148272	2.51077992	H	4.72451744	0.37921376	0.95129433
C	2.24401552	-1.59208037	3.36604910	C	3.40445209	1.47805017	-0.44200456
O	1.02776929	-1.53558835	3.45652268	H	3.75304414	2.50246430	-0.23523650
O	2.95882065	-2.39081439	4.21870318	H	3.90707471	1.16684569	-1.37206797
C	4.32759506	-2.42201987	3.78251697	H	2.33134404	1.53059606	-0.64603361
H	4.48391403	-3.32016850	3.17279330	O	-1.25466153	0.77082323	1.15133164
H	4.97166502	-2.46372992	4.66237868	C	-2.33903443	1.40665717	1.45839205
C	4.48596158	-1.13545883	2.96439887	N	-3.27833763	0.65456561	2.29930224
H	5.14564339	-1.29616799	2.10814527	C	-4.73077112	0.64653867	2.11514336
C	4.98459092	0.06752915	3.80594591	C	-5.15945031	-0.19230477	3.33455295
H	4.81620975	0.97388572	3.21573878	H	-5.46704343	0.43695706	4.17750621
H	4.35267569	0.14276369	4.69925115	H	-5.95582010	-0.90507751	3.11186467
C	6.43976478	-0.04987625	4.20176893	O	-3.98265630	-0.92407155	3.71747341
C	7.45608840	0.16992794	3.25907166	C	-2.88523435	-0.30024934	3.18921826
C	8.79973480	0.03606866	3.60749060	O	-1.75637968	-0.61489450	3.53628732
C	9.15487827	-0.31987133	4.91080470	H	-5.13504286	1.65956339	2.19261179
C	8.15613350	-0.53668423	5.86036806	C	-5.14236853	0.04544446	0.75033303
C	6.81188336	-0.40240949	5.50642505	H	-4.57047773	0.57672072	-0.01918190
H	6.03960493	-0.56195990	6.25609898	H	-4.83084267	-1.00595533	0.72401781
H	8.42103710	-0.80659621	6.87943467	C	-6.62556416	0.16297190	0.47851334

C	-7.47800246	-0.94331326	0.59278459
C	-8.85096762	-0.81906738	0.36880409
C	-9.39471475	0.41901075	0.02600697
C	-8.55630339	1.52988565	-0.09550580
C	-7.18599739	1.40099612	0.12789485
H	-6.53770853	2.26833267	0.02029446
H	-8.96986830	2.49680664	-0.37034986
H	-10.46236076	0.51786082	-0.15067490
H	-9.49325448	-1.69130201	0.45869457
H	-7.06051600	-1.91499147	0.84860301
C	-2.72074104	2.66317182	1.10517845
C	-1.91011929	3.55844301	0.21332943
H	-1.68514161	4.52274127	0.69339912
H	-0.95638209	3.08635815	-0.04003593
H	-2.42612375	3.79961309	-0.73005537
H	-3.64979027	3.06163447	1.50268644
O	0.56543717	1.56534458	3.82778622
C	0.81848338	2.80623787	3.12105374
C	0.19293384	3.92431721	3.97287657
C	-0.83394886	3.16523622	4.83023380
C	-0.11190468	1.84035697	5.06675306
H	-0.76883216	0.99278082	5.27297151
H	0.62610727	1.92902097	5.87845697
H	-1.75134312	2.99488354	4.25567237
H	-1.09103855	3.68309251	5.75993680
H	-0.25934893	4.70673045	3.35625016
H	0.94884927	4.39480471	4.61322193
H	1.89953055	2.92034042	2.98818019
H	0.35016021	2.71692712	2.13801124
O	-0.47667988	-1.98146162	-0.35773118
C	-1.88852367	-2.30284384	-0.34434523
C	-2.03521251	-3.60983883	0.45533688
C	-0.73445918	-3.66009543	1.27479345
C	0.26292025	-3.02676331	0.30947420
H	0.61977938	-3.75107342	-0.43864421
H	1.11486739	-2.55160894	0.79620809
H	-0.45154159	-4.67669763	1.56574388
H	-0.81418570	-3.04994509	2.17958617
H	-2.09680523	-4.47023546	-0.22172596
H	-2.93235790	-3.61166843	1.08185553
H	-2.40341643	-1.46224768	0.12998612
H	-2.24101976	-2.39757185	-1.37842868
O	0.21839509	0.51320090	-1.92850377
C	-0.06066991	1.75496831	-2.60661915
C	0.27203018	1.49708002	-4.07594739
C	1.45504793	0.52320790	-3.96030531
C	1.05687665	-0.33279684	-2.75343972
H	1.90973550	-0.66075765	-2.15252042
H	0.47144132	-1.21172592	-3.04508163
H	2.37968865	1.07287969	-3.75018783
H	1.61358423	-0.07716333	-4.86120721
H	0.51685549	2.41594037	-4.61724649
H	-0.57435396	1.01711052	-4.58180258
H	-1.10637647	2.01280937	-2.42293687
H	0.57588163	2.54552465	-2.18653644

Table 38. Geometric coordinates and thermally corrected MP2 energies for **5** D_{2d} tetramer

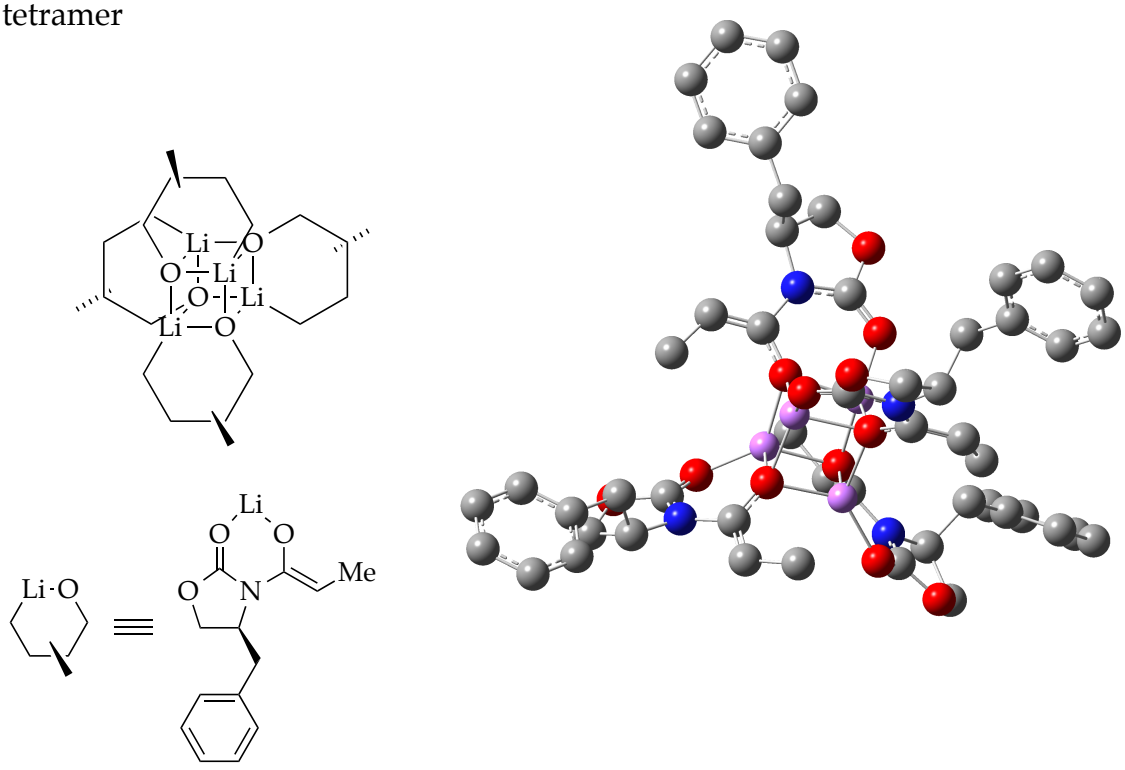


G = -3166.662534 Hartree
G_{MP2} = -1980930.794 kcal/mol
ΔG_{MP2} = 0.375561044 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.26428982	1.99018207	-6.10391756
O	0.00000000	0.00000000	1.89861070	H	-1.29118253	3.78066966	-6.22229477
C	1.05585130	0.00000000	2.52402978	C	-1.92064642	2.98500716	-4.25853369
O	1.12651741	-0.59231240	3.74489124	H	-2.82262435	2.37091814	-4.30870624
C	2.50137875	-0.59782195	4.18227305	N	-0.95399263	2.35428375	-3.34779468
H	2.91749791	-1.59017164	3.98345487	C	-1.30389776	1.62759451	-2.14149057
H	2.50872415	-0.39220160	5.25391674	C	-2.51844401	1.82556346	-1.57783798
C	3.17781310	0.49877718	3.34189588	H	-3.18305215	2.57926802	-1.98217944
H	4.16626791	0.18314087	2.99581318	C	-2.99438943	1.06416526	-0.37019718
N	2.26657711	0.53607049	2.19012104	H	-2.59131260	0.04451436	-0.34260460
C	2.64016857	0.95192206	0.85098338	H	-2.71374752	1.54719054	0.57873746
C	3.69779669	1.77859681	0.67780146	H	-4.08745118	0.97571288	-0.36893686
H	4.21004590	2.18878057	1.53828089	O	-0.38806896	0.77865933	-1.73170696
C	4.20137889	2.17854646	-0.68327539	Li	-0.01973221	-1.03106286	-2.49492021
H	3.67767766	3.05574343	-1.09407348	O	-0.29270694	-1.07497797	-4.37329619
H	5.26669231	2.43481941	-0.64615718	C	0.60921506	-0.76095601	-5.14394454
H	4.09136604	1.36805456	-1.41464629	O	0.31566577	-0.20466281	-6.34840040
O	1.91456735	0.42211923	-0.10906251	C	1.54258265	0.21819224	-6.97883753
Li	1.55502468	0.97865032	-1.93350744	H	1.65326183	1.29511017	-6.81933748
O	1.39380755	2.30442534	-3.29685634	H	1.45933624	0.00014348	-8.04479982
C	0.30965783	2.50810502	-3.83698836	C	2.64015445	-0.59357477	-6.26983272
O	0.25857136	2.98092212	-5.11391698	H	3.52025717	0.02194645	-6.06248136
C	-1.11762441	2.92962831	-5.56274456	N	1.96141851	-0.88569767	-5.00006409

C	2.63442461	-1.13326491	-3.73847330
C	3.91025443	-1.58519171	-3.73829876
H	4.39538785	-1.83534211	-4.67272286
C	4.70369053	-1.77659578	-2.47342918
H	4.54491543	-2.76383502	-2.01229470
H	5.77877359	-1.68808094	-2.66917762
H	4.45237947	-1.02447135	-1.71511423
O	1.92589375	-0.83362023	-2.67215027
Li	2.02399625	-1.43203668	-0.82819381
O	2.48122320	-2.71027372	0.51335988
C	1.60387382	-3.22923745	1.19859453
O	1.88658772	-3.66540840	2.45817005
C	0.64238730	-4.03523705	3.10095144
H	0.28979213	-3.17627251	3.67956500
H	0.83916284	-4.88287767	3.75835927
C	-0.28210093	-4.36744056	1.92457225
H	-1.31338985	-4.06383030	2.11811287
N	0.29868188	-3.48779868	0.89960133
C	-0.42951179	-2.93396175	-0.22670589
C	-1.58962902	-3.51306422	-0.61497172
C	-2.44650780	-2.96492025	-1.72406874
H	-2.39445369	-1.87080114	-1.78073969
H	-2.16391030	-3.35247264	-2.71528466
H	-3.50018829	-3.22708096	-1.57058009
H	-1.92146240	-4.42685102	-0.13735196
O	0.10745189	-1.85154012	-0.74380530
C	-0.21934411	-5.86457803	1.52546649
H	-0.67956097	-5.98204870	0.53947201
H	0.83546271	-6.14444563	1.41482335
C	-0.89574915	-6.76737888	2.53527464
C	-0.14783387	-7.58159975	3.39621336
C	-0.77562379	-8.39588797	4.34147672
C	-2.16692970	-8.40718045	4.44117447
C	-2.92556148	-7.60256720	3.58762981
C	-2.29466474	-6.79220938	2.64443602
H	-2.89585652	-6.17648166	1.97840309
H	-4.01039066	-7.60954720	3.65349266
H	-2.65798285	-9.04089709	5.17467872
H	-0.17618863	-9.02312141	4.99610882
H	0.93731670	-7.58697907	3.31700307
C	3.08848239	-1.84352170	-7.07867600
H	3.52522479	-1.46694662	-8.01314308
H	3.90061567	-2.33790231	-6.53813405
C	1.99971230	-2.84876529	-7.38587567
C	1.39296970	-2.89817868	-8.64807137
C	0.38241242	-3.82094751	-8.92323591
C	-0.03606692	-4.71354003	-7.93611004
C	0.56816950	-4.68316579	-6.67737120
C	1.57967297	-3.76167261	-6.40590449
H	2.05355824	-3.75092519	-5.42748951
H	0.25589155	-5.38118221	-5.90519611
H	-0.82240822	-5.43314494	-8.14759130
H	-0.07362597	-3.84413160	-9.90958802
H	1.72300798	-2.21555350	-9.42887887
C	-2.27063653	4.43620771	-3.83881216
H	-2.59797238	4.42768235	-2.79451128
H	-1.35105396	5.03309284	-3.87459170
C	-3.33214590	5.05957908	-4.72022930
C	-4.66965354	4.64507999	-4.62662679
C	-5.65006310	5.19637888	-5.45075399
C	-5.31053114	6.17692870	-6.38600986
C	-3.98574503	6.60169457	-6.48757954
C	-3.00673072	6.04574187	-5.66104625
H	-1.97767295	6.39055064	-5.73850614
H	-3.71196117	7.36883396	-7.20718153
H	-6.07446573	6.60887797	-7.02677761
H	-6.68075303	4.86372387	-5.35985339
H	-4.94703174	3.88859036	-3.89523453
C	3.32644400	1.84430271	4.10679056
H	3.98833360	1.64375929	4.95970592
H	3.85779343	2.55437463	3.46677069
C	2.03507475	2.46758824	4.59071825
C	1.63137114	2.35463825	5.92787246
C	0.43453407	2.92317978	6.36694327
C	-0.37837431	3.61838011	5.47132229
C	0.01754474	3.74871394	4.13839016
C	1.21540686	3.18176551	3.70287015
H	1.52311115	3.29660402	2.66647921
H	-0.60412635	4.29701291	3.43561711
H	-1.31053469	4.06221548	5.81040796
H	0.14086640	2.82589022	7.40890901
H	2.26617602	1.82667188	6.63698233

Table 39. Geometric coordinates and thermally corrected MP2 energies for **5** S_4 tetramer

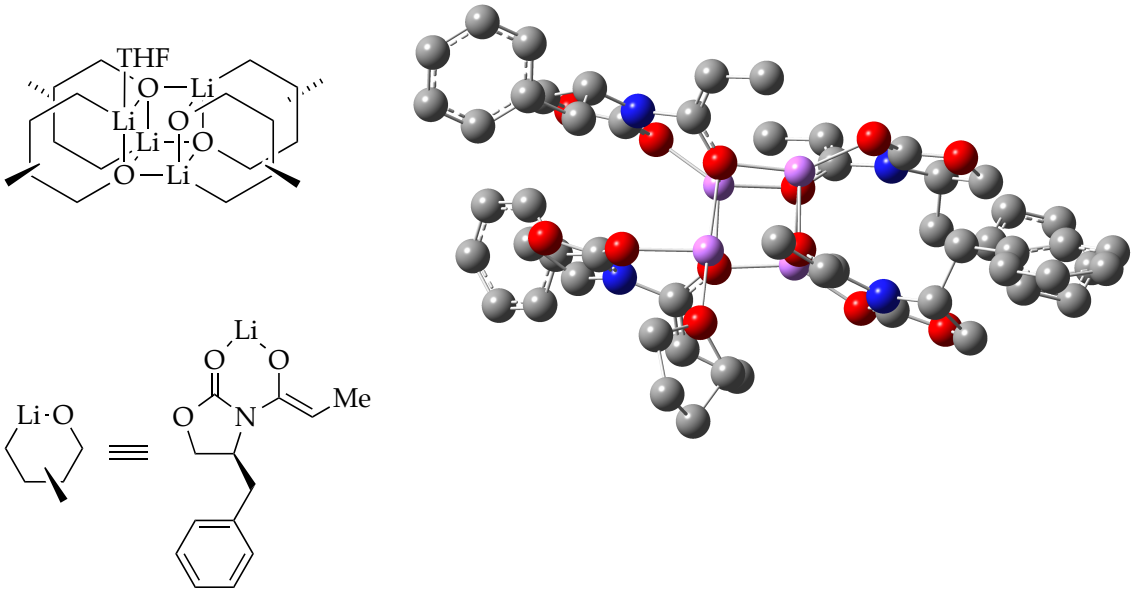


G = - 3166.66637 Hartree
G_{MP2} = -1980924.053 kcal/mol
ΔG_{MP2} = 2.060914038 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	Li	-6.08024768	-0.33358165	-1.75858171
H	0.00000000	0.00000000	1.09545220	O	-7.18504687	-0.53093955	-0.23339699
H	1.02940245	0.00000000	-0.36155046	C	-7.86452798	0.40186683	0.18511489
C	-0.85358200	-1.14028366	-0.58071920	O	-8.96551594	0.15902924	0.94358691
H	-0.99117400	-1.92370996	0.16798276	C	-9.44592336	1.40412810	1.48387871
N	-2.11755103	-0.42884150	-0.81837010	H	-9.09878617	1.48615128	2.51963196
C	-1.92354790	0.92138729	-0.80196390	H	-10.53676351	1.38962556	1.46823563
O	-0.64201997	1.20691152	-0.45183666	C	-8.83430757	2.48721961	0.57893825
O	-2.71197332	1.82843814	-1.05221038	H	-8.47615380	3.32278477	1.18457669
Li	-4.24039960	1.53089789	-2.12975726	N	-7.70217586	1.74461473	0.00704132
O	-4.12947756	-0.42356407	-2.01640366	C	-6.65814419	2.36831676	-0.79028964
C	-3.35272068	-1.09771088	-1.19483725	O	-6.17334715	1.62505593	-1.76257427
C	-3.58574006	-2.33924197	-0.71197270	Li	-6.37919715	1.46176276	-3.68871290
H	-2.90648903	-2.76141619	0.02119815	O	-6.85557812	2.77549953	-4.93471900
C	-4.78251431	-3.16188089	-1.10491242	C	-6.04459983	3.32709732	-5.67199006
H	-5.62800790	-3.03845102	-0.41179186	O	-6.47707039	4.26537336	-6.55624420
H	-5.13915771	-2.89213943	-2.10633590	C	-5.33436454	4.91181100	-7.14416487
H	-4.53634441	-4.23100042	-1.12216654	H	-5.14541115	5.84505539	-6.60178122

H	-5.56181642	5.13558281	-8.18724113
C	-4.20022829	3.89662159	-6.96702583
H	-3.26537404	4.40746276	-6.72678704
N	-4.69122053	3.15864337	-5.79160781
C	-3.84785057	2.28026495	-4.99329293
O	-4.48019396	1.55050226	-4.10168505
Li	-4.54607395	-0.40739784	-3.91517633
O	-4.47279337	-1.81631146	-5.14601389
C	-5.46871862	-2.41164983	-5.54504032
O	-5.32712324	-3.41865953	-6.44791670
C	-6.58920907	-4.09338187	-6.59353030
H	-6.58524464	-4.98100690	-5.95093198
H	-6.70108377	-4.39740309	-7.63510066
C	-7.62117671	-3.05405978	-6.14287501
H	-8.42553852	-3.53406877	-5.58143379
N	-6.79227132	-2.23619947	-5.24213779
C	-7.35008585	-1.29032425	-4.28595020
O	-6.47688147	-0.50365855	-3.69768749
C	-8.68962156	-1.29217933	-4.07691819
H	-9.31774094	-2.00780700	-4.59297540
C	-9.38665076	-0.35319348	-3.13292598
H	-8.72097912	0.44868780	-2.79964055
H	-10.25748170	0.11680432	-3.61088737
H	-9.75388025	-0.86595909	-2.23141700
C	-8.20664497	-2.21643042	-7.30664954
H	-8.71929823	-1.35344385	-6.86952107
H	-7.37188889	-1.82855937	-7.90330938
C	-9.15221575	-3.01041265	-8.18127328
C	-10.44698229	-3.31607752	-7.73479886
H	-10.78052641	-2.94733858	-6.76687654
C	-11.31648153	-4.07211920	-8.52015497
H	-12.31673576	-4.29387201	-8.15734458
C	-10.90669693	-4.53669234	-9.77214591
C	-9.62438710	-4.23584275	-10.23177430
C	-8.75642273	-3.47939412	-9.44123182
H	-7.76259155	-3.23820664	-9.81287481
H	-9.29836617	-4.58529812	-11.20792416
H	-11.58452435	-5.12338746	-10.38622502
C	-2.51118158	2.28145896	-5.21992913
H	-2.08756119	2.94878514	-5.96033062
C	-1.53972390	1.40734166	-4.47772865
H	-2.05576138	0.64035666	-3.89235789
H	-0.85894272	0.89288512	-5.17022559
H	-0.91268496	1.98150836	-3.77939976
C	-4.00326064	2.96715149	-8.19016038
H	-3.36804649	2.13315679	-7.87457087
H	-4.97920116	2.54586537	-8.46094090
C	-3.39312863	3.68187551	-9.37607191
C	-4.17326036	4.05993362	-10.47723228
H	-5.23059705	3.80364708	-10.49586884
C	-3.60965066	4.74447917	-11.55624892
H	-4.23227030	5.02376569	-12.40219256
C	-2.25157533	5.06335513	-11.55023574
C	-1.46074938	4.68892493	-10.46137135
C	-2.02746148	4.00441367	-9.38680348
H	-1.40007239	3.70519091	-8.54958060
H	-0.39987965	4.92509396	-10.45166294
H	-1.81034251	5.59415784	-12.38947096
C	-6.29943984	3.63965040	-0.50064109
H	-6.71663244	4.12387998	0.37606905
C	-5.29890252	4.41585459	-1.31295061
H	-4.27592916	4.33432987	-0.91622528
H	-5.27467565	4.06754762	-2.35261410
H	-5.55083264	5.48361148	-1.33132770
C	-9.78605657	3.02008279	-0.51726444
H	-9.17756208	3.59784607	-1.22195347
H	-10.19909086	2.16641196	-1.06780431
C	-10.89863653	3.87676640	0.04573207
C	-10.63543140	5.18371764	0.48382881
H	-9.63101118	5.58936182	0.38017454
C	-11.64526978	5.97182233	1.03465190
H	-11.42175686	6.98342657	1.36343061
C	-12.94190866	5.46640524	1.15626546
C	-13.21948944	4.17092514	0.71946421
C	-12.20472562	3.38447916	0.16956955
H	-12.43230364	2.37992908	-0.18103266
H	-14.22694277	3.77137947	0.80154873
H	-13.73031342	6.08082200	1.58256673
C	-0.29177331	-1.76534169	-1.87883656
H	-1.08511123	-2.38677852	-2.30906107
H	-0.08487279	-0.96041387	-2.59418737
C	0.95220182	-2.59099055	-1.63484050
C	0.85728366	-3.85812758	-1.03928670
H	-0.12321517	-4.25807082	-0.78865415
C	1.99912437	-4.61505227	-0.77938114
H	1.90361911	-5.59637007	-0.32189761
C	3.26124070	-4.11785664	-1.11309685
C	3.37034293	-2.86223909	-1.71112160
C	2.22414474	-2.10683535	-1.96846409
H	2.31667492	-1.13423757	-2.44734382
H	4.34695827	-2.47002957	-1.98265494
H	4.15150830	-4.70821329	-0.91378454

Table 40. Geometric coordinates and thermally corrected MP2 energies for **5** D_{2d} tetramer with one THF

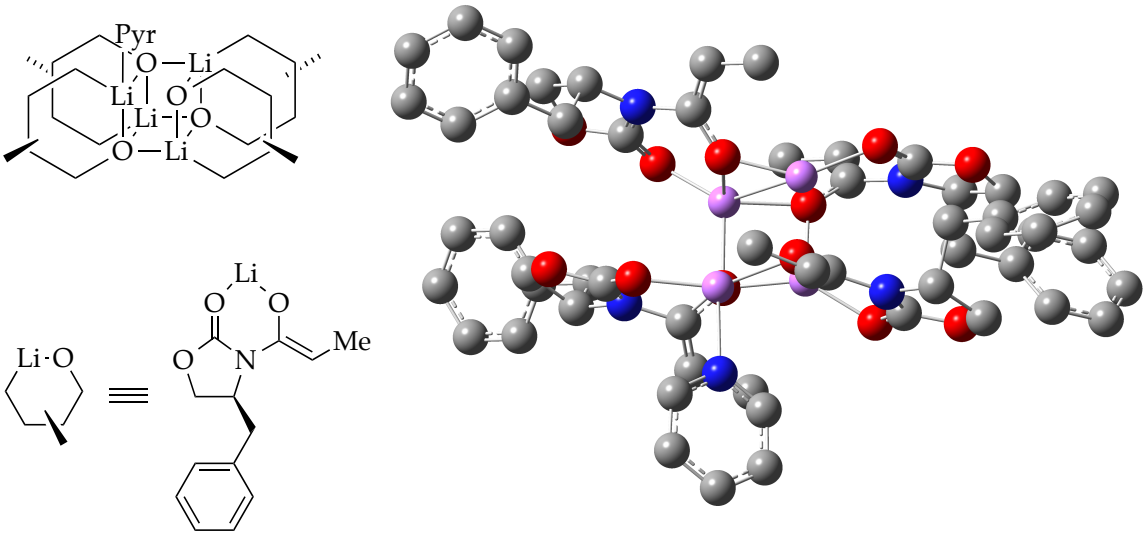


G = -3399.01452 Hartree
G_{MP2} = -2126253.179 kcal/mol
ΔG_{MP2} = -2.148099694 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-5.63036611	2.28873669	2.48291072
Li	0.00000000	0.00000000	2.73154670	C	-6.34514490	1.73226371	3.60255504
O	2.07881221	0.00000000	2.76560556	H	-7.37396998	1.53839137	3.29613405
C	2.72496736	0.72180885	2.01580723	H	-6.34140182	2.47045674	4.41204035
O	4.03478483	0.46077342	1.75053272	C	-5.56795218	0.45708472	3.96972267
C	4.50875161	1.36504314	0.72954873	N	-4.26040084	0.75004329	3.35569038
H	4.63721890	0.78956781	-0.19076588	C	-3.07519606	-0.09002879	3.54900856
H	5.47238027	1.76544979	1.04935389	O	-2.17621677	-0.01710421	2.60159350
C	3.41433787	2.44788571	0.58663850	Li	-2.08766237	-1.20230465	1.03939044
N	2.32037779	1.83625754	1.35047463	O	-3.83222521	-1.75848754	0.38502665
C	0.97254944	2.37368842	1.45608980	C	-4.49867208	-0.92925447	-0.22902539
C	0.84389441	3.71204078	1.60680139	O	-5.85638533	-0.91082824	-0.13251324
H	1.75122098	4.29800436	1.72920333	C	-6.36096590	0.25960957	-0.81033563
C	-0.45794729	4.46231211	1.60558134	H	-6.64856599	0.99445253	-0.05130710
H	-0.72601158	4.84110819	2.60369814	H	-7.24031236	-0.03049698	-1.38684121
H	-0.41170041	5.33811398	0.94371275	C	-5.19344348	0.77062837	-1.67921834
H	-1.29166057	3.84122069	1.26507697	N	-4.07115491	0.05556771	-1.05955319
O	0.02407663	1.46852557	1.35313362	C	-2.66751789	0.25927485	-1.37892669
Li	-1.90306781	1.37383436	1.27832316	C	-2.33069475	0.47268145	-2.66904254
O	-3.52300525	2.27803840	1.72635271	H	-3.10412965	0.38261546	-3.42674469
C	-4.36288144	1.78334179	2.47534698	C	-0.93601223	0.80140295	-3.12383028

H	-0.35015685	-0.09231056	-3.38375073
H	-0.95342778	1.44414888	-4.01276120
H	-0.37659356	1.33330696	-2.34496533
O	-1.87455831	0.24771531	-0.33048378
C	-5.03130860	2.30208238	-1.64922751
H	-4.81226670	2.60332485	-0.61902139
H	-4.15444636	2.56007723	-2.25257093
C	-6.26302405	3.01899819	-2.16074352
C	-6.57765610	3.02596774	-3.52827494
C	-7.72611455	3.66431208	-3.99610823
C	-8.58141976	4.31286936	-3.10230827
C	-8.27721087	4.31939555	-1.74054940
C	-7.12791496	3.67700865	-1.27498757
H	-6.88906774	3.69385528	-0.21374237
H	-8.93169730	4.82920634	-1.03812431
H	-9.47414166	4.81438761	-3.46637829
H	-7.94997382	3.66166670	-5.05981305
H	-5.90995467	2.53646336	-4.23453901
H	-5.31809821	0.43743582	-2.71875485
O	-0.19169042	-1.52872183	1.23483659
C	0.43663839	-2.64608542	0.94717560
N	1.82392001	-2.48106259	0.52997527
C	2.23246277	-1.53460567	-0.34726006
O	1.57126455	-0.64930363	-0.89235558
O	3.56094653	-1.65152938	-0.60050229
C	4.12835574	-2.64138481	0.28427509
H	4.72182514	-2.11410311	1.03573434
H	4.77499901	-3.29419697	-0.30402666
C	2.92338102	-3.37564540	0.91370290
H	2.78467411	-4.35640944	0.44028396
C	3.04475093	-3.55886065	2.43846083
C	4.20943623	-4.44900320	2.81725713
C	5.38040405	-3.91096754	3.36842961
C	6.46357806	-4.73061849	3.69300049
C	6.39302682	-6.10599122	3.46968445
C	5.23057342	-6.65672535	2.92498897
C	4.15036766	-5.83502801	2.60428751
H	3.24378291	-6.27440126	2.19306929
H	5.16282756	-7.72835177	2.75592114
H	7.23411169	-6.74569348	3.72338274
H	7.36059387	-4.29340207	4.12403458
H	5.43785975	-2.84081548	3.55453026
H	2.10177487	-3.98587885	2.79645064
H	3.14506209	-2.56713062	2.89261892
C	-0.04638822	-3.90747019	1.02040920
C	-1.42587627	-4.25058978	1.51098092
H	-2.16057604	-4.33568038	0.69664672
H	-1.42824662	-5.21058106	2.04283138
H	-1.80481439	-3.49489262	2.20872303
H	0.58282946	-4.72438785	0.67893129
C	-3.04060018	-0.87137059	4.65696272
H	-3.84004417	-0.79679063	5.38594764
C	-1.95906705	-1.87110076	4.94954673
H	-2.37857896	-2.86962742	5.13988371
H	-1.26287955	-1.96228239	4.11133395
H	-1.37217835	-1.60293173	5.84017019
C	-6.20149252	-0.84751445	3.43351000
H	-6.36241684	-0.75128929	2.35452656
H	-5.47058213	-1.65052655	3.57134286
C	-7.49796883	-1.18108737	4.13921849
C	-8.73521524	-1.01511224	3.50230582
C	-9.93077949	-1.29673974	4.16725490
C	-9.90777334	-1.74992189	5.48635470
C	-8.68189393	-1.92559503	6.13275275
C	-7.49092876	-1.64458495	5.46413202
H	-6.54068730	-1.79916930	5.97148819
H	-8.65338789	-2.28853041	7.15695964
H	-10.83633350	-1.97151430	6.00551576
H	-10.87861267	-1.16614986	3.65150456
H	-8.76066846	-0.67715210	2.46855770
H	-5.46274888	0.39062678	5.05536057
C	3.03679021	2.74389669	-0.87744514
H	2.70567681	1.80748904	-1.33974065
H	2.18008283	3.42685605	-0.86991298
C	4.18657699	3.34635538	-1.65728323
C	4.58422628	4.67428660	-1.43803107
C	5.65748588	5.22631645	-2.13687140
C	6.35359408	4.45865188	-3.07356870
C	5.96533845	3.13898408	-3.30630821
C	4.89158938	2.58897722	-2.60277499
H	4.58743303	1.56301260	-2.79783772
H	6.49455937	2.53575124	-4.03945762
H	7.18736473	4.88896477	-3.62189110
H	5.94617449	6.25854240	-1.95579164
H	4.03836601	5.28507959	-0.72162548
H	3.73317188	3.37967761	1.07252450
O	0.04190953	0.75659509	4.65626579
C	1.00575978	0.43079599	5.67628466
H	0.92843760	-0.64036959	5.88619581
H	2.01291093	0.63883762	5.29649260
C	0.65018497	1.31707699	6.87086654
H	-0.14419418	0.85415303	7.46854426
H	1.50701438	1.50235542	7.52613468
C	0.12804864	2.58294896	6.17425522
C	-0.61869521	2.00420187	4.96784063
H	-0.57239496	2.64681031	4.08440018
H	-1.66708170	1.78352323	5.19965878
H	0.96672358	3.20665473	5.84277815
H	-0.51859627	3.19520832	6.81045341

Table 41. Geometric coordinates and thermally corrected MP2 energies for **5** D_{2d} tetramer 1 pyridine

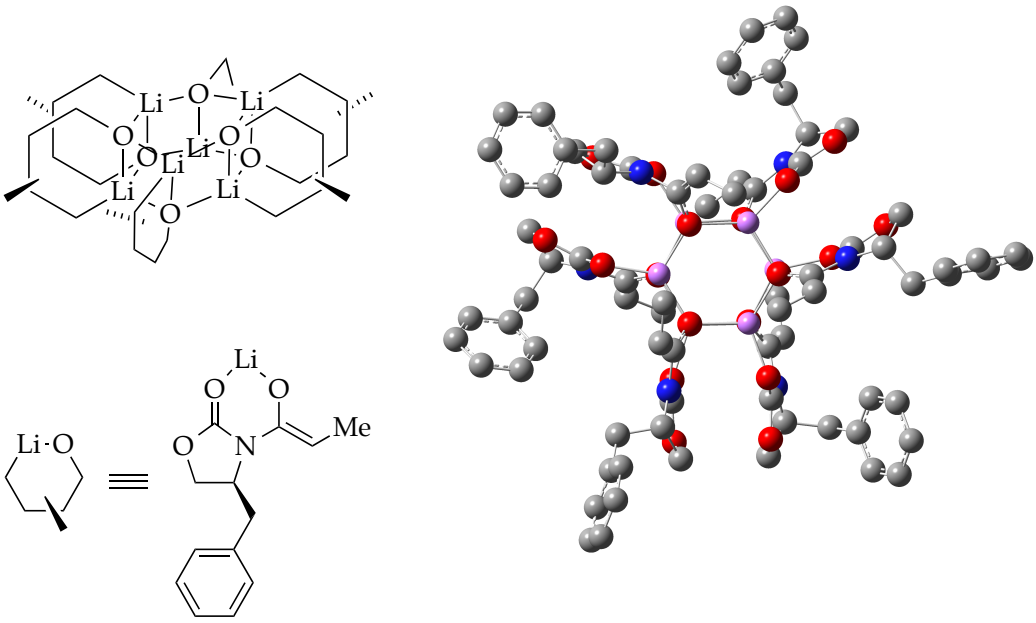


G = -3414.881206 Hartree
G_{MP2} = -2136193.804 kcal/mol
ΔG_{MP2} = -2.338561749 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-7.06176862	-1.05802231	3.60412764
Li	0.00000000	0.00000000	3.05734620	H	-6.45399628	-0.09239081	4.97166948
O	1.96747092	0.00000000	3.03044663	C	-5.00384188	-1.57967664	4.22277030
C	2.57488810	0.80625885	2.33047955	N	-3.89189931	-0.80115973	3.65128901
O	3.91359876	0.68434761	2.13628182	C	-2.50314443	-1.24482277	3.67085732
C	4.34795165	1.67490571	1.17770175	O	-1.76104653	-0.79588638	2.68327490
H	4.53761309	1.16393206	0.23055609	Li	-1.70765001	-1.70832491	0.88299419
H	5.27090694	2.12405505	1.54720121	O	-3.45462526	-2.40967589	0.37639176
C	3.18114997	2.67854470	1.06243181	C	-4.30675164	-1.64268784	-0.06400284
N	2.09617004	1.89721511	1.67392974	O	-5.63252828	-1.88536725	0.13389854
C	0.69510501	2.28186244	1.70375889	C	-6.39688589	-0.75488797	-0.33814043
C	0.38916477	3.59157016	1.83473182	H	-6.75176324	-0.19841610	0.53481276
H	1.19864906	4.29681969	2.00149934	H	-7.25094298	-1.13117227	-0.90306708
C	-1.01022759	4.13699739	1.78215731	C	-5.41719162	0.08264218	-1.18781319
H	-1.42925580	4.32445487	2.78251505	N	-4.13606746	-0.49715681	-0.76911575
H	-1.04532427	5.09147635	1.24122082	C	-2.82173093	0.00054106	-1.15219213
H	-1.69058486	3.44689525	1.27121668	C	-2.65047848	0.42374287	-2.42313747
O	-0.13572218	1.26932460	1.56554666	H	-3.46558266	0.28067827	-3.12754394
Li	-2.01709633	0.81292114	1.57596764	C	-1.38570254	1.05309336	-2.93557234
O	-3.71150600	1.18968665	2.42148104	H	-0.72245026	0.32833142	-3.43003706
C	-4.33955744	0.31673691	3.02138903	H	-1.60487695	1.83862243	-3.67020289
O	-5.69343746	0.41097086	3.12200874	H	-0.80895532	1.51120715	-2.12446743
C	-6.17583021	-0.59219926	4.03838184	O	-1.95033147	0.00991585	-0.16957961

C	-5.51386749	1.59662118	-0.92057187
H	-5.28165802	1.77390652	0.13564007
H	-4.73424261	2.09038502	-1.51050607
C	-6.87912180	2.15305256	-1.26537089
C	-7.27229417	2.31839592	-2.60225545
C	-8.53959957	2.80543973	-2.92157948
C	-9.43866376	3.14049942	-1.90637242
C	-9.05871059	2.98705154	-0.57270156
C	-7.78978814	2.49708350	-0.25670273
H	-7.49497300	2.39039953	0.78502035
H	-9.74776132	3.25333303	0.22473910
H	-10.42482000	3.52395624	-2.15422652
H	-8.82314407	2.92995859	-3.96351614
H	-6.57396916	2.07403262	-3.40023858
H	-5.58015657	-0.10756975	-2.25734228
O	0.14425872	-1.83120577	0.57739005
C	0.91655827	-2.73399547	0.04863147
N	2.19485276	-2.23623845	-0.46645668
C	2.40035854	-0.97734225	-0.92158318
O	1.60066469	-0.05539353	-1.08144705
O	3.72120184	-0.78733518	-1.21746342
C	4.40310738	-2.05543824	-1.12325650
H	5.37954151	-1.88985860	-0.66543405
H	4.53709370	-2.44697482	-2.13742953
C	3.47127165	-2.93972689	-0.27643728
H	3.41792192	-3.94399433	-0.70339115
C	3.85472805	-3.03681744	1.21841167
C	5.14242479	-3.79928743	1.43819766
C	6.32217085	-3.13369134	1.79848798
C	7.51747335	-3.83453340	1.97393145
C	7.55202646	-5.21702963	1.78982201
C	6.38251951	-5.89427880	1.43574399
C	5.19072426	-5.19094045	1.26329809
H	4.28124427	-5.72788964	1.00119566
H	6.39753523	-6.97267851	1.29991090
H	8.48061402	-5.76462593	1.92728773
H	8.41977879	-3.29952566	2.25907399
H	6.29672903	-2.05776956	1.95798740
H	3.02086841	-3.53163363	1.72877579
H	3.93242420	-2.02522048	1.63224211
C	0.69697810	-4.06878098	-0.03656021
C	-0.52691521	-4.72710292	0.53771562
H	-1.38218013	-4.73209149	-0.15542850
H	-0.32523808	-5.77245917	0.80282570
H	-0.86209585	-4.21914000	1.45154219
H	1.40628466	-4.69155258	-0.57201881
C	-2.11131917	-2.08179918	4.65966019
H	-2.80900765	-2.33415240	5.45151048
C	-0.73630251	-2.68475490	4.73523093
H	-0.78414985	-3.74907113	5.00122017
H	-0.21509606	-2.61087328	3.77463779
H	-0.10359254	-2.19956824	5.49428726
C	-5.20672222	-2.94349518	3.52594930
H	-5.40452067	-2.77414664	2.46341393
H	-4.26163502	-3.49231609	3.59102682
C	-6.33014333	-3.74017175	4.15373462
C	-7.54623051	-3.92179915	3.48087019
C	-8.59266233	-4.63727410	4.06720099
C	-8.43924395	-5.18353659	5.34162553
C	-7.23085411	-5.01539194	6.02211391
C	-6.18792855	-4.30203107	5.43203025
H	-5.24528168	-4.19134728	5.96449415
H	-7.09822379	-5.44680424	7.01099915
H	-9.25118125	-5.74221949	5.79940285
H	-9.52495367	-4.77134589	3.52465137
H	-7.66436204	-3.51218670	2.48009717
H	-4.82667706	-1.74260036	5.28977626
C	2.89232131	3.11100420	-0.38762646
H	2.61693504	2.21945707	-0.95976999
H	2.02003948	3.77271748	-0.37702517
C	4.07936267	3.80783445	-1.01919820
C	4.40396244	5.12949181	-0.67755325
C	5.51161716	5.76435545	-1.23924268
C	6.31608438	5.08704773	-2.15847258
C	6.00174232	3.77420404	-2.51176888
C	4.89298586	3.14093561	-1.94629989
H	4.64738307	2.12024268	-2.23103216
H	6.61658255	3.24168409	-3.23292009
H	7.17686177	5.58192899	-2.60036470
H	5.74297980	6.79047315	-0.96485721
H	3.77462330	5.67026459	0.02668461
H	3.38290577	3.56929712	1.67401556
N	-0.20921402	1.01504616	4.93927061
C	-1.29807492	1.73839202	5.24266074
H	-2.09107252	1.74162653	4.49947891
C	-1.42780607	2.45772206	6.42989056
H	-2.32944124	3.03146740	6.62124958
C	-0.38148486	2.42118295	7.35084439
C	0.75365349	1.67194297	7.04444675
C	0.79631543	0.99150320	5.82775214
H	1.66624186	0.40927469	5.53614954
H	1.59499446	1.61544547	7.72835181
H	-0.44828045	2.96823646	8.28755211

Table 42. Geometric coordinates and thermally corrected MP2 energies for **5** hexamer



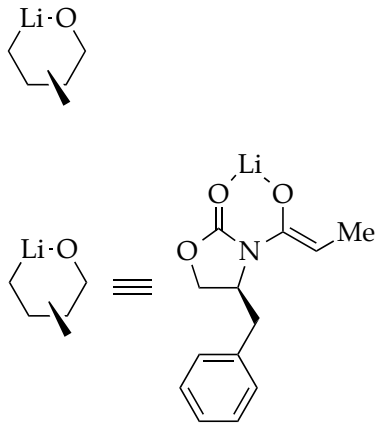
G = -4749.986807 Hartree
G_{MP2} = -2971414.86 kcal/mol
ΔG_{MP2} = -2.735898515 kcal/mol Li vs. **5** spirocyclic dimer with three THF

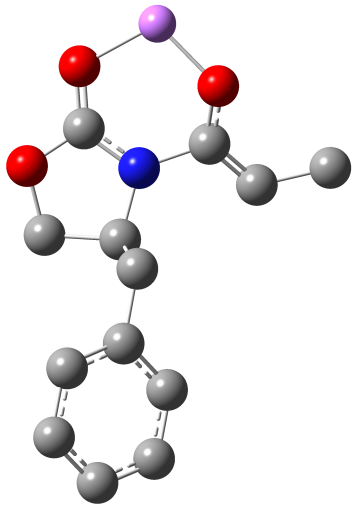
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	0.36159619	5.48288395	-1.41053305
O	0.00000000	0.00000000	1.91383380	C	-1.01399171	5.87040688	-1.63926229
C	1.02658669	0.00000000	2.58753598	H	-1.20917188	5.80796285	-2.71312398
O	0.99089934	-0.42959575	3.87686383	H	-1.14143554	6.89429807	-1.28586302
C	2.34094063	-0.51115690	4.37604326	C	-1.81200647	4.83798982	-0.83693342
H	2.67123224	-1.55130792	4.29790588	H	-2.74388022	4.56791380	-1.33871304
H	2.32914672	-0.19237805	5.41933476	N	-0.88091382	3.70096737	-0.89646097
C	3.14096643	0.42258204	3.45597227	C	-1.27574256	2.30814313	-0.79349364
H	4.11666635	-0.00532353	3.20926739	C	-2.49814426	2.01566723	-0.28779291
N	2.29288256	0.38348297	2.25445409	H	-3.12820894	2.81898520	0.07466458
C	2.76251888	0.66116617	0.90609503	C	-3.05700436	0.62632032	-0.16175071
C	3.94636659	1.30177390	0.75445529	H	-2.41794709	-0.11857422	-0.64465610
H	4.49393378	1.61807621	1.63270337	H	-3.17291404	0.32971017	0.89149180
C	4.57289291	1.64450750	-0.56688848	H	-4.05111470	0.54793131	-0.62348312
H	4.64309714	2.73264120	-0.70755212	O	-0.38768698	1.44333219	-1.24788352
H	5.59443184	1.24691798	-0.64586094	Li	-0.15515047	1.13950931	-3.19584372
H	4.00768571	1.24215067	-1.41097227	O	-0.39014394	2.79673943	-4.11625529
O	1.97528127	0.22576418	-0.06185575	C	0.54506604	3.54830204	-4.36948237
Li	1.57887192	1.65980822	-1.36004135	O	0.31756367	4.87685176	-4.55532319
O	1.45880387	3.55568679	-1.06152289	C	1.58553069	5.55759773	-4.64185087
C	0.38773692	4.15266625	-1.11388524	H	1.80948567	5.98470930	-3.65982384

H	1.48807027	6.34798668	-5.38775742
C	2.57881523	4.45547782	-5.03915022
H	3.52631136	4.56358006	-4.50390662
N	1.87487166	3.27570255	-4.51493945
C	2.52988847	2.04189148	-4.11200829
C	3.77819956	1.79422518	-4.57590433
H	4.23367405	2.49192610	-5.26701699
C	4.59953108	0.58599311	-4.22732821
H	4.76530317	-0.05682101	-5.10346368
H	5.59104493	0.86878363	-3.84637775
H	4.12608548	-0.02915037	-3.45831674
O	1.83398676	1.27836993	-3.28723193
Li	1.75432911	-0.58356078	-3.89020013
O	1.89121407	-1.26784856	-5.66969668
C	0.92706970	-1.75969982	-6.24712464
O	1.12176198	-2.66576003	-7.24709388
C	-0.15970107	-3.23431424	-7.60350448
H	-0.28542718	-4.16666290	-7.04607418
H	-0.15869145	-3.42938524	-8.67676032
C	-1.15989283	-2.15558374	-7.17604525
H	-2.08169302	-2.59190907	-6.78499075
N	-0.40729945	-1.53576815	-6.07592013
C	-1.01550038	-0.83271089	-4.96172376
C	-2.31263299	-0.45544754	-5.06425132
C	-3.07646987	0.24336599	-3.97591906
H	-2.52994475	0.23927816	-3.02898138
H	-3.28449585	1.29307979	-4.22973655
H	-4.04669779	-0.23870540	-3.79195697
H	-2.84779178	-0.63248842	-5.98942433
O	-0.23024163	-0.65579387	-3.91463471
C	-1.47045665	-1.14999522	-8.31579612
H	-1.95539740	-0.27133149	-7.87876242
H	-0.51578506	-0.80928249	-8.73575041
C	-2.33591297	-1.74392930	-9.40653850
C	-1.79821801	-2.08657752	-10.65442911
C	-2.59666547	-2.65434931	-11.64979380
C	-3.95062087	-2.89013015	-11.41074104
C	-4.50098193	-2.55116769	-10.17236338
C	-3.70046376	-1.98312920	-9.18206135
H	-4.14147553	-1.71378874	-8.22449760
H	-5.55631862	-2.72499120	-9.97912448
H	-4.57437352	-3.33033267	-12.18403420
H	-2.15984304	-2.90819762	-12.61212990
H	-0.74545150	-1.89592389	-10.85243238
C	2.87306370	4.42258749	-6.56596090
H	3.42110441	5.34676509	-6.79297172
H	3.55891711	3.59637857	-6.77267826
C	1.66363737	4.31160824	-7.46903823
C	1.14871296	5.43704327	-8.12688000
C	0.02773916	5.33743742	-8.95255013
C	-0.59660745	4.10340953	-9.13531325
C	-0.08679795	2.97169773	-8.49546579
C	1.03615140	3.07301820	-7.67391979
H	1.43327270	2.18451253	-7.18935602
H	-0.56136132	2.00474804	-8.63888012
H	-1.46981214	4.02170310	-9.77703346
H	-0.35350635	6.22271059	-9.45499752
H	1.63841977	6.40097603	-8.00157255
C	-2.08908402	5.30688990	0.61578987
H	-2.40768199	4.44290944	1.20728989
H	-1.14147824	5.65428707	1.04631881
C	-3.12637784	6.40739082	0.68752988
C	-4.48230042	6.12501497	0.46117742
C	-5.44122994	7.13656799	0.50087703
C	-5.06147202	8.45355412	0.77059737
C	-3.71793426	8.74845570	1.00226649
C	-2.76062757	7.73240723	0.96005324
H	-1.71618171	7.96893361	1.15246310
H	-3.41236179	9.76857509	1.21971299
H	-5.80862030	9.24186619	0.80399533
H	-6.48651812	6.89594714	0.32555509
H	-4.79094906	5.10131230	0.25922629
C	3.35880615	1.83722302	4.06348253
H	4.03967885	1.70336855	4.91452203
H	3.89082722	2.45338105	3.33382069
C	2.11066377	2.56130131	4.52060295
C	1.28231371	3.21523616	3.59540878
C	0.12761004	3.87494850	4.01731460
C	-0.21495058	3.90175623	5.37078492
C	0.60807439	3.26791450	6.30192226
C	1.76080374	2.60552739	5.87721530
H	2.40591932	2.12753018	6.61208136
H	0.35733755	3.29211464	7.35926723
H	-1.11300139	4.41939207	5.69721826
H	-0.50337457	4.37288271	3.28615183
H	1.54797582	3.21232418	2.54114961
Li	0.12464572	-2.14380758	-2.64959758
O	0.19841623	-3.72845966	-3.71769720
C	1.23909551	-4.24228097	-4.11122203
O	1.19847949	-5.16499360	-5.11062578
C	2.54573368	-5.47911515	-5.50943031
H	2.77964544	-4.90005259	-6.40839104
H	2.58968935	-6.54783299	-5.72562617
C	3.40668694	-5.05859214	-4.30893772
H	4.32724226	-4.57165380	-4.64269977
N	2.52758594	-4.04923439	-3.70289266
C	2.99045972	-2.98511611	-2.83178506
C	4.26323045	-3.03196883	-2.36994859
H	4.89638363	-3.86862973	-2.63599987
C	4.87866350	-2.00710106	-1.46109112
H	5.12023564	-2.43420024	-0.47704838
H	5.81606229	-1.60900538	-1.87444760
H	4.21594038	-1.15462892	-1.29322121
O	2.10444500	-2.03531380	-2.58350955
Li	1.86489626	-1.66081036	-0.70527645
O	2.06796317	-3.07784090	0.61166404

C	1.14031780	-3.22175817	1.40469904
O	1.38052038	-3.34600823	2.73634538
C	0.13059150	-3.58084503	3.41634300
H	0.12442243	-2.99497754	4.33439705
H	0.06738061	-4.64911420	3.65504762
C	-0.95389175	-3.15126489	2.41593564
H	-1.20576749	-2.09439682	2.56179946
N	-0.19553882	-3.27021084	1.14628769
C	-0.72696377	-2.86698535	-0.15455496
C	-1.74857895	-3.59709072	-0.65517286
H	-2.02209196	-4.50632475	-0.13145088
C	-2.51673917	-3.26563481	-1.90362275
H	-2.24794081	-3.92297408	-2.74108371
H	-3.59716036	-3.37657726	-1.73927005
H	-2.34456485	-2.23301338	-2.22527260
O	-0.15457980	-1.80936330	-0.71181744
C	-2.23023698	-3.99888072	2.52425211
H	-2.92803190	-3.67420465	1.74683043
H	-1.98487585	-5.04904381	2.32307438
C	-2.87569426	-3.86559379	3.89059683
C	-3.52686833	-2.67812867	4.25799268
C	-4.10752996	-2.54135217	5.51839509
C	-4.05113224	-3.59324839	6.43587760
C	-3.41132776	-4.78115577	6.08184199
C	-2.82867190	-4.91330340	4.81944771
H	-2.34025485	-5.84673215	4.54769569
H	-3.36742764	-5.60861960	6.78532938
H	-4.50668391	-3.48822980	7.41689454
H	-4.60817367	-1.61363857	5.78277878
H	-3.58413089	-1.85635263	3.54749884
C	3.77987444	-6.23877855	-3.36793283
H	4.43049132	-6.90574989	-3.94918806
H	4.38642969	-5.84634101	-2.54711839
C	2.61339752	-7.02036801	-2.80348277
C	2.23536001	-8.25267138	-3.35397662
C	1.15033773	-8.96607088	-2.84229568
C	0.42426991	-8.45505424	-1.76602492
C	0.79785419	-7.23426927	-1.20003484
C	1.88651957	-6.52538365	-1.70920057
H	2.17549114	-5.58323373	-1.25005608
H	0.24358564	-6.82794034	-0.35832637
H	-0.42249097	-9.00713356	-1.36675152
H	0.87549952	-9.92101303	-3.28296172
H	2.80429504	-8.66573477	-4.18497023

Table 43. Geometric coordinates and thermally corrected MP2 energies for **5** monomer with no THF

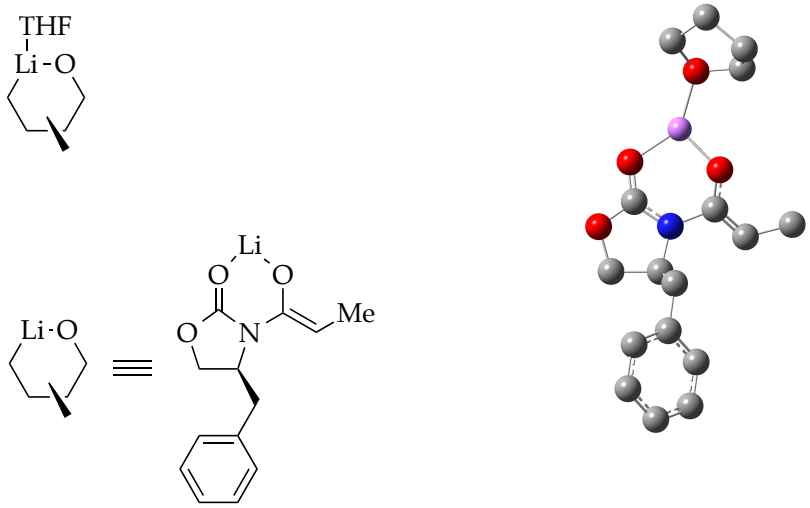




G = -791.626405 Hartree
G_{MP2} = -495177.2338 kcal/mol
ΔG_{MP2} = 55.84024071 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	2.20195589	-2.09667712	-2.00789260
H	0.00000000	0.00000000	1.09522300	H	2.29732397	-1.11536793	-2.46829647
H	1.02888286	0.00000000	-0.36285900	H	4.32232685	-2.47320896	-2.04572825
C	-0.85989390	-1.13278175	-0.58448864	H	4.11978511	-4.73089164	-1.02021858
H	-0.99621882	-1.92407742	0.15562016	H	1.87083625	-5.61597362	-0.42857983
N	-2.12615868	-0.41786311	-0.80753267	H	-0.15118001	-4.25529866	-0.85320184
C	-1.91615814	0.92010477	-0.80171682				
O	-0.64090962	1.21220808	-0.44880084				
O	-2.70046398	1.84505961	-1.06270013				
Li	-4.19521848	1.33738395	-1.97511019				
O	-4.14225086	-0.39370968	-2.01268292				
C	-3.38220253	-1.08526978	-1.22459252				
C	-3.58552869	-2.34384488	-0.76161231				
H	-2.88344697	-2.78088152	-0.05865091				
C	-4.78951069	-3.15569871	-1.14474376				
H	-5.38185919	-2.62374376	-1.89443332				
H	-4.51125914	-4.13421085	-1.56347574				
H	-5.44464616	-3.35917279	-0.28409724				
C	-0.31091992	-1.74201426	-1.89510186				
H	-1.11446594	-2.34909777	-2.32614477				
H	-0.10253972	-0.92685006	-2.59910966				
C	0.92940374	-2.57930886	-1.67444289				
C	0.83022395	-3.85735277	-1.10325806				
C	1.96917276	-4.62642741	-0.86727286				
C	3.23204501	-4.13082027	-1.20080601				
C	3.34520026	-2.86426624	-1.77443243				

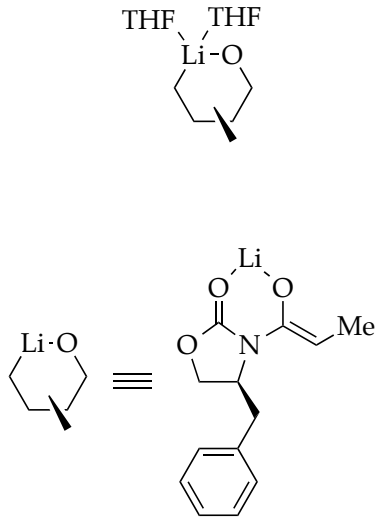
Table 44. Geometric coordinates and thermally corrected MP2 energies for **5** monomer with one THF

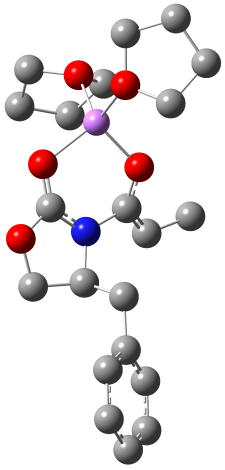


G = -1023.997533 Hartree
G_{MP2} = -640527.7041 kcal/mol
ΔG_{MP2} = 17.66023664 kcal/mol Li vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-7.23371222	3.43595423	-5.15993745
H	0.00000000	0.00000000	1.09560600	H	-5.79017263	4.20778178	-3.41982294
H	1.02978539	0.00000000	-0.36116898	H	-4.35829463	3.44230169	-4.14765575
C	-0.85634521	-1.13699797	-0.58130218	C	-0.30428854	-1.75038333	-1.88935602
H	-0.98895164	-1.92732524	0.16090767	H	-1.10943737	-2.35584958	-2.31984631
N	-2.12302697	-0.42821125	-0.80736568	H	-0.09180130	-0.93708412	-2.59424851
C	-1.92264561	0.91307394	-0.80217834	C	0.93203144	-2.59210988	-1.66529964
O	-0.64230888	1.20811414	-0.45132802	C	0.82688464	-3.86747877	-1.08880572
O	-2.70983118	1.83087324	-1.05597588	C	1.96185106	-4.64109054	-0.84847601
Li	-4.24845674	1.36237374	-1.98633705	C	3.22757575	-4.15325222	-1.18275691
O	-4.11734580	-0.40813458	-2.03901172	C	3.34697675	-2.88956159	-1.76144203
C	-3.37089249	-1.09761362	-1.24307013	C	2.20761354	-2.11748589	-1.99917054
C	-3.57123020	-2.36061732	-0.78383048	H	2.30853214	-1.13810540	-2.46250220
H	-2.87706792	-2.79229859	-0.06968281	H	4.32630799	-2.50383093	-2.03275099
C	-4.76379890	-3.18067890	-1.18482871	H	4.11236610	-4.75661447	-0.99836438
H	-5.34124176	-2.65578267	-1.95142015	H	1.85814605	-5.62820400	-0.40536180
H	-4.47567430	-4.16194680	-1.59139177	H	-0.15653535	-4.25951160	-0.83730516
H	-5.43974777	-3.38038295	-0.33896441				
O	-5.59227423	2.16669006	-3.08505826				
C	-5.42952621	3.31998586	-3.94874543				
C	-6.22539271	3.01183885	-5.22588906				
C	-6.29412293	1.47501737	-5.22404705				
C	-6.42684831	1.16945431	-3.73590578				
H	-6.05049981	0.19128672	-3.42866186				
H	-7.46061938	1.29467399	-3.38714627				
H	-5.36635512	1.04259931	-5.61621766				
H	-7.13013301	1.08221537	-5.81011618				
H	-5.74603805	3.42267193	-6.11906672				

Table 45. Geometric coordinates and thermally corrected MP2 energies for **5** monomer with two THF



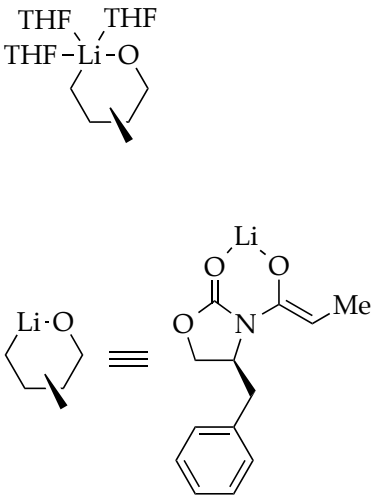


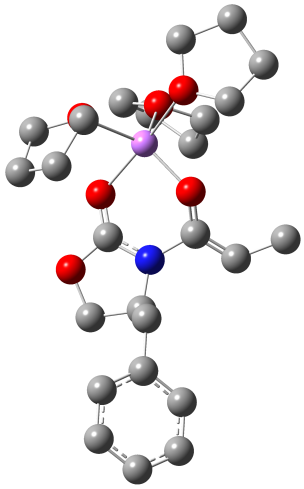
G = - 1256.35369 Hartree
G_{MP2} = - 785850.9491 kcal/mol
ΔG_{MP2} = 6.705758941 kcal/mol vs. **5** spirocyclic dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	3.23191972	-4.14942853	-1.18862772
H	0.00000000	0.00000000	1.09591670	C	3.34834282	-2.88375789	-1.76365751
H	1.03039198	0.00000000	-0.35988750	C	2.20708940	-2.11403361	-1.99978247
C	-0.85548735	-1.14040296	-0.57873722	H	2.30536927	-1.13303073	-2.46015724
H	-0.98374107	-1.93338445	0.16194467	H	4.32682134	-2.49474419	-2.03343954
N	-2.12155385	-0.43327616	-0.80001351	H	4.11819928	-4.75110581	-1.00574954
C	-1.92468851	0.90937628	-0.80761702	H	1.86617340	-5.63013797	-0.41592370
O	-0.64225263	1.20675652	-0.45352409	H	-0.15223295	-4.26450490	-0.84427621
O	-2.71813403	1.81422659	-1.06929285	C	-5.39356538	2.90253188	-4.50843032
Li	-4.22598888	1.36376188	-2.17654212	O	-4.35741118	2.00750838	-4.04039326
O	-4.02646528	-0.45852551	-2.16686227	C	-4.08295332	1.00489802	-5.04553468
C	-3.36269252	-1.09556148	-1.26535991	C	-5.38347536	0.89207005	-5.83603537
C	-3.63168630	-2.30730779	-0.70638681	C	-5.86052734	2.35460656	-5.86920881
H	-2.99562381	-2.68220567	0.09013946	H	-5.37137528	2.89342560	-6.68877056
C	-4.79669522	-3.15319056	-1.13540525	H	-6.94180988	2.45217990	-6.00456134
H	-5.28402529	-2.70791390	-2.00834354	H	-5.23839859	0.46529200	-6.83318888
H	-4.48938820	-4.17447701	-1.40721007	H	-6.09631945	0.26154051	-5.29225496
H	-5.55901876	-3.26013739	-0.34745711	H	-3.25431259	1.34817155	-5.68166082
C	-0.30566048	-1.75319124	-1.88814654	H	-3.79216470	0.09743187	-4.51265551
H	-1.11076229	-2.36174940	-2.31463758	H	-6.18899432	2.89968882	-3.75651043
H	-0.09818527	-0.94031143	-2.59488504	H	-4.98127085	3.91532256	-4.58077796
C	0.93261128	-2.59281683	-1.66755968	C	-6.68366416	0.83748089	-0.76200001
C	0.83050215	-3.87004374	-1.09470920	O	-5.90334689	1.95194338	-1.24276453
C	1.96735052	-4.64144175	-0.85615709	C	-5.80130139	2.87235589	-0.14278373

C	-5.62860532	1.99652152	1.10955690
C	-6.24226535	0.62847862	0.69802526
H	-5.49256763	-0.16532919	0.75236588
H	-7.08670600	0.34117756	1.33208269
H	-4.56734743	1.88601678	1.34687941
H	-6.12485353	2.43851491	1.97905856
H	-4.95429447	3.53104420	-0.34545860
H	-6.72246850	3.47174900	-0.09284268
H	-7.74999157	1.09723693	-0.83331256
H	-6.45948532	-0.01027718	-1.41054894

Table 46. Geometric coordinates and thermally corrected MP2 energies for **5** monomer with three THF



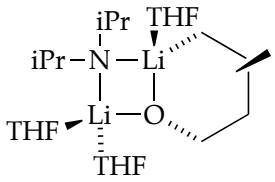


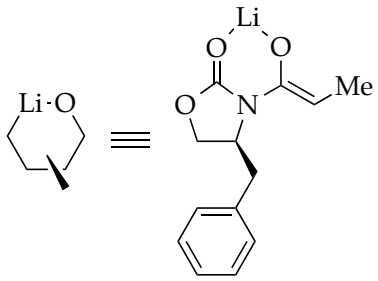
G = -1488.697668 Hartree
G_{MP2} = -931168.1672 kcal/mol
ΔG_{MP2} = 1.777728882 kcal/mol Li vs. **5** spirocyclic dimer with three THF

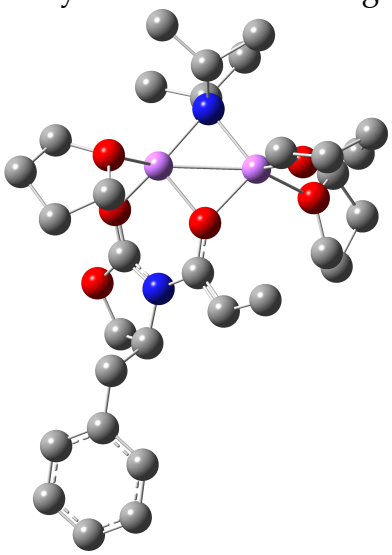
Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-6.80171037	2.60700094	-3.59975795
H	0.00000000	0.00000000	1.09594000	H	-6.31410918	2.67479076	-5.31025337
H	1.03066998	0.00000000	-0.35974383	O	-3.32136783	2.90205065	-3.76041224
C	-0.85316631	-1.14441615	-0.57725508	C	-2.85974559	2.47204057	-5.04842001
H	-0.98029291	-1.93649274	0.16534604	C	-1.34964607	2.25033660	-4.87083115
N	-2.11842155	-0.44096168	-0.80121795	C	-0.96978914	3.24248220	-3.73607744
C	-1.93456686	0.90087743	-0.80409189	C	-2.32693566	3.82694767	-3.29082687
O	-0.64453267	1.20553213	-0.45424963	H	-2.50912249	4.80845278	-3.75440419
O	-2.73602623	1.79426663	-1.06148375	H	-2.43639544	3.90177402	-2.21024045
C	-3.34485027	-1.08936684	-1.31776815	H	-0.29145113	4.02946614	-4.08072996
O	-3.94969478	-0.45044848	-2.25651827	H	-0.48651079	2.72260351	-2.90494278
Li	-4.21593375	1.39759846	-2.49053784	H	-0.79773129	2.43127560	-5.79860894
O	-5.57440760	1.08006719	-4.19391830	H	-1.15511072	1.21838809	-4.56204428
C	-6.63423766	2.00849569	-4.49905687	H	-3.43105001	1.58350758	-5.31587396
C	-7.86470437	1.16241863	-4.89526286	H	-3.05813696	3.26450037	-5.78780773
C	-7.48655499	-0.25387141	-4.42289714	O	-5.77654675	2.12760340	-1.31084364
C	-5.96920194	-0.24331523	-4.59354319	C	-5.55171938	3.20328131	-0.36813717
H	-5.69196602	-0.41288884	-5.64697535	C	-6.20389452	2.76558038	0.95139395
H	-5.42006442	-0.93340955	-3.95272046	C	-6.18305332	1.23294871	0.83754632
H	-7.97754996	-1.04411460	-4.99970343	C	-6.44674952	1.02758075	-0.65219153
H	-7.74046493	-0.39221189	-3.36576493	H	-7.52277834	1.07753907	-0.87734773
H	-8.00653569	1.17357414	-5.98212222	H	-6.02719185	0.10468583	-1.05784732
H	-8.78746392	1.53393194	-4.43899665	H	-6.92952530	0.74144810	1.46927937

H	-5.19541249	0.83775181	1.09814018
H	-7.23714986	3.12819324	1.01272392
H	-5.66267094	3.14306848	1.82431946
H	-4.47055600	3.33292473	-0.26424186
H	-5.98776997	4.12185564	-0.77686145
C	-3.65265587	-2.28855273	-0.75162469
H	-3.05586139	-2.64819289	0.08202871
C	-4.80763651	-3.13596707	-1.20166318
H	-5.28107373	-2.69786790	-2.08585431
H	-4.49742560	-4.15938598	-1.46344715
H	-5.58542299	-3.23902695	-0.42809985
C	-0.29872778	-1.76128376	-1.88291290
H	-1.10608630	-2.36181030	-2.31660968
H	-0.07845946	-0.95007159	-2.58790179
C	0.92905743	-2.61367528	-1.65328589
C	0.80857337	-3.88536082	-1.07149601
C	1.93417077	-4.67054093	-0.82518845
C	3.20612267	-4.19847288	-1.15865892
C	3.34091939	-2.93853995	-1.74203639
C	2.21070224	-2.15475958	-1.98548926
H	2.32357864	-1.17786268	-2.45129386
H	4.32519422	-2.56475485	-2.01236111
H	4.08366141	-4.81104786	-0.96983251
H	1.81846032	-5.65458290	-0.37810616
H	-0.17999370	-4.26448076	-0.82042804

Table 47. Geometric coordinates and thermally corrected MP2 energies for **5** LDA mixed dimer with three THF





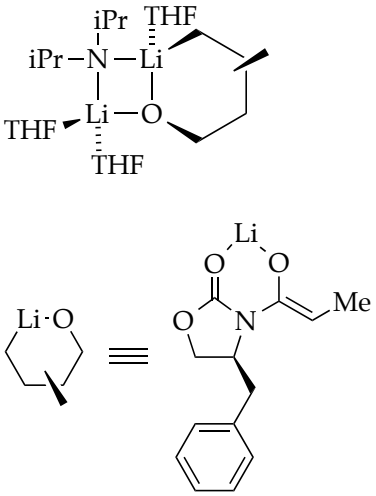


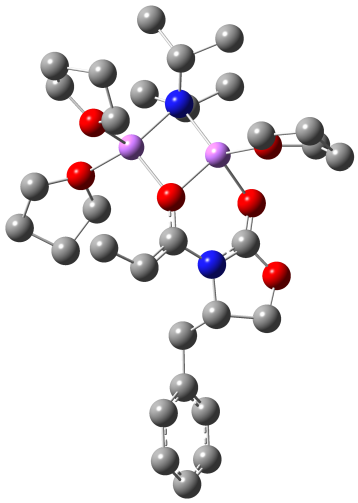
G = -1787.915892 Hartree
G_{MP2} = -1118227.787 kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.37823608	0.15904441	4.55541500
O	0.00000000	0.00000000	1.95527310	H	-5.00957212	-1.13231849	2.57142406
C	0.81677532	0.00000000	2.96012211	H	-3.68121045	-2.05630954	3.31902711
N	0.86336440	-1.25049413	3.72021522	N	-1.62880436	-1.15561486	-0.35706991
C	1.79873533	-1.52869629	4.81768955	C	-2.79402158	-0.45997865	-0.91510556
C	1.73906511	-3.05949988	4.82987813	H	-2.94590531	0.40138762	-0.24044276
H	2.47498393	-3.50931433	4.15309160	C	-2.60424514	0.17761214	-2.32042560
H	1.84234736	-3.49590858	5.82446021	H	-2.59045835	-0.56851309	-3.12149205
O	0.41878550	-3.35356258	4.33777452	H	-3.41988556	0.88159084	-2.54563655
C	-0.01030452	-2.29654314	3.58584778	H	-1.65758240	0.72808454	-2.35735951
O	-1.05352614	-2.38130518	2.95222075	C	-4.15093636	-1.20719898	-0.89977196
Li	-1.60196420	-1.01790348	1.65312489	H	-4.97307454	-0.52050149	-1.14664786
O	-3.17268196	-0.16877952	2.65474479	H	-4.18220751	-2.02305911	-1.63132648
C	-4.14611398	-1.06788624	3.24103793	H	-4.35095076	-1.63489513	0.08886877
C	-4.49450081	-0.48672830	4.61974407	C	-1.30184465	-2.51169766	-0.81578543
C	-3.24907053	0.35031306	4.95412108	H	-0.27908561	-2.69076714	-0.43384351
C	-2.86645497	0.89408490	3.57906752	C	-1.21224699	-2.74465874	-2.34488342
H	-1.80693666	1.13203475	3.46290128	H	-0.75201513	-3.71877729	-2.56400519
H	-3.46500004	1.78098483	3.32297081	H	-2.20243431	-2.74703528	-2.81543969
H	-2.44858932	-0.29022317	5.34201444	H	-0.61428407	-1.96586672	-2.83144184
H	-3.44178883	1.14227780	5.68457171	C	-2.13643300	-3.66823885	-0.19591145
H	-4.70210151	-1.26811167	5.35686772	H	-2.16431602	-3.57777562	0.89509827

H	-3.16684010	-3.68211951	-0.56560736
H	-1.68823204	-4.64366739	-0.43710313
H	2.79615785	-1.16844311	4.55482436
C	1.33464490	-0.89955373	6.15763737
H	1.13712428	0.16230775	5.98083211
H	0.37930906	-1.36155505	6.43642879
C	2.34315313	-1.07456927	7.27209315
C	3.51581682	-0.30401532	7.29926346
C	4.46504201	-0.47785123	8.30583652
C	4.25800259	-1.42742768	9.30920869
C	3.09455192	-2.19706269	9.29851281
C	2.14726157	-2.02041747	8.28760766
H	1.23707324	-2.61666664	8.29299534
H	2.91980715	-2.93331473	10.07868455
H	4.99570111	-1.56134536	10.09574262
H	5.36451024	0.13235824	8.31064683
H	3.68120297	0.44691548	6.52927166
C	1.64274449	1.01148344	3.35192052
H	2.27420385	0.89551893	4.22458771
C	1.70128412	2.33429163	2.63984709
H	1.21296861	2.27146624	1.66338001
H	1.20945069	3.14221604	3.20615909
H	2.73849715	2.66203795	2.47719136
O	1.88498098	-0.40807203	-0.73275030
C	3.06609920	-0.08405751	0.03289678
C	4.02250377	-1.25102408	-0.20177448
C	3.72754416	-1.60212551	-1.66828398
C	2.21365993	-1.36841124	-1.76585118
H	1.64280187	-2.28135772	-1.57158429
H	1.90271879	-0.96425905	-2.73461539
H	4.00553554	-2.62601657	-1.93533071
H	4.26900447	-0.92134143	-2.33594323
H	3.76381068	-2.09069817	0.45432199
H	5.06815984	-0.98316738	-0.02116547
H	3.49330235	0.85740839	-0.34324412
H	2.76589838	0.05440411	1.07390894
O	-0.04598026	1.98298805	-0.57443947
C	-1.04981245	2.89659415	-0.08657295
C	-0.62465764	4.26987350	-0.60387140
C	-0.02240942	3.91081410	-1.97174993
C	0.66222143	2.56670067	-1.68780703
H	1.71163779	2.69575247	-1.39583512
H	0.61760305	1.87530657	-2.53519427
H	0.67700653	4.66215392	-2.35083385
H	-0.81893016	3.78416484	-2.71383240
H	0.13889366	4.70533971	0.05158547
H	-1.46114362	4.97217859	-0.67056435
H	-2.02872455	2.60073968	-0.48455330
H	-1.06845886	2.81126843	1.00241946

Table 48. Geometric coordinates and thermally corrected MP2 energies for **5** LDA mixed spirocyclic dimer with three THF



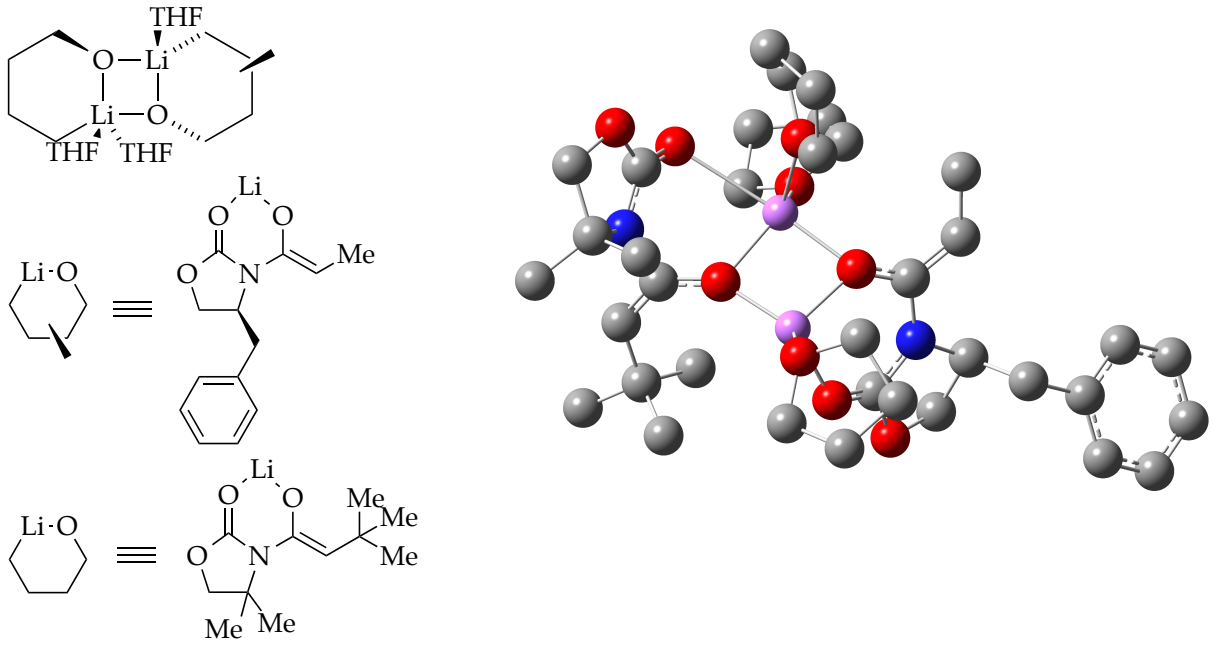


G = -1787.914072 Hartree
G_{MP2} = -1118226.969 kcal/mol
ΔG_{MP2} = 0.409071258 kcal/mol Li vs. **5** LDA mixed dimer with three THF

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.57693330	-2.07636022	3.26136163
O	0.00000000	0.00000000	1.94667770	N	-1.74875205	0.96219277	-0.33587249
C	0.75186238	0.00000000	3.00030639	C	-1.59252690	2.40754298	-0.55675899
N	0.45661276	1.05169231	3.98307140	H	-0.94150317	2.73814906	0.27231128
C	1.32148232	1.36938551	5.12829914	C	-0.82346752	2.83806863	-1.83865905
C	0.36548147	2.22358551	5.96862194	H	-1.43120978	2.75021231	-2.74540621
H	-0.19336219	1.62361231	6.69662555	H	-0.50728107	3.88914534	-1.76315087
H	0.85673288	3.05125162	6.48289821	H	0.07103620	2.21943168	-1.97106742
O	-0.55949489	2.76254797	5.01072387	C	-2.86250948	3.28506332	-0.42951143
C	-0.56517872	1.95910513	3.90414013	H	-2.59629854	4.35086619	-0.40242113
O	-1.41370475	2.13219052	3.03935697	H	-3.54544688	3.14441236	-1.27609839
Li	-1.73823887	0.76326655	1.67853986	H	-3.41037085	3.05093577	0.49061957
O	-3.21903224	-0.18537937	2.75767016	C	-2.74123744	0.21280986	-1.10991280
C	-3.47451327	-1.60172355	2.84885659	H	-2.47321173	-0.84782045	-0.94694108
C	-4.69756080	-1.76403426	3.76948056	C	-2.73439130	0.39442757	-2.64821312
C	-4.71394648	-0.43935740	4.55130394	H	-3.35382157	-0.37329721	-3.13385174
C	-4.21757613	0.54554624	3.49564130	H	-3.13949624	1.36822035	-2.94657005
H	-3.73524418	1.44105166	3.89091535	H	-1.71747534	0.32146750	-3.05031590
H	-5.02857469	0.84588907	2.81642378	C	-4.21399332	0.30952139	-0.61918942
H	-4.01249649	-0.47752741	5.39326760	H	-4.26002334	0.14722658	0.46285536
H	-5.70368033	-0.18126862	4.94028956	H	-4.66003621	1.28678931	-0.83133634
H	-4.61910855	-2.64583129	4.41241858	H	-4.84250502	-0.45064618	-1.10811706
H	-5.61347512	-1.86206605	3.17571527	H	1.58997751	0.45634886	5.66439740
H	-3.65049195	-1.99771301	1.84210063	C	2.60218302	2.12413583	4.69410914

H	3.07715378	1.53088747	3.90631939
H	2.30128842	3.07986725	4.24741880
C	3.56713610	2.35903215	5.83512371
C	4.33943832	1.30278372	6.34282416
C	5.21340424	1.50225754	7.41089914
C	5.33356415	2.76666308	7.99260253
C	4.57580381	3.82730302	7.49558969
C	3.70065669	3.62251370	6.42665217
H	3.12197446	4.45761514	6.03740378
H	4.66711989	4.81684293	7.93582758
H	6.01662821	2.92379064	8.82299218
H	5.80581952	0.67164719	7.78592089
H	4.26203202	0.31728881	5.88787470
C	1.77262045	-0.85548892	3.28954868
H	2.29970335	-0.77803111	4.23293882
C	2.16959929	-1.98717384	2.38492818
H	1.71557774	-1.87429798	1.39697691
H	3.26030678	-2.03875240	2.25034814
H	1.86259494	-2.97097460	2.77739945
O	0.12257454	-1.94139624	-0.71788146
C	-0.59593857	-2.97572070	-0.00527299
C	-1.28980121	-3.81452362	-1.07936510
C	-0.30297368	-3.70740424	-2.25191033
C	0.18174826	-2.26056468	-2.12741028
H	-0.47033475	-1.56604258	-2.66866937
H	1.21135837	-2.11758226	-2.46930856
H	-0.76074245	-3.91025235	-3.22465131
H	0.53054970	-4.40671865	-2.11510670
H	-2.25251873	-3.36674374	-1.35045883
H	-1.46790180	-4.84433739	-0.75480843
H	0.12487631	-3.56998636	0.57038023
H	-1.28093526	-2.48832728	0.69235647
O	1.81427539	0.74787215	-0.59447830
C	2.24292451	1.92490172	0.12737127
C	3.68230164	1.63377204	0.54571135
C	4.19640547	0.82282462	-0.65367560
C	2.96313123	-0.00469391	-1.04029282
H	2.95051481	-0.97786862	-0.53678024
H	2.87941564	-0.16477610	-2.12088059
H	5.05947004	0.19380637	-0.41552879
H	4.48214447	1.49364389	-1.47241922
H	3.68939004	1.02164703	1.45451271
H	4.25999916	2.54440620	0.73187090
H	2.18011430	2.79485442	-0.53985938
H	1.55419718	2.06571703	0.96284052

Table 49. Geometric coordinates and thermally corrected MP2 energies for **5 18** mixed dimer with three THF

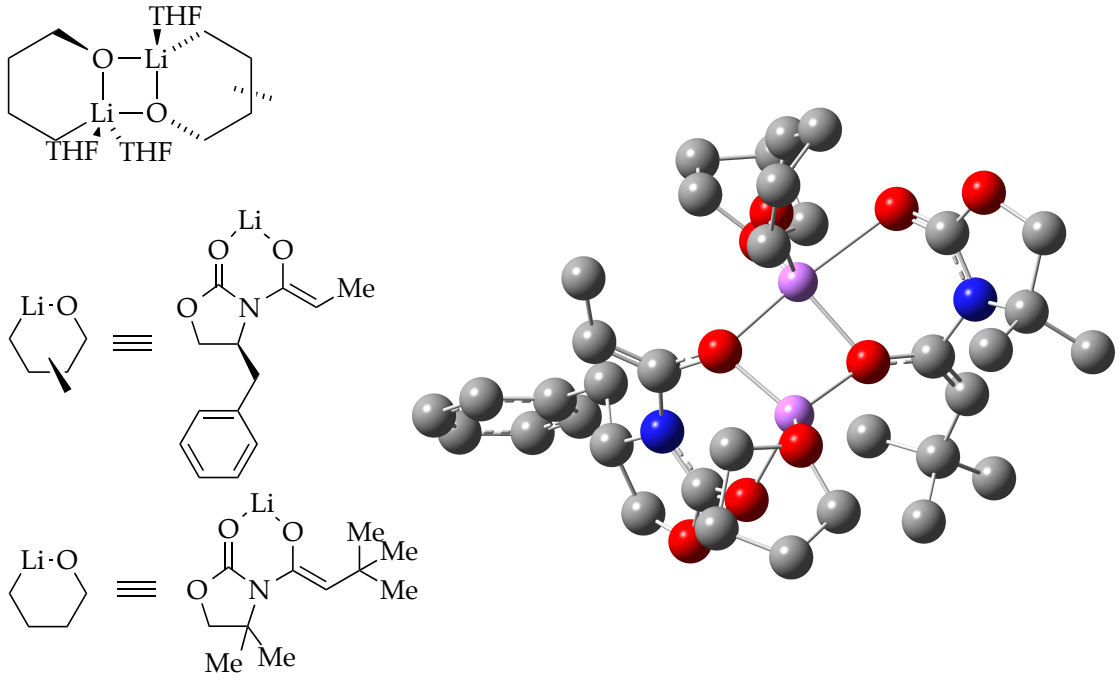


G = -2206.530974 Hartree
G_{MP2} = -1380179.361 kcal/mol
ΔG_{MP2} = 1.654267068 kcal/mol Li vs. **5 18** mixed dimer with three THF isomer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-2.47747561	0.77800261	-3.32883304
O	0.00000000	0.00000000	2.03020200	C	-1.67716660	-0.10470801	-2.64379118
C	0.98463157	0.00000000	2.87369909	O	-0.47073609	0.06214084	-2.55656956
N	1.23308890	-1.28113404	3.54494361	C	-4.43148373	-0.20121979	-0.95946738
C	2.38700454	-1.56439255	4.40993424	H	-5.50037246	0.01875890	-1.07099605
C	2.39267618	-3.09455571	4.34339983	H	-4.30144779	-0.88466589	-0.11610738
H	2.98073065	-3.47200983	3.49906633	H	-3.90933251	0.72967032	-0.71615684
H	2.72242930	-3.57487646	5.26569132	C	-4.69192596	-2.04429859	-2.66586035
O	1.00805568	-3.42837584	4.12598901	H	-4.29154709	-2.49414794	-3.58016026
C	0.39680014	-2.36045986	3.53616481	H	-4.67303848	-2.80107975	-1.87705407
O	-0.75310501	-2.46810847	3.12324018	H	-5.73474128	-1.75670550	-2.84675161
Li	-1.44791896	-1.20554438	1.83177858	C	-1.88178306	-3.31264988	-1.38201052
O	-1.40736534	-1.36587195	-0.03170272	H	-2.26980658	-3.57233917	-2.36221633
C	-1.85633781	-1.98902224	-1.08828220	C	-1.42951786	-4.47398358	-0.50570231
N	-2.42814547	-1.11162085	-2.12536766	C	0.02775580	-4.28913127	-0.02871595
C	-3.87421188	-0.81776175	-2.25440305	H	0.14227179	-3.34859339	0.51502648
C	-3.80139256	0.22364519	-3.39577264	H	0.32958107	-5.11275307	0.63224777
H	-3.93311340	-0.24650617	-4.37804132	H	0.71132539	-4.27335488	-0.88626933
H	-4.52277018	1.03686498	-3.28408574	C	-2.35763583	-4.62841939	0.72160881

H	-2.05289871	-5.48321190	1.34048736
H	-2.32506881	-3.73696077	1.35342683
H	-3.39550541	-4.79042547	0.40470098
C	-1.50944106	-5.76844254	-1.34146931
H	-2.53374154	-5.95319585	-1.68996624
H	-0.86141979	-5.70663907	-2.22468245
H	-1.19354417	-6.63715827	-0.75067844
O	-3.16954640	-0.61277883	2.74323178
C	-3.96235635	-1.63449264	3.40035707
C	-4.21608680	-1.13575172	4.83315393
C	-3.08688914	-0.11318352	5.04255276
C	-2.95761142	0.49234428	3.64761191
H	-1.97287987	0.90666389	3.42143606
H	-3.72661611	1.25933741	3.47184456
H	-2.15485463	-0.62001200	5.31520424
H	-3.31588179	0.63277648	5.80994549
H	-4.19850880	-1.95170779	5.56151685
H	-5.19260241	-0.64242326	4.90422337
H	-4.88672999	-1.78163474	2.83133517
H	-3.38254472	-2.56206937	3.38510297
H	3.29106059	-1.13816032	3.96924561
C	2.18270918	-1.03297980	5.85335698
H	1.91732125	0.02666266	5.79023708
H	1.31964022	-1.55364650	6.28658017
C	3.39996517	-1.22571505	6.73131460
C	4.53443031	-0.41600644	6.56667733
C	5.67017610	-0.60412053	7.35360444
C	5.69283381	-1.60783086	8.32493481
C	4.57098518	-2.41751226	8.50337258
C	3.43627339	-2.22624008	7.71210008
H	2.56162598	-2.85505104	7.86534680
H	4.57502637	-3.19689163	9.26093476
H	6.57645662	-1.75326882	8.94045333
H	6.53657856	0.03684521	7.21237620
H	4.52365109	0.37577080	5.82027460
C	1.81637591	1.03561695	3.17719992
H	2.59123977	0.90966479	3.92355856
C	1.69019210	2.39899050	2.55613868
H	1.09748922	2.35798673	1.63854810
H	1.21100934	3.12903321	3.22968495
H	2.67429105	2.81793230	2.30156329
O	1.89371434	-0.43206698	-0.52907401
C	2.99195156	0.49231981	-0.36527637
C	4.14012724	-0.07015304	-1.20863763
C	3.38411816	-0.80184759	-2.32886884
C	2.19430475	-1.39041532	-1.57208246
H	2.45151172	-2.34837609	-1.10152327
H	1.29506416	-1.51066793	-2.17650120
H	3.98406306	-1.56825645	-2.82949323
H	3.03614613	-0.08913743	-3.08572061
H	4.73509499	-0.78183003	-0.62320331
H	4.81182553	0.71323594	-1.57343633
H	2.67622071	1.47799231	-0.73159874
H	3.21297221	0.57009362	0.70262198
O	-0.46114263	2.02659303	-0.24224136
C	-1.52206105	2.62121570	0.53790341
C	-1.78669635	4.00254562	-0.07878983
C	-1.27874210	3.83039578	-1.51967493
C	-0.07595536	2.91237987	-1.31401351
H	0.81350249	3.48321580	-1.00717145
H	0.16032288	2.28957994	-2.17709924
H	-1.01172014	4.77687925	-2.00028354
H	-2.02521298	3.32367075	-2.14123821
H	-1.20172004	4.77169943	0.43943298
H	-2.84173430	4.28804876	-0.02026822
H	-2.39735702	1.96458773	0.47114585
H	-1.20379071	2.66523481	1.58278009

Table 50. Geometric coordinates and thermally corrected MP2 energies for **5 18** mixed dimer with three THF isomer



G = -2206.53395 Hartree
G_{MP2} = -1380182.669kcal/mol
ΔG_{MP2} = 0 kcal/mol Li vs. **5 18** mixed dimer with three THF isomer

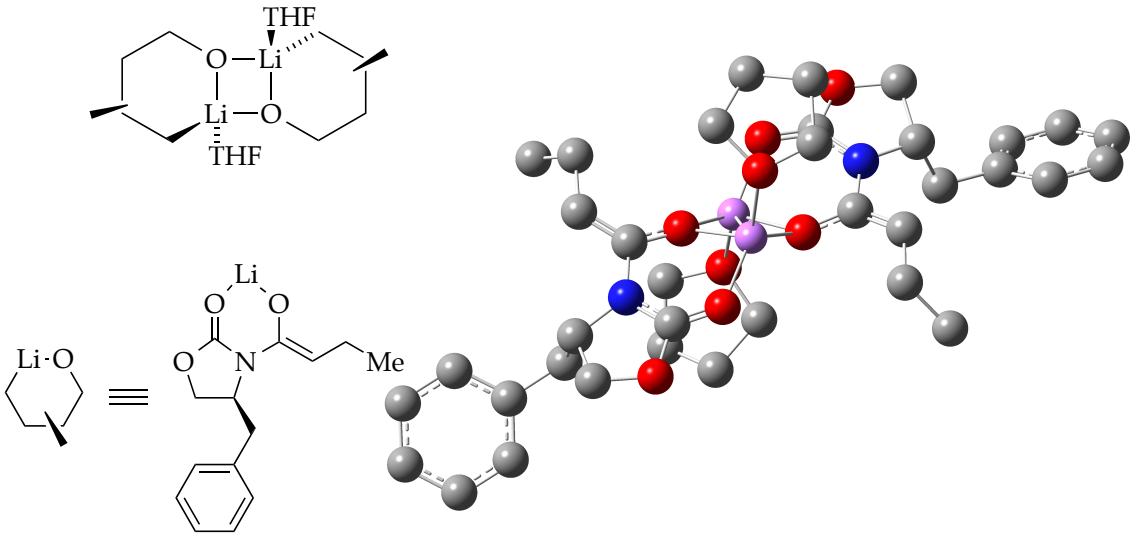
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.42188982	3.43137927	2.43247071
O	0.00000000	0.00000000	2.02253570	H	7.56866782	4.08919554	3.46982494
C	0.88330000	0.00000000	2.96846562	H	8.51223071	2.75099640	5.34385558
N	1.29414259	1.33868580	3.42915803	H	7.28587268	0.74611289	6.16144092
C	0.40214017	2.34615443	3.63120299	H	5.14259799	0.08973344	5.11924497
O	1.00897687	3.42064518	4.20024092	H	2.72286692	1.14582064	4.96985692
C	2.42655034	3.18453991	4.25536072	O	-0.80115138	2.37002811	3.38348142
H	2.90405329	3.77939381	3.46901015	Li	-1.40176729	1.25677279	1.88294199
H	2.79503953	3.51505742	5.22774543	O	-1.24521357	1.57640554	0.04910699
C	2.59857347	1.67136534	4.01251696	C	-1.48555455	2.29183762	-1.01321839
C	3.78909994	1.33310420	3.09690234	N	-2.11862915	1.54774424	-2.12011696
H	3.64235366	1.84515976	2.13874326	C	-3.57352064	1.56058438	-2.40189719
H	3.75803129	0.25758844	2.89558257	C	-3.60967759	0.47654658	-3.50487616
C	5.11781508	1.72287697	3.70986718	H	-3.53626679	0.91823775	-4.50604962
C	5.66603374	0.97462179	4.76308521	H	-4.49478431	-0.16214928	-3.45470044
C	6.87703727	1.34179325	5.34932338	O	-2.44802005	-0.34070930	-3.28135942
C	7.56687177	2.46618928	4.88995577	C	-1.56144802	0.37661038	-2.52095161
C	7.03694545	3.21642534	3.83989736	O	-0.44076888	-0.04852547	-2.27486877
C	5.82305226	2.84623233	3.25722807	C	-4.37566212	1.13921847	-1.15858230

H	-5.44860303	1.11824799	-1.38499448
H	-4.20731768	1.84622355	-0.34144651
H	-4.07086202	0.14704239	-0.81109298
C	-4.06159287	2.91151249	-2.92958449
H	-3.48243459	3.22229516	-3.80518289
H	-3.96021226	3.68263603	-2.16126697
H	-5.11803268	2.84404717	-3.21638757
C	-1.23600185	3.60095225	-1.26370475
H	-1.47446598	3.95242157	-2.26287614
C	-0.63004491	4.62152064	-0.30894696
C	0.74907072	4.15001061	0.20702860
H	0.66817426	3.17340623	0.69171782
H	1.16292186	4.86813255	0.92860752
H	1.45885862	4.05619847	-0.62432252
C	-1.56550187	4.88124841	0.89436293
H	-1.14555220	5.64710168	1.56042760
H	-1.70753645	3.97352477	1.48672121
H	-2.54754685	5.23074166	0.55236821
C	-0.44153094	5.94734383	-1.07433756
H	-1.40192612	6.33165451	-1.44132539
H	0.21758051	5.81220125	-1.94110456
H	0.00257566	6.71489831	-0.42843011
O	-3.19388963	0.68689610	2.64698659
C	-4.08754810	1.77763957	2.98363525
C	-4.58824497	1.50242485	4.40754881
C	-3.45355626	0.64874438	4.99695374
C	-3.03603063	-0.18706397	3.78951620
H	-1.99553838	-0.51866015	3.80615278
H	-3.69014138	-1.06151103	3.66074319
H	-2.62162037	1.28577944	5.31400795
H	-3.77086828	0.03439563	5.84530113
H	-4.76924756	2.42553088	4.96598705
H	-5.52400443	0.93108661	4.38449564
H	-4.89222310	1.80825301	2.24156614
H	-3.51760986	2.71163452	2.92884353
C	1.47584569	-1.06768625	3.56642985
H	2.14813797	-0.90297293	4.40358130
C	1.19047863	-2.48931694	3.16815749
H	0.68654686	-2.52036616	2.19763033
H	0.54752489	-3.01266023	3.89433768
H	2.11204200	-3.08442232	3.09038798
O	1.98452558	0.06818347	-0.42426407
C	2.80322160	-1.08848857	-0.15066611
C	4.12651946	-0.83092642	-0.87199106
C	3.65885866	-0.04366147	-2.10637567
C	2.53600721	0.82316969	-1.52938974
H	2.92063052	1.77319499	-1.13641018
H	1.72707521	1.02604332	-2.23284663
H	4.45159708	0.55228513	-2.56919892
H	3.26068452	-0.72801772	-2.86494341
H	4.78866544	-0.21446747	-0.25181941
H	4.65628223	-1.75610145	-1.11969299
H	2.30368794	-1.98260324	-0.54779881
H	2.88834785	-1.18914960	0.93412016
O	-0.70653053	-2.02594604	-0.06566208
C	-1.90553128	-2.30652816	0.69235148
C	-2.50788933	-3.58037249	0.08396542
C	-1.97503730	-3.54340798	-1.35691402
C	-0.57593570	-2.96490966	-1.15153221
H	0.14021017	-3.74953012	-0.86402487
H	-0.19623820	-2.41542208	-2.01375648
H	-1.96022538	-4.52569727	-1.83991227
H	-2.56877567	-2.86217656	-1.97672073
H	-2.13297502	-4.47014699	0.60418811
H	-3.60085507	-3.59243417	0.14448034
H	-2.57986144	-1.44709998	0.59500615
H	-1.63351774	-2.40892197	1.74581551

Part 7: 6 Ground State Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 51. Geometric coordinates and thermally corrected MP2 energies for **6** trans disolvated dimer with two THF

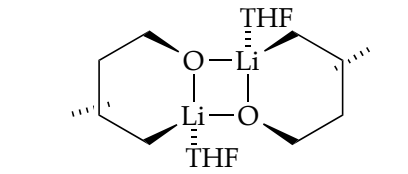


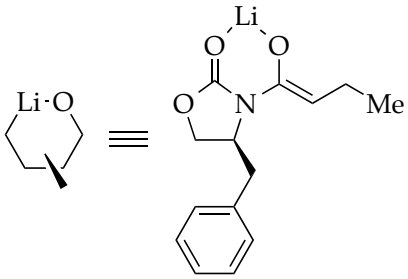
G = - 2126.597799 Hartree
G_{MP2} = - 1330208.34 kcal/mol
ΔG_{MP2} = 0.610451832 kcal/mol Li vs. **6** D_{2d} tetramer

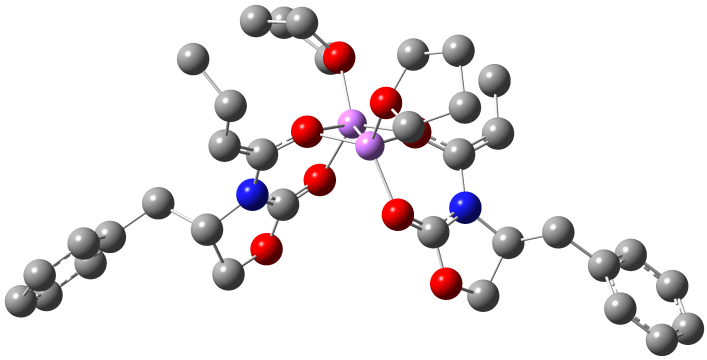
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.58841284	-1.50851022	1.44389266
O	0.00000000	0.00000000	1.93137090	C	4.38820692	-1.95079010	-0.71792228
C	1.07112132	0.00000000	2.52826923	H	3.61019840	-1.79979087	-1.47432302
O	1.12827218	0.44855761	3.81465172	H	4.57749525	-3.03681224	-0.68633445
C	2.43026038	0.15849867	4.35162481	C	5.68205539	-1.25405686	-1.17484966
H	2.36579817	-0.76227708	4.94304630	H	6.48623003	-1.38708841	-0.43928843
H	2.73052883	0.98380914	4.99914224	H	6.03756326	-1.65742634	-2.13127943
C	3.32305898	-0.00884992	3.11522137	H	5.52229358	-0.17620453	-1.29738214
H	4.03467606	-0.82256129	3.27016921	O	1.70314841	-0.84628305	-0.09210844
N	2.31630022	-0.39009858	2.11440795	Li	0.74025655	-2.20689892	-1.03357623
C	2.64790166	-0.92956468	0.79440992	O	0.73897278	-2.56695519	-2.92928651
C	3.89073507	-1.45577322	0.61422695	C	-0.22109605	-2.28505878	-3.63646267

O	-0.13344265	-2.40981118	-4.99129675
C	-1.44708567	-2.26622268	-5.55769413
H	-1.84676193	-3.26545302	-5.76420386
H	-1.36299764	-1.71198207	-6.49409139
C	-2.26045630	-1.52961970	-4.48030006
H	-3.25970355	-1.96447064	-4.40024925
N	-1.46470835	-1.84014945	-3.28706980
C	-1.87788729	-1.50273863	-1.92153923
C	-3.20946389	-1.50956312	-1.64967534
C	-3.78686934	-1.13638724	-0.31125418
H	-2.97106531	-0.92363713	0.38870048
H	-4.33839650	-1.99116277	0.11300189
C	-4.74490111	0.06728040	-0.36519044
H	-5.57738393	-0.11880685	-1.05616570
H	-5.17364866	0.28263668	0.62166030
H	-4.22478865	0.96819443	-0.71255255
H	-3.91111260	-1.81678946	-2.42010954
O	-0.90470268	-1.22436374	-1.10836940
C	-2.38521076	-0.00490417	-4.70993240
H	-2.76323502	0.42730607	-3.77671229
H	-1.38101678	0.40288288	-4.88062192
C	-3.30058250	0.34463182	-5.86197500
C	-2.78967090	0.75926614	-7.09921229
C	-3.64140745	1.05073083	-8.16702546
C	-5.02273143	0.93078831	-8.01324865
C	-5.54629532	0.52262471	-6.78406005
C	-4.69249459	0.23409433	-5.72008058
H	-5.10899927	-0.07106477	-4.76214576
H	-6.62156244	0.43447473	-6.65218120
H	-5.68743668	1.15831455	-8.84219037
H	-3.22396873	1.37442935	-9.11691935
H	-1.71407769	0.86597643	-7.22477437
O	0.50958489	-3.87830401	0.04003657
C	1.48812923	-4.43182146	0.93948413
H	1.68973030	-5.47202413	0.64936094
H	2.40069580	-3.84261158	0.82689496
C	0.87013001	-4.35118527	2.35755837
H	0.89990411	-5.32905801	2.84892166
H	1.41545703	-3.64672137	2.99220640
C	-0.58531313	-3.87930168	2.10938590
C	-0.78257720	-4.13781825	0.61412956
H	-1.49434087	-3.46799238	0.12980891
H	-1.06537898	-5.18311535	0.41561419
H	-1.31557556	-4.41195701	2.72638974
H	-0.68386131	-2.80820472	2.30964466
C	4.07968339	1.27761267	2.70480771
H	4.46914304	1.11308302	1.69455832
H	3.35554181	2.09984824	2.64732365
C	5.20214162	1.62850165	3.65585101
C	6.41029400	0.91524860	3.62226628
C	7.44134286	1.20943477	4.51385435
C	7.28384791	2.22727975	5.45762122
C	6.09063303	2.94887110	5.49881543
C	5.06016938	2.65011669	4.60467266
H	4.13793026	3.22682934	4.63456847
H	5.96107801	3.74863579	6.22336046
H	8.08797216	2.45946290	6.15064839
H	8.37111720	0.64835917	4.46779644
H	6.54663259	0.13066502	2.88068176
O	0.08368522	1.86457362	-0.71867156
C	1.25271738	2.16816326	-1.51229528
H	1.75292060	3.05334442	-1.09349635
H	1.91967481	1.30637735	-1.44227148
C	0.71241253	2.44620503	-2.91226055
C	-0.60903941	3.16809574	-2.59991856
C	-1.09046595	2.45975229	-1.32278288
H	-1.79793722	1.65151681	-1.53866278
H	-1.54820614	3.14508556	-0.60144494
H	-1.34082259	3.10092700	-3.41043991
H	-0.42310002	4.23047649	-2.40399163
H	1.39834117	3.04440136	-3.51983758
H	0.52438105	1.50036248	-3.43316764

Table 52. Geometric coordinates and thermally corrected MP2 energies for **6** cis disolvated dimer with two THF





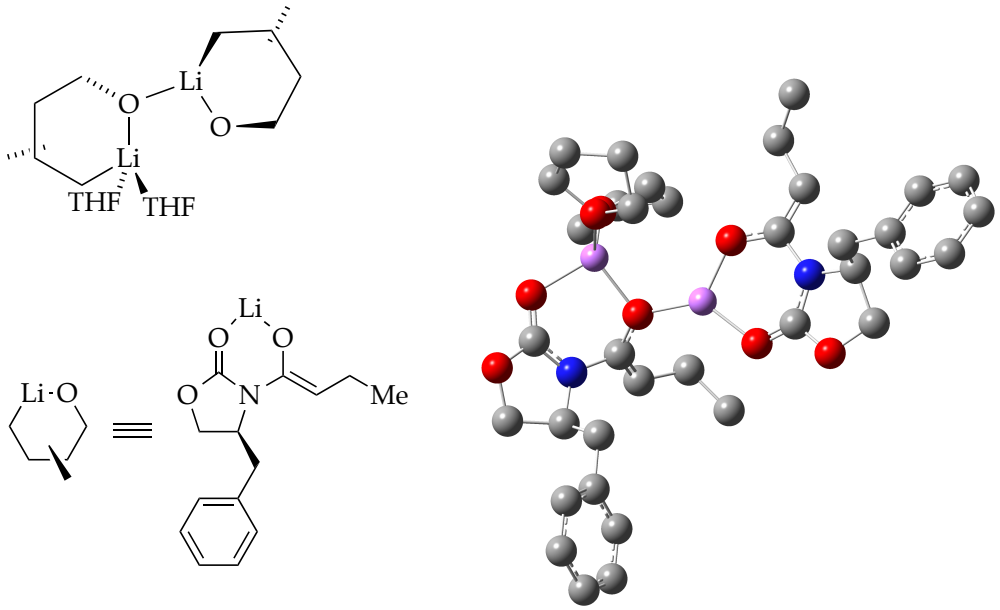


G = - 2126.59718 Hartree
G_{MP2} = - 1330205.291 kcal/mol
ΔG_{MP2} = 2.13512188 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.00222845	-3.34661783	-4.08697370
O	0.00000000	0.00000000	1.90304040	H	-1.94275996	-2.78833870	-4.04352687
C	1.00651828	0.00000000	2.72648419	H	-0.23448140	-2.65359017	-4.45318679
N	1.37391908	-1.31816589	3.24403447	C	-1.12614743	-4.52784067	-5.02467389
C	2.56504891	-1.58536119	4.06094667	C	-0.13012993	-4.81166091	-5.96897424
C	2.72719593	-3.08783450	3.80791528	C	-0.23499983	-5.91791830	-6.81488664
H	3.35477804	-3.29565063	2.93386282	C	-1.34242136	-6.76177826	-6.72867177
H	3.10211830	-3.64157099	4.66990343	C	-2.34495263	-6.48947892	-5.79478532
O	1.38651262	-3.53528183	3.52775819	C	-2.23660084	-5.38301668	-4.95298182
C	0.66045531	-2.47173956	3.07707916	H	-3.02832644	-5.17432603	-4.23627008
O	-0.47067333	-2.65241684	2.63584958	H	-3.21518391	-7.13695938	-5.72528926
Li	-1.41790513	-1.25033788	1.71302490	H	-1.42742217	-7.62228513	-7.38679981
O	-1.51884284	-1.13246482	-0.18123010	H	0.54732768	-6.11640474	-7.54286219
C	-1.77680294	-2.03527577	-1.08002260	H	0.73145860	-4.15211781	-6.05016707
N	-0.59689551	-2.60901757	-1.72781244	C	-3.00230677	-2.49617700	-1.44566563
C	-0.62676231	-3.75975421	-2.64029549	C	-4.27527796	-2.02659496	-0.79615915
C	0.82361779	-4.23719861	-2.51205865	H	-4.96049479	-1.61381554	-1.55478798
H	0.95095446	-4.96342228	-1.70126118	H	-4.04334715	-1.20732525	-0.10745721
H	1.23717708	-4.64222691	-3.43673158	C	-5.01867227	-3.13785323	-0.03237398
O	1.55061631	-3.03978646	-2.17467412	H	-5.95697307	-2.76798294	0.40206832
C	0.68590013	-2.15686801	-1.59735200	H	-5.26849503	-3.97734467	-0.69401869
O	1.11927576	-1.12492947	-1.09303964	H	-4.39667038	-3.53481332	0.77877267
H	-1.32825346	-4.50805688	-2.26441633	H	-3.09671485	-3.26129245	-2.20854983

O	-3.01229464	-0.76505211	2.81841091	H	6.83496415	-1.84370224	8.50939696
C	-3.60548222	-1.74034989	3.71127061	H	6.57200698	0.12243802	7.00676734
C	-3.86687405	-1.00851521	5.03874196	H	4.50873167	0.40333957	5.67735318
C	-2.89398054	0.18046007	4.97031656	C	1.74445476	1.07458758	3.11184252
C	-2.91804803	0.51492032	3.48113909	H	2.56412834	0.95491961	3.81172767
H	-2.01294366	1.00151709	3.11127812	C	1.46554364	2.47182564	2.62753792
H	-3.79641927	1.12297072	3.22056120	H	0.72916317	2.43227116	1.81790058
H	-1.88476393	-0.12636233	5.26812454	H	2.37866148	2.91031022	2.19430361
H	-3.19733125	1.02292111	5.59951046	C	0.95831581	3.41415326	3.73517772
H	-3.69976571	-1.65429701	5.90593484	H	1.67586100	3.47626685	4.56345333
H	-4.90136162	-0.64844523	5.08298767	H	0.79912734	4.43226301	3.35624884
H	-4.52025323	-2.12751372	3.25057150	H	0.00995626	3.05211641	4.15008080
H	-2.88970707	-2.56160334	3.82198355	O	-0.19978885	1.74298418	-0.94636597
H	3.41417414	-1.02072259	3.66932473	C	-1.57884097	2.14830163	-1.15164071
C	2.33303534	-1.24440276	5.55581031	C	-1.68279865	2.60768176	-2.61740468
H	1.96090873	-0.21650460	5.61069428	C	-0.45033658	1.96097731	-3.27310906
H	1.53505840	-1.89572962	5.93380831	C	0.56746790	2.00936584	-2.13604742
C	3.57937772	-1.40617159	6.39830964	H	1.03401762	3.00204427	-2.05640717
C	4.61776193	-0.46492144	6.32411416	H	1.34825360	1.24799475	-2.19670422
C	5.78165806	-0.62045360	7.07618784	H	-0.11190361	2.48997385	-4.16945576
C	5.92941566	-1.72314938	7.92095060	H	-0.65888294	0.91959727	-3.54384602
C	4.90385401	-2.66465925	8.00871966	H	-1.61821151	3.69976303	-2.68577736
C	3.74034472	-2.50530411	7.25291963	H	-2.62483829	2.29839504	-3.07931199
H	2.94035553	-3.23814071	7.33630260	H	-2.20271662	1.27585267	-0.93569272
H	5.00526285	-3.52256811	8.66834375	H	-1.81857196	2.94698385	-0.44128744

Table 53. Geometric coordinates and thermally corrected MP2 energies for **6** unsymmetrically solvated dimer with two THF

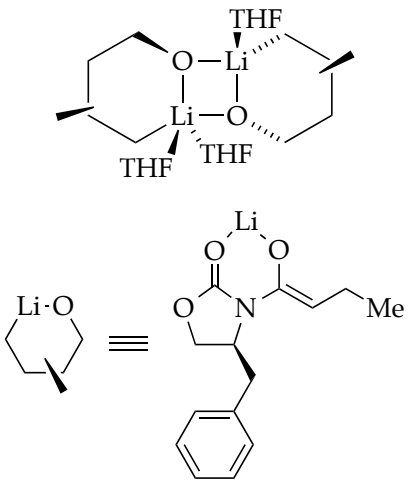


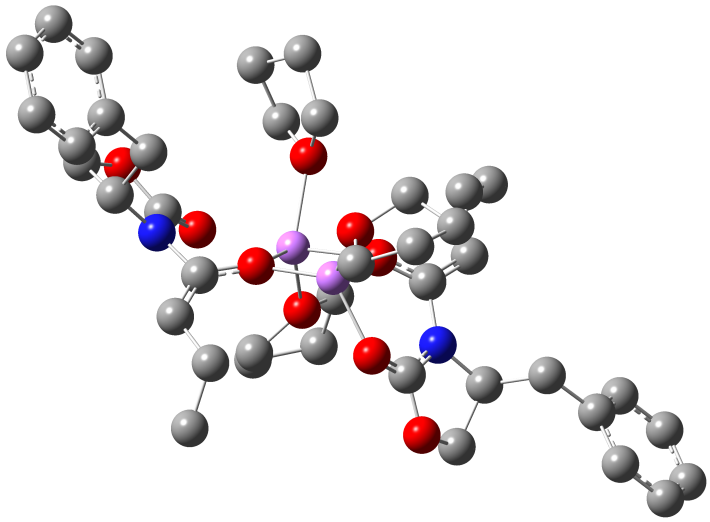
G = -2126.589616 Hartree
G_{MP2} = -1330200.128 kcal/mol
ΔG_{MP2} = 4.716502092 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.20840330	-1.67494359	-1.78413681
O	0.00000000	0.00000000	3.73418690	O	-0.64568028	-0.58307555	-1.74017617
C	0.18254924	0.00000000	5.01380745	H	-1.52373002	-4.78297115	-1.33363912
N	-0.57700271	-1.01877831	5.76603644	C	-3.08436864	-3.84034598	-0.15891148
C	-1.08627112	-0.81258810	7.12877811	H	-2.57052387	-3.95234317	0.80284022
C	-1.60076658	-2.22464903	7.44958227	H	-3.59836489	-2.87157079	-0.13978841
H	-0.85601129	-2.82428119	7.98493805	C	-4.07741877	-4.96471318	-0.35576747
H	-2.53875234	-2.23196011	8.00718373	C	-5.35654271	-4.72346650	-0.87469376
O	-1.82902884	-2.82852960	6.16305150	C	-6.25793552	-5.77053224	-1.07914321
C	-1.10489563	-2.15137579	5.23018272	C	-5.89151536	-7.07987740	-0.76693780
O	-1.00909789	-2.60202726	4.08842005	C	-4.62085277	-7.33440657	-0.24527393
Li	-0.36600482	-1.47081911	2.72663855	C	-3.72422614	-6.28591366	-0.04190541
O	-0.22002905	-1.65682445	0.90198907	H	-2.74151535	-6.49019159	0.37834841
C	-0.12976197	-2.74443510	0.17483776	H	-4.33034438	-8.35009593	0.01033931
N	-0.99486385	-2.76451287	-1.00272514	H	-6.59215256	-7.89587467	-0.92219442
C	-1.99958305	-3.80127264	-1.26059688	H	-7.24739483	-5.56071404	-1.47705538
C	-2.50433224	-3.33824735	-2.64026889	H	-5.65526587	-3.70316119	-1.10644867
H	-1.98457038	-3.84609779	-3.45998495	C	0.64100696	-3.83789740	0.37871628
H	-3.58195238	-3.44805247	-2.77095009	C	1.53734821	-4.04926788	1.56761449
O	-2.17877052	-1.93328012	-2.70086501	H	2.54687324	-4.31774174	1.21970247

H	1.64885999	-3.10631981	2.11789616	H	2.05407373	4.14195768	5.43907761
C	1.04435246	-5.14471054	2.53149058	H	0.40425845	3.60230776	5.81912210
H	1.76434636	-5.30965803	3.34310552	O	1.89117418	0.56955771	0.00245804
H	0.08604963	-4.86422927	2.98028841	C	2.46237043	0.86055514	1.30764891
H	0.91048456	-6.09863442	2.00574592	C	3.67513306	-0.06037775	1.43458232
H	0.60442813	-4.63313691	-0.36243485	C	4.14944365	-0.17070683	-0.02259812
H	-0.27203351	-0.54515908	7.80567398	C	2.82341729	-0.21206443	-0.78555109
C	-2.17257179	0.28788037	7.17322844	H	2.43834491	-1.23582087	-0.86640014
H	-1.74619321	1.17312762	6.68902687	H	2.87472744	0.22724312	-1.78625603
H	-3.02687632	-0.04055783	6.56832313	H	4.76516076	-1.05471861	-0.21401908
C	-2.61485531	0.61649077	8.58160000	H	4.72941261	0.71625938	-0.30485833
C	-1.79192141	1.38384543	9.42054102	H	3.36588292	-1.04206744	1.81114740
C	-2.17099358	1.66666512	10.73224218	H	4.43473016	0.34217444	2.11128479
C	-3.38485847	1.18727014	11.23083354	H	2.75742144	1.91839504	1.32423233
C	-4.21560098	0.42802306	10.40654598	H	1.69749918	0.68813687	2.06990897
C	-3.83170929	0.14641496	9.09351617	O	-1.01844484	1.59748614	0.49187624
H	-4.49135628	-0.43546953	8.45302769	C	-1.77900094	1.90667279	1.68495178
H	-5.16577160	0.05710814	10.78211881	C	-1.85778328	3.43127983	1.70861770
H	-3.68225611	1.40930820	12.25219249	C	-1.95990644	3.76531738	0.21109186
H	-1.52138796	2.26658467	11.36440892	C	-1.03988851	2.71593895	-0.42588264
H	-0.85071242	1.77018399	9.03459315	H	-0.01226916	3.08329913	-0.53441253
C	0.96100447	0.83925722	5.74963101	H	-1.38936026	2.35992730	-1.39988428
H	1.07029038	0.67868119	6.81823357	H	-1.65145511	4.78713812	-0.02972139
C	1.72112080	1.99115505	5.15308175	H	-2.99124906	3.63339226	-0.13660873
H	1.44488295	2.08894478	4.09728565	H	-0.94052950	3.85197378	2.13739300
H	2.80736634	1.79730043	5.16839075	H	-2.70723991	3.79907214	2.29221243
C	1.46391414	3.32535193	5.87504222	H	-2.77986432	1.46012707	1.59246537
H	1.73038012	3.25773945	6.93794416	H	-1.25826590	1.45797799	2.53482395

Table 54. Geometric coordinates and thermally corrected MP2 energies for **6** dimer with three THF



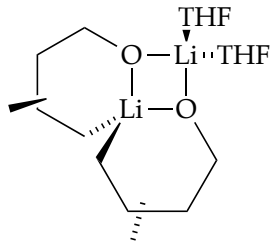


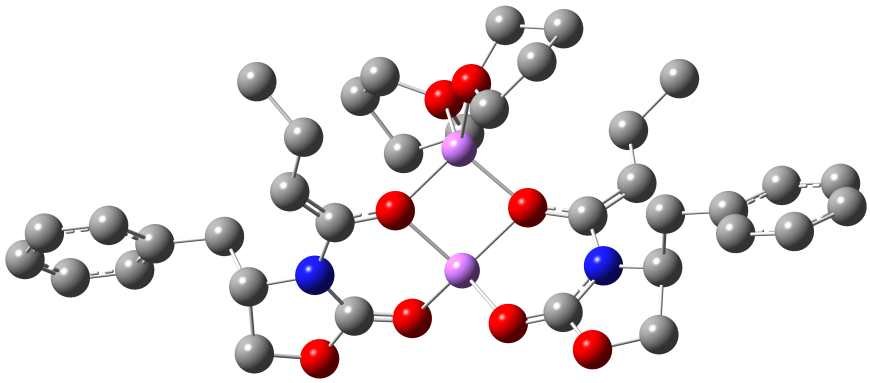
G = - 2358.937168 Hartree
G_{MP2} = - 1475522.775 kcal/mol
ΔG_{MP2} = -0.461912607 kcal/mol Li vs. **6** D_{2d} tetramer

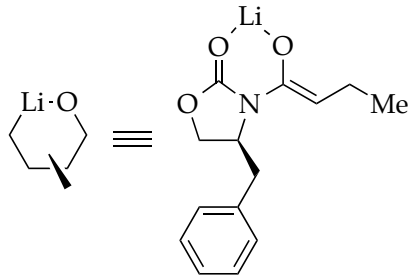
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-6.06192569	-0.12231777	-2.26838214
O	0.00000000	0.00000000	2.09927980	C	-6.58378541	1.08624406	-2.74880081
C	0.98404283	0.00000000	2.93885918	C	-7.87693125	1.15382856	-3.27214974
N	1.35832435	-1.32043239	3.46369260	C	-8.67127477	0.00818892	-3.32399789
C	2.57338415	-1.60175241	4.23850864	C	-8.16549371	-1.20308507	-2.84572897
C	2.70975266	-3.10490850	3.97496200	C	-6.87429526	-1.26549867	-2.32292112
H	3.29139010	-3.31799123	3.07059198	H	-6.49097233	-2.20998062	-1.94210435
H	3.12119010	-3.66435293	4.81646347	H	-8.77999742	-2.09921675	-2.87485790
O	1.35176224	-3.53636783	3.76193650	H	-9.67848800	0.05845839	-3.72886430
C	0.62072021	-2.46210884	3.34112798	H	-8.26342019	2.10274340	-3.63508290
O	-0.53481592	-2.62189941	2.96091757	H	-5.97466425	1.98664001	-2.70111741
Li	-1.39610397	-1.24502847	1.90478164	C	-2.56487364	-3.14501309	-0.94676072
O	-1.50749987	-1.22538105	0.04083159	C	-2.46766886	-4.12456698	0.18934361
C	-2.10329403	-1.87027090	-0.91734447	H	-3.47357060	-4.39715957	0.55247880
N	-2.34605999	-1.07797159	-2.12916150	H	-1.94734657	-3.66475840	1.03581994
C	-3.67168516	-0.88699912	-2.71811903	C	-1.73165262	-5.41965863	-0.19691834
C	-3.30155161	-0.02889531	-3.94290900	H	-1.70329692	-6.12753598	0.64088078
H	-3.16724059	-0.63904392	-4.84320818	H	-2.22341368	-5.91990782	-1.04136253
H	-4.01915106	0.76690206	-4.15110695	H	-0.69979121	-5.20348550	-0.49638878
O	-2.03579217	0.57085412	-3.60649595	H	-2.99639669	-3.50971544	-1.87684888
C	-1.45776061	-0.16756747	-2.60340286	O	-3.07112937	-0.81308062	2.95318520
O	-0.30329665	0.03221562	-2.25223151	C	-3.77653166	-1.91354246	3.58021572
H	-4.09175235	-1.84570288	-3.03499506	C	-4.07775314	-1.46992231	5.02044510
C	-4.65176731	-0.21217507	-1.72930974	C	-3.01233193	-0.38950979	5.27094197
H	-4.63188929	-0.80387410	-0.80686466	C	-2.91172910	0.26784589	3.89641471
H	-4.27044470	0.78612285	-1.48168107	H	-1.94914174	0.73937309	3.68598519

H	-3.71701135	1.00195097	3.74596210
H	-2.05358828	-0.84793404	5.53860164
H	-3.28997646	0.31713193	6.05920703
H	-4.02341533	-2.30250231	5.72810888
H	-5.08168457	-1.03462636	5.08951530
H	-4.68079994	-2.12541893	3.00013979
H	-3.11973158	-2.78859523	3.54824625
H	3.41143951	-1.03790466	3.82222233
C	2.39869942	-1.27793188	5.74592200
H	2.02577473	-0.25266837	5.83176292
H	1.61768668	-1.93657413	6.14586310
C	3.67755381	-1.44719388	6.53708318
C	4.72040038	-0.51579854	6.41493954
C	5.91296471	-0.67831897	7.11910419
C	6.08576726	-1.77816965	7.96294480
C	5.05619921	-2.70957774	8.09827890
C	3.86390950	-2.54329072	7.39023701
H	3.06147819	-3.26836495	7.50982187
H	5.17711886	-3.56521452	8.75755591
H	7.01389389	-1.90407509	8.51392460
H	6.70650449	0.05690108	7.01320496
H	4.59231327	0.34998155	5.76828080
C	1.71412617	1.07111147	3.36080515
H	2.49280471	0.94407361	4.10497072
C	1.45755695	2.47792117	2.88727928
H	0.93700916	2.44613867	1.92450013
H	0.78291850	3.01090337	3.58161457
C	2.74295698	3.30905053	2.75218048
H	2.52467073	4.33905436	2.44320374
H	3.28629443	3.36040426	3.70511370
H	3.42339579	2.87131930	2.01134872
O	1.92120760	-0.60479262	-0.31927707
C	3.02224536	0.32012804	-0.20873689
C	4.21683944	-0.39223808	-0.84383640
C	3.53737735	-1.20894086	-1.95452681
C	2.22604746	-1.63622531	-1.28746656
H	2.33487152	-2.58760271	-0.75088295
H	1.38505407	-1.70677880	-1.97925421
H	4.13201304	-2.06318417	-2.29289102
H	3.33287736	-0.57157061	-2.82278245
H	4.69659213	-1.05861352	-0.11637671
H	4.97314725	0.30558508	-1.21661740
H	2.77482822	1.24072898	-0.75635861
H	3.14755197	0.56236480	0.84996573
O	-0.39084956	2.06845744	-0.11828132
C	-1.63598612	2.45729621	0.50637641
C	-2.05856031	3.76984188	-0.16726265
C	-1.38379243	3.66848706	-1.54475799
C	-0.06932390	2.97235700	-1.19388193
H	0.68345133	3.69316068	-0.84244869
H	0.34200552	2.37753016	-2.01077870
H	-1.23227790	4.63966922	-2.02653643
H	-1.96818529	3.03543785	-2.22194732
H	-1.66336842	4.63050887	0.38552279
H	-3.14661372	3.87712195	-0.22149817
H	-2.36241391	1.65284906	0.33911802
H	-1.46678161	2.55085260	1.58228095

Table 55. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with two THF





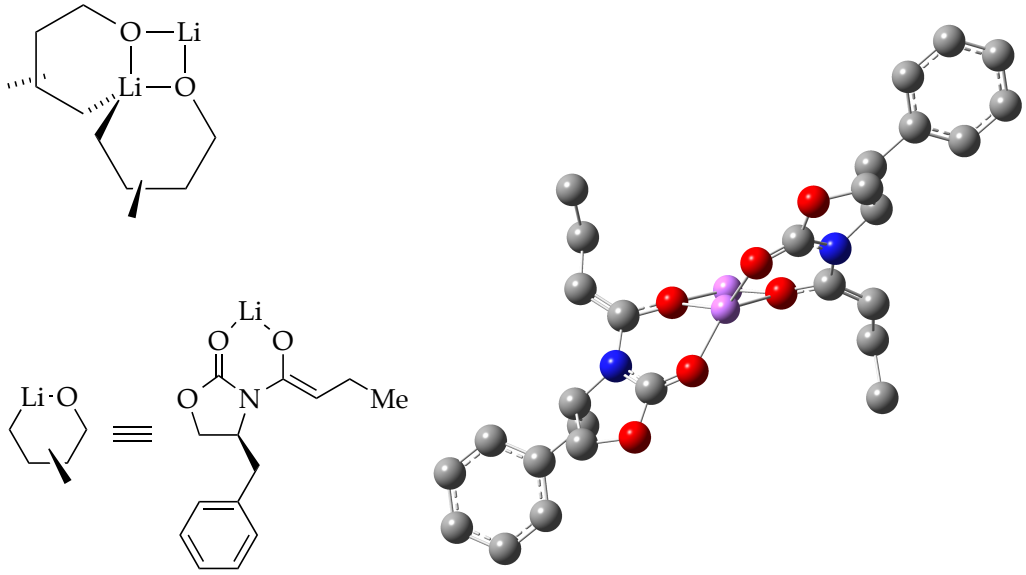


G = -2126.593455 Hartree
G_{MP2} = -1330207.175 kcal/mol
ΔG_{MP2} = 1.193116682 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	1.47913403	1.46328177	-1.49470886
O	0.00000000	0.00000000	1.91010250	O	-0.39169782	1.36272574	-1.28286746
C	1.03172090	0.00000000	2.56771136	C	-1.55699077	1.65541948	-1.77315416
O	0.97189531	0.07790988	3.92786664	N	-2.48316311	0.52567274	-1.88531865
C	2.27540297	-0.19715318	4.46557040	C	-3.70291806	0.54536955	-2.70353249
H	2.30950246	-1.24790198	4.77526672	C	-4.39758180	-0.72614430	-2.19769776
H	2.43476492	0.44103048	5.33638711	H	-5.09883402	-0.51691389	-1.38191549
C	3.23964775	0.09486386	3.30666120	H	-4.91095859	-1.28428278	-2.98243568
H	4.03369208	-0.65442186	3.28136489	O	-3.32822352	-1.53700370	-1.68353695
N	2.33650144	-0.06905317	2.16011075	C	-2.27119000	-0.72990281	-1.38062732
C	2.78987798	-0.12848285	0.76779242	O	-1.32433443	-1.17983611	-0.74779542
C	4.07605049	-0.51051828	0.54576405	H	-4.30475601	1.42560583	-2.46659849
H	4.68869598	-0.84873957	1.37542680	C	-3.38387796	0.52221474	-4.21865466
C	4.69242264	-0.60666476	-0.82412430	H	-2.67994053	1.33872147	-4.41217448
H	4.57119449	-1.62197622	-1.24020408	H	-2.86840249	-0.41920973	-4.44663125
H	4.16101991	0.05839214	-1.51519367	C	-4.61648729	0.66861959	-5.08276803
C	6.19030221	-0.26497440	-0.83335633	C	-5.17385413	-0.43136799	-5.74859825
H	6.75059492	-0.92777301	-0.16135642	C	-6.32886695	-0.29407686	-6.52169140
H	6.62089998	-0.37308364	-1.83642731	C	-6.94718777	0.95074571	-6.64068795
H	6.36581014	0.76481428	-0.49809142	C	-6.40065994	2.05695448	-5.98555349
O	1.90445931	0.20939132	-0.12138737	C	-5.24657658	1.91559559	-5.21582892

H	-4.82078817	2.78482007	-4.71863248
H	-6.87113427	3.03235851	-6.07859680
H	-7.84505133	1.06055393	-7.24283564
H	-6.74181441	-1.15983972	-7.03284825
H	-4.69138044	-1.40349422	-5.66980917
C	-1.99453170	2.87647520	-2.18473577
C	-1.15946883	4.12627122	-2.11861938
H	-1.48067768	4.76036664	-1.27394495
H	-0.11653402	3.86067467	-1.91655392
C	-1.23285611	4.97118945	-3.40150696
H	-2.26784712	5.25787020	-3.62949982
H	-0.64806397	5.89518076	-3.30855887
H	-0.85087037	4.41267967	-4.26503480
H	-3.01741275	3.00050014	-2.52513118
O	2.00300706	0.83227204	-3.33536773
C	1.23275518	1.39658482	-4.42989291
C	0.78439524	0.21166137	-5.29856776
C	0.81615234	-0.96205465	-4.30669212
C	2.02898714	-0.61224076	-3.45041554
H	2.96708840	-0.91395739	-3.93721745
H	2.00354033	-1.01755021	-2.43724375
H	0.91194490	-1.93722970	-4.79386881
H	-0.08558682	-0.97117913	-3.68528887
H	1.49595620	0.03906790	-6.11467476
H	-0.20180004	0.37756291	-5.74217964
H	0.38058830	1.93224536	-3.99849198
H	1.86555358	2.10859891	-4.97056030
O	2.37668452	3.22915861	-1.26398048
C	3.70258800	3.48148420	-1.77431750
C	4.56129038	3.73121458	-0.53713046
C	3.57917746	4.48941123	0.37141188
C	2.23798678	3.80946851	0.06041851
H	1.39199736	4.50287764	0.04764060
H	2.01346320	2.99254193	0.75388316
H	3.54776145	5.54996386	0.09571153
H	3.83804949	4.42602049	1.43235015
H	5.47073209	4.29766095	-0.75945637
H	4.84684711	2.77582834	-0.08251419
H	3.99814008	2.61086078	-2.36466546
H	3.67554027	4.36384987	-2.42957388
C	3.86462553	1.50985219	3.34877914
H	4.31349851	1.68914289	2.36565746
H	3.05604638	2.23939348	3.48285693
C	4.90111473	1.66624303	4.43892969
C	6.17477503	1.09467442	4.29484642
C	7.12859061	1.20626523	5.30591222
C	6.82643547	1.89547511	6.48296501
C	5.56631617	2.47353403	6.63767028
C	4.61357646	2.35845606	5.62302952
H	3.63694463	2.82181370	5.74733213
H	5.32332085	3.01810798	7.54636056
H	7.56995384	1.98485297	7.27034361
H	8.11055923	0.75960326	5.17307793
H	6.42220573	0.56658717	3.37610422

Table 56. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with with no THF isomer 1

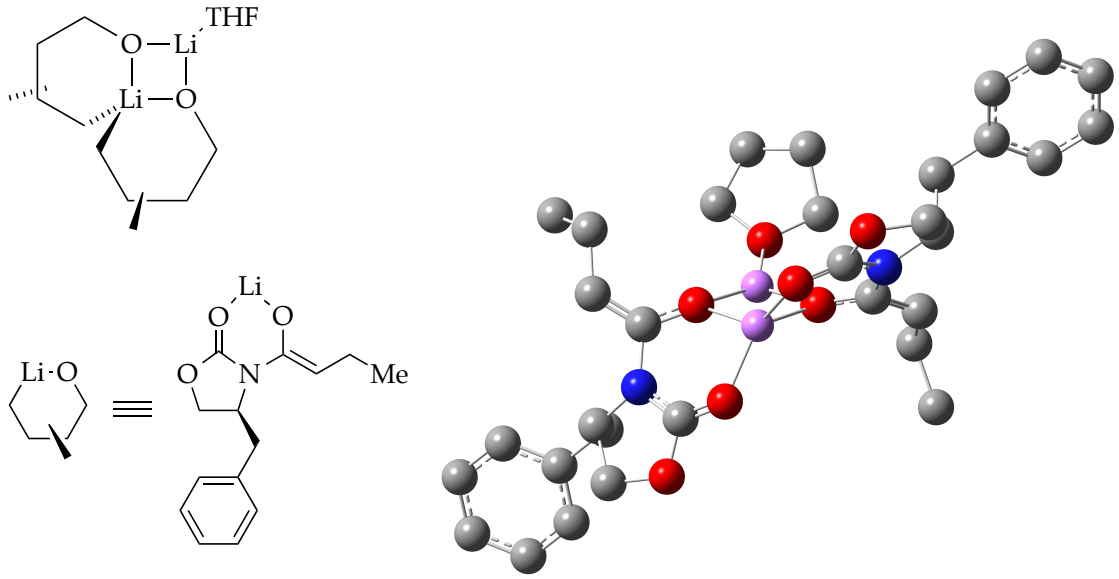


G = -1661.875946 Hartree
G_{MP2} = -1039554.194 kcal/mol
ΔG_{MP2} = 15.39328341 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	1.61495347	1.34730143	-1.29267628
O	0.00000000	0.00000000	1.91522680	O	-0.13389916	1.37778904	-1.43607910
C	1.01729158	0.00000000	2.59806762	C	-1.26283738	1.64190723	-2.04222192
O	0.95279516	0.23833870	3.93566152	N	-2.01568510	0.46934491	-2.46217578
C	2.23507662	-0.05239927	4.52177969	C	-2.74474163	0.38198132	-3.73347939
H	2.19327653	-1.05385915	4.96398552	C	-3.45720052	-0.96746677	-3.54350002
H	2.43205749	0.68140601	5.30482999	H	-4.46925574	-0.84520270	-3.14223981
C	3.22612903	0.01937962	3.34816616	H	-3.49800324	-1.57107029	-4.45148486
H	3.96354994	-0.78340277	3.42466220	O	-2.66330641	-1.66556934	-2.56641128
N	2.31245479	-0.22187600	2.22461468	C	-1.92646228	-0.75859951	-1.87029014
C	2.75350243	-0.39835419	0.84897819	O	-1.31208481	-1.09465945	-0.86492442
C	3.89627325	-1.08802500	0.62595162	H	-3.47665080	1.18935330	-3.81447353
H	4.39458815	-1.56992700	1.46238707	C	-1.78693334	0.43332334	-4.94707168
C	4.47530549	-1.31243847	-0.74389313	H	-1.17887727	1.33881122	-4.83869243
H	5.56227241	-1.14198870	-0.72245060	H	-1.10817678	-0.42654507	-4.89043115
H	4.06026047	-0.57345419	-1.44134630	C	-2.51618955	0.44520541	-6.27230447
C	4.20906219	-2.72432387	-1.29899640	C	-2.58646989	-0.70232330	-7.07353489
H	4.61421904	-3.49325654	-0.63016369	C	-3.28583218	-0.69234249	-8.28239463
H	3.13239888	-2.90289088	-1.39489016	C	-3.92876382	0.46984711	-8.70914804
H	4.67132172	-2.86031248	-2.28517895	C	-3.86400643	1.62220428	-7.92214300
O	1.98695327	0.16813866	-0.04721048	C	-3.16347855	1.60834699	-6.71649376

H	-3.10775562	2.51360214	-6.11512015
H	-4.35490094	2.53455339	-8.25076039
H	-4.47201491	0.48055797	-9.65015435
H	-3.32377370	-1.59205314	-8.89092170
H	-2.07745468	-1.60927021	-6.75382554
C	-1.76719285	2.86418323	-2.33026347
C	-1.07240735	4.15133697	-1.98007746
H	-0.00704541	3.95492147	-1.80335388
H	-1.12223534	4.84638650	-2.83179952
C	-1.66170677	4.84915566	-0.73982840
H	-2.72740850	5.06698809	-0.87973723
H	-1.56815121	4.20728511	0.14308614
H	-1.14980868	5.79788759	-0.53343185
H	-2.75614385	2.93672195	-2.77398186
C	3.95626578	1.37615937	3.21076515
H	4.44095312	1.38235204	2.22769539
H	3.20570157	2.17612391	3.21168299
C	4.97777342	1.60797585	4.30208592
C	6.20586604	0.92934073	4.28131395
C	7.14272294	1.11255492	5.29780417
C	6.86845499	1.98202180	6.35624866
C	5.65361334	2.66711927	6.38733825
C	4.71749221	2.47966949	5.36798251
H	3.77753463	3.02712034	5.39326185
H	5.43359743	3.35157869	7.20240408
H	7.59909038	2.12757253	7.14727038
H	8.09003014	0.58094795	5.26104193
H	6.43217865	0.25942302	3.45413015

Table 57. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with one THF isomer 1

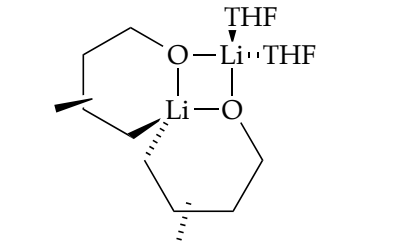


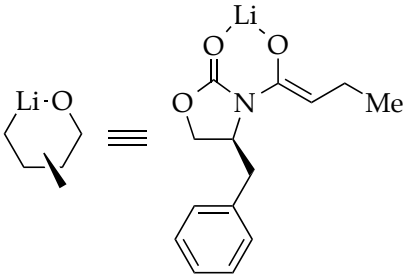
G = -1894.241229 Hartree
G_{MP2} = -1184881.842 kcal/mol
ΔG_{MP2} = 7.714645714 kcal/mol Li vs. **6** D_{2d} tetramer

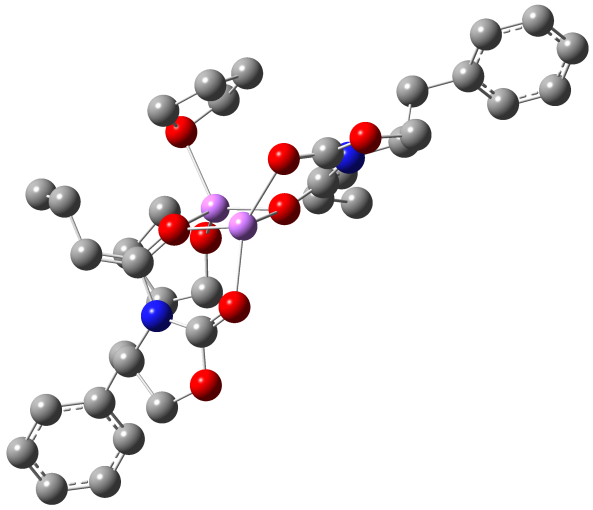
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.33060076	1.38566865	-1.34159709
O	0.00000000	0.00000000	1.91814910	C	-1.45870396	1.41551329	-1.99650605
C	1.02412744	0.00000000	2.58807300	N	-1.86971349	0.13430569	-2.56683868
O	0.95206720	0.07313102	3.94667232	C	-2.39874623	-0.02494500	-3.92446453
C	2.24998089	-0.20112971	4.49894138	C	-2.77820598	-1.51681252	-3.89539117
H	2.27478908	-1.24726073	4.82384497	H	-3.83600883	-1.66657129	-3.65258211
H	2.40501532	0.44845538	5.36201952	H	-2.54249844	-2.04421662	-4.82133847
C	3.23061231	0.07007247	3.34631165	O	-1.98517298	-2.08019544	-2.83462753
H	4.00720145	-0.69843333	3.32431812	C	-1.57627876	-1.07590424	-2.01089478
N	2.33312150	-0.07135945	2.19387402	O	-1.03757127	-1.32405639	-0.93881342
C	2.78703298	-0.10545375	0.80681731	H	-3.29102257	0.59049513	-4.06514645
C	4.05111352	-0.53684413	0.55623645	C	-1.34941095	0.34926392	-4.99739261
H	4.66211133	-0.91152623	1.37188509	H	-1.00562402	1.36450262	-4.76749687
C	4.61691847	-0.67492167	-0.83148975	H	-0.48769883	-0.32107080	-4.89091182
H	5.59826781	-0.17792425	-0.89783199	C	-1.89988262	0.28652560	-6.40479567
H	3.95954409	-0.16361219	-1.54420611	C	-1.57548600	-0.77008509	-7.26624050
C	4.78528155	-2.14050187	-1.27401345	C	-2.11275170	-0.83827764	-8.55358512
H	5.43653308	-2.68976060	-0.58262333	C	-2.98670379	0.15289402	-9.00057637
H	3.81601513	-2.65075053	-1.29201954	C	-3.31540917	1.21457566	-8.15414184
H	5.22939111	-2.20788294	-2.27562088	C	-2.77551677	1.27962519	-6.87005288
O	1.91339449	0.30771218	-0.06394029	H	-3.02721580	2.11634116	-6.22128770
Li	1.47230927	1.58236160	-1.28723232	H	-3.98905079	1.99583131	-8.49665198

H	-3.40505644	0.10258963	-10.00220844
H	-1.84451753	-1.66459848	-9.20672090
H	-0.88579127	-1.54126625	-6.92945926
C	-2.27005261	2.47929430	-2.20905427
C	-1.96390325	3.87146465	-1.73364868
H	-2.75910895	4.21965200	-1.05597837
H	-1.04641060	3.84780768	-1.13403768
C	-1.81993073	4.89686484	-2.87300410
H	-0.99364937	4.62814172	-3.54276325
H	-2.73165201	4.94095701	-3.48197556
H	-1.63319497	5.90714546	-2.48575244
H	-3.21410581	2.32554529	-2.72555051
O	2.67719523	2.97384100	-1.85993384
C	2.22777033	4.27736741	-2.31965997
C	3.26991300	5.29248513	-1.81925491
C	3.97946397	4.53446493	-0.68376945
C	3.96487874	3.10340555	-1.21016841
H	4.02499015	2.32694013	-0.44420796
H	4.75972984	2.93774224	-1.94995057
H	3.40393211	4.60018539	0.24690287
H	4.99107184	4.90241918	-0.48887175
H	2.80748221	6.22676036	-1.48882388
H	3.98269692	5.53475237	-2.61535657
H	2.14427439	4.25584430	-3.41089255
H	1.23368456	4.44918464	-1.89594088
C	3.89078435	1.46875170	3.39420822
H	4.37090246	1.62992403	2.42255995
H	3.09934356	2.22099199	3.49966702
C	4.90206222	1.60647422	4.51058704
C	6.15497263	0.98127991	4.41539176
C	7.08431814	1.07721649	5.45053101
C	6.77788512	1.80452595	6.60323550
C	5.53842256	2.43578323	6.70949618
C	4.60993324	2.33572904	5.67100648
H	3.64948830	2.83966140	5.75737571
H	5.29266346	3.00968656	7.59917586
H	7.50225594	1.88176369	7.40950922
H	8.05042605	0.58831936	5.35561140
H	6.40637410	0.42248487	3.51603741

Table 58. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with two THF isomer 1





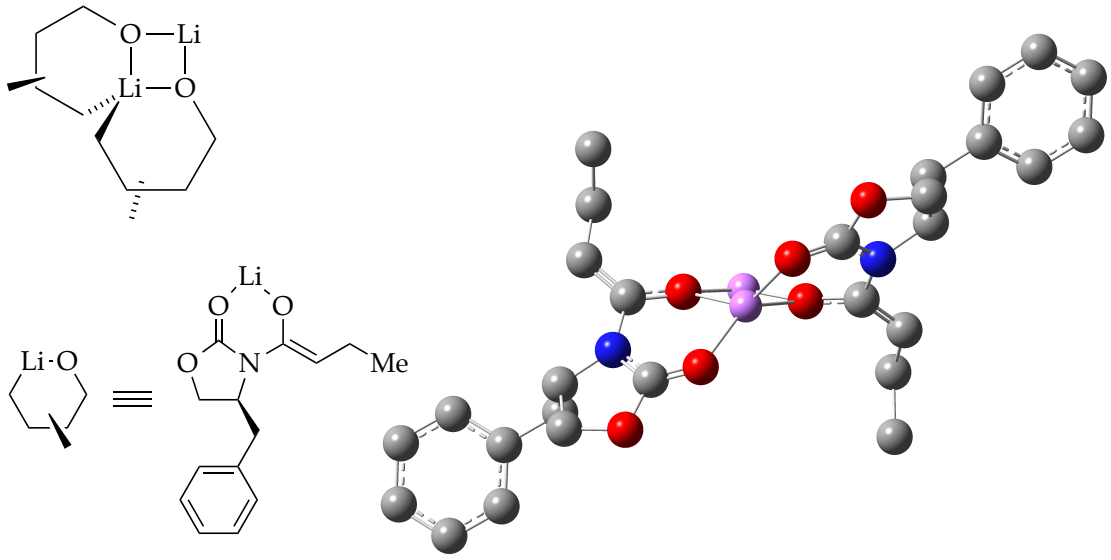


G = - 2126.593648 Hartree
G_{MP2} = - 1330206.864 kcal/mol
ΔG_{MP2} = 1.348809468 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.87912306	1.32263911	-1.29040239
O	0.00000000	0.00000000	2.18222390	C	-1.46196808	1.13446757	-2.40743173
C	1.09418993	0.00000000	2.71579528	N	-0.79671556	0.08354206	-3.22391611
O	1.29803016	-0.80922379	3.82996287	C	-0.78764032	0.12763986	-4.71932943
C	2.68474703	-0.69264622	4.28601243	C	-0.03794534	-1.17673719	-5.08773448
H	3.14784815	-1.67331317	4.09392508	H	-0.66876267	-1.92029298	-5.59965691
H	2.61660762	-0.50246284	5.36877245	H	0.90350015	-1.02443129	-5.63885655
C	3.30801403	0.46459328	3.46434807	O	0.34962937	-1.79761233	-3.82080252
H	4.25208139	0.14602593	2.95464767	C	-0.11679231	-1.03767795	-2.74916975
N	2.25236353	0.72902787	2.43604758	O	0.09919872	-1.42590519	-1.61749617
C	2.49757212	1.49858009	1.19060420	H	-1.84016157	0.10617146	-5.10127021
C	3.49493725	2.41619041	1.16690978	C	-0.07870328	1.40121460	-5.21043261
H	4.11287076	2.62653090	2.02858856	H	-0.64225586	2.29042263	-4.83830438
C	3.81636128	3.19256699	-0.07023916	H	0.92293870	1.48917945	-4.72628520
H	3.13130290	4.07404076	-0.14259862	C	0.02580691	1.44519797	-6.70658861
H	3.62221398	2.57934752	-0.97604178	C	1.25779526	1.21853167	-7.33841595
C	5.26823276	3.67596351	-0.09291341	C	1.34852695	1.26441879	-8.73270204
H	5.48395203	4.34172005	0.74907301	C	0.21434284	1.53560723	-9.50365423
H	5.96330634	2.83096990	-0.02711652	C	-1.01477637	1.76347650	-8.87544090
H	5.49065611	4.22084516	-1.01515132	C	-1.11142368	1.72012179	-7.48271673
O	1.67575157	1.19090202	0.27081781	H	-2.06969423	1.90362535	-6.99904964
Li	0.73064292	2.53802900	-0.92206352	H	-1.89987443	1.97625938	-9.47393995

H	0.28685995	1.56965873	-10.58890572
H	2.30689458	1.08686541	-9.21908677
H	2.14639999	1.00561954	-6.74780853
C	-2.54582949	1.75947670	-2.92191095
C	-3.24368523	2.84415189	-2.16654186
H	-4.32847118	2.61865153	-2.11703622
H	-2.88691374	2.86336099	-1.10798131
C	-3.02702576	4.22024794	-2.80363917
H	-1.96373434	4.48153304	-2.81788765
H	-3.38394391	4.23707975	-3.83855315
H	-3.55904574	5.00193769	-2.25349832
H	-2.97716852	1.49885176	-3.87452190
O	-0.14096473	4.39573245	0.00938084
C	-1.33610908	3.88350248	0.67416039
C	-0.86704384	3.33509522	2.02321044
C	0.45180737	4.07518275	2.31905926
C	0.79262989	4.84394187	1.03680175
H	1.79969166	4.62030417	0.62354153
H	0.65343876	5.93147053	1.13659295
H	1.25516223	3.36216232	2.58422906
H	0.34540469	4.75636363	3.17932398
H	-0.70406801	2.23794889	1.98655022
H	-1.61594170	3.49993510	2.81493441
H	-2.03379658	4.73042335	0.77390106
H	-1.75519139	3.12846555	-0.03196289
C	3.57011299	1.71032334	4.33133837
H	3.85811212	2.56098287	3.66198428
H	2.63250098	2.04500359	4.81902201
C	4.65676536	1.45736816	5.33654847
C	5.99428686	1.37030113	4.91813108
C	7.00565255	1.13257476	5.85161789
C	6.69225773	0.98200151	7.20676110
C	5.36172680	1.07266551	7.62600509
C	4.34490505	1.30900276	6.69617263
H	3.31283254	1.38402099	7.03321935
H	5.11491263	0.95972486	8.68079515
H	7.48198053	0.79716790	7.93196059
H	8.04189434	1.06591858	5.52281138
H	6.24541160	1.49330143	3.86565812
C	2.42600874	3.30796747	-3.63949907
O	1.85682484	3.81699627	-2.40274039
C	1.21756985	5.10474173	-2.63674183
C	1.03860678	5.24995305	-4.14933598
C	2.07189208	4.28922633	-4.76248291
H	1.66612193	3.77240845	-5.65056869
H	2.96536834	4.83956314	-5.10763700
H	0.01325828	4.97409128	-4.45822410
H	1.19533539	6.28832340	-4.48577887
H	0.27301406	5.06820211	-2.06239850
H	1.89734127	5.85916993	-2.20658978
H	3.50785313	3.22085854	-3.44779242
H	1.97277515	2.30524487	-3.78215076

Table 59. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with no THF isomer 2

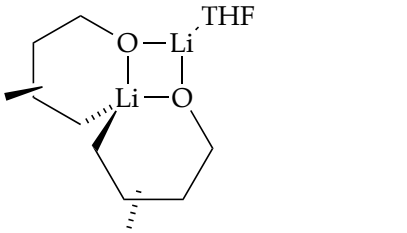


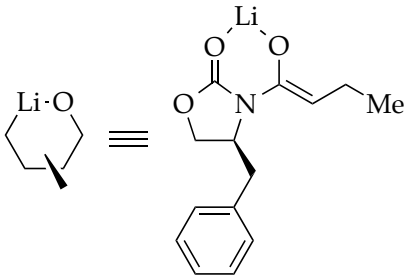
G = -1661.875945 Hartree
G_{MP2} = -1039554.194 kcal/mol
ΔG_{MP2} = 15.3933466 kcal/mol vs. **6** D_{2d} tetramer

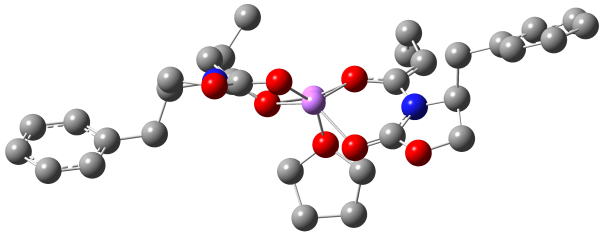
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	1.61465982	1.34721341	-1.29298275
O	0.00000000	0.00000000	1.91517720	O	-0.13420287	1.37776171	-1.43613406
C	1.01728616	0.00000000	2.59802520	C	-1.26337057	1.64138540	-2.04208625
O	0.95274838	0.23810925	3.93565776	N	-2.01545801	0.46848068	-2.46246574
C	2.23505051	-0.05258111	4.52175038	C	-2.74409085	0.38090436	-3.73399021
H	2.19335397	-1.05410783	4.96381657	C	-3.45575454	-0.96904188	-3.54447125
H	2.43195351	0.68113399	5.30490378	H	-4.46803059	-0.84748522	-3.14355356
C	3.22611718	0.01946957	3.34816436	H	-3.49585278	-1.57252925	-4.45256575
H	3.96359003	-0.78327643	3.42453433	O	-2.66177591	-1.66680120	-2.56720647
N	2.31248110	-0.22165786	2.22455173	C	-1.92571669	-0.75947821	-1.87071429
C	2.75357450	-0.39793141	0.84891806	O	-1.31147658	-1.09527210	-0.86517377
C	3.89651884	-1.08727865	0.62579009	H	-3.47649132	1.18782738	-3.81503220
H	4.39496595	-1.56920358	1.46212641	C	-1.78597682	0.43312292	-4.94730144
C	4.47543890	-1.31139793	-0.74416143	H	-1.17854629	1.33899013	-4.83856167
H	5.56263627	-1.14254672	-0.72234239	H	-1.10666986	-0.42630934	-4.89065732
H	4.06165057	-0.57121068	-1.44110657	C	-2.51487106	0.44481212	-6.27273529
C	4.20720820	-2.72241043	-1.30053154	C	-2.58414883	-0.70258345	-7.07424313
H	4.61110592	-3.49251310	-0.63228956	C	-3.28317362	-0.69280004	-8.28329898
H	3.13029013	-2.89927278	-1.39674731	C	-3.92676502	0.46905195	-8.70997488
H	4.66941556	-2.85822929	-2.28676504	C	-3.86300997	1.62127655	-7.92269234
O	1.98688873	0.16841119	-0.04724638	C	-3.16281593	1.60761846	-6.71684699

H	-3.10787470	2.51277389	-6.11525104
H	-4.35442559	2.53336883	-8.25124215
H	-4.46975459	0.47960984	-9.65113361
H	-3.32033144	-1.59239687	-8.89204337
H	-2.07461022	-1.60925590	-6.75459349
C	-1.76862774	2.86341041	-2.32958515
C	-1.07482974	4.15096945	-1.97896800
H	-0.00961063	3.95504058	-1.80092459
H	-1.12397244	4.84579453	-2.83092305
C	-1.66594737	4.84883684	-0.73961465
H	-2.73159504	5.06609747	-0.88084092
H	-1.57311179	4.20727805	0.14360243
H	-1.15477533	5.79788728	-0.53289282
H	-2.75764807	2.93537489	-2.77325818
C	3.95615843	1.37632569	3.21101473
H	4.44084282	1.38273815	2.22794537
H	3.20553700	2.17623648	3.21208703
C	4.97765215	1.60801631	4.30237664
C	6.20576372	0.92941659	4.28152168
C	7.14261305	1.11252902	5.29803625
C	6.86831781	1.98185402	6.35658981
C	5.65345533	2.66691019	6.38776658
C	4.71734231	2.47956344	5.36838578
H	3.77736921	3.02698442	5.39373052
H	5.43341698	3.35125776	7.20291974
H	7.59894811	2.12732349	7.14763132
H	8.08993522	0.58095382	5.26120954
H	6.43209535	0.25960820	3.45425363

Table 60. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with one THF isomer 2





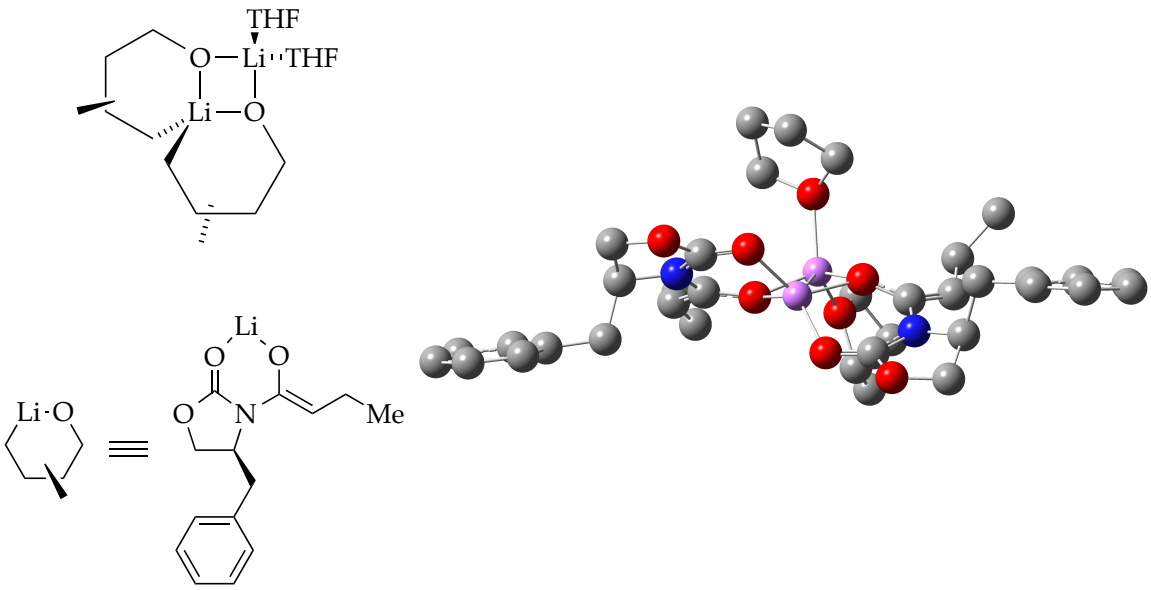


G = -1894.239434 Hartree
G_{MP2} = -1184882.872 kcal/mol
ΔG_{MP2} = 7.199447576 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.56521106	-1.19680514	-1.41982614
O	0.00000000	0.00000000	1.91054780	C	-1.62075689	-1.13464034	-2.18064299
C	1.07089690	0.00000000	2.50862880	N	-2.47982741	0.02082907	-1.94771922
O	1.17252059	0.53670784	3.75385891	C	-3.93264499	0.01897824	-2.16358414
C	2.46730262	0.21553212	4.29639021	C	-4.23661982	1.51632931	-1.99290770
H	2.35062638	-0.62240487	4.99232681	H	-4.25431148	2.04659640	-2.95173148
H	2.83973285	1.08577525	4.83943979	H	-5.16478727	1.71333065	-1.45415968
C	3.32756678	-0.16079095	3.07581749	O	-3.13956639	2.02586358	-1.21259314
H	3.93609033	-1.04096527	3.29776796	C	-2.09251177	1.16148764	-1.30173086
N	2.27641251	-0.49209864	2.10836570	O	-0.99768609	1.46254488	-0.83593481
C	2.53700429	-1.05257793	0.78731582	H	-4.16911361	-0.29881187	-3.18163396
C	3.45411556	-2.04991688	0.71217088	C	-4.65886999	-0.90004687	-1.15351956
H	3.86410608	-2.45805167	1.63139681	H	-4.18599408	-1.88607711	-1.21884020
C	3.87666682	-2.69422092	-0.57957637	H	-4.47657688	-0.51783450	-0.14168534
H	4.95675667	-2.90162286	-0.55681793	C	-6.14429596	-1.00350227	-1.41970669
H	3.72828124	-1.98918624	-1.40964275	C	-7.07429964	-0.32060557	-0.62436896
C	3.13721698	-4.00961678	-0.89798784	C	-8.44280557	-0.39713491	-0.89268064
H	3.29365583	-4.74778927	-0.10275064	C	-8.90388411	-1.16004671	-1.96573320
H	2.05480839	-3.84627722	-0.97462511	C	-7.98846200	-1.84942787	-2.76467552
H	3.48661682	-4.45042656	-1.84098919	C	-6.62306971	-1.77145460	-2.49234782
O	1.87815713	-0.49594777	-0.19192525	H	-5.91781201	-2.32248462	-3.11139994
Li	1.23251482	-1.14726212	-1.79618004	H	-8.33914929	-2.45407919	-3.59709282

H	-9.96830688	-1.22308264	-2.17517850	H	1.32726187	2.47773800	-5.12236282
H	-9.14699144	0.13614080	-0.25939245	H	3.95562664	2.00233573	-4.55616242
H	-6.72389492	0.26554341	0.22264738	H	2.86398363	2.39142606	-3.21348283
C	-1.99981862	-2.03404680	-3.12557615	H	3.60784429	0.25086449	-2.41948229
C	-1.25236189	-3.31538516	-3.38128766	H	3.85187652	-0.37091688	-4.07588814
H	-0.63595698	-3.55191030	-2.50507040	C	4.24441303	0.97178749	2.55866653
H	-1.96981527	-4.14346395	-3.48338839	H	4.62053413	0.65517341	1.57897854
C	-0.35911990	-3.29507051	-4.63733191	H	3.63562120	1.87011751	2.39975072
H	-0.94342356	-3.05385139	-5.53418046	C	5.39483528	1.26869356	3.49490993
H	0.43151252	-2.54048743	-4.54477203	C	6.48742666	0.39209795	3.57980908
H	0.11974939	-4.26902310	-4.80303963	C	7.53811883	0.64016055	4.46249533
H	-2.87391845	-1.83587576	-3.73826947	C	7.51660102	1.77435429	5.27786823
O	1.88550886	-0.31101649	-3.42436432	C	6.43950463	2.65744535	5.20024822
C	3.22031645	0.26282143	-3.44162158	C	5.38863884	2.40442566	4.31585275
C	3.06267985	1.67301415	-4.01669636	H	4.55795039	3.10425194	4.25271025
C	1.82497561	1.52572628	-4.91564490	H	6.41670083	3.54678484	5.82465308
C	0.95179715	0.58270251	-4.09242299	H	8.33626764	1.96992763	5.96396783
H	0.26813765	-0.03439954	-4.67948802	H	8.37727677	-0.04904017	4.51015228
H	0.37996032	1.12306170	-3.32868027	H	6.51747884	-0.48729890	2.93947816
H	2.09486622	1.06373518	-5.87273262				

Table 61. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with two THF isomer 2

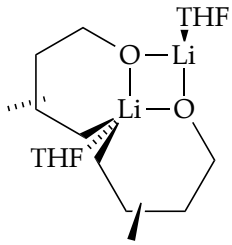


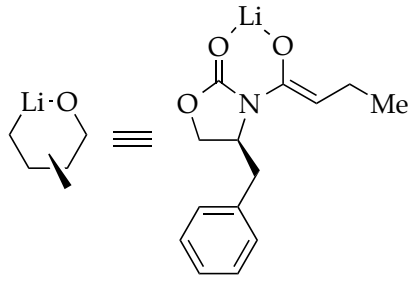
G = - 2126.595319 Hartree
G_{MP2} = - 1330207.012 kcal/mol
ΔG_{MP2} = 1.274348253 kcal/mol Li vs. **6** D_{2d} tetramer

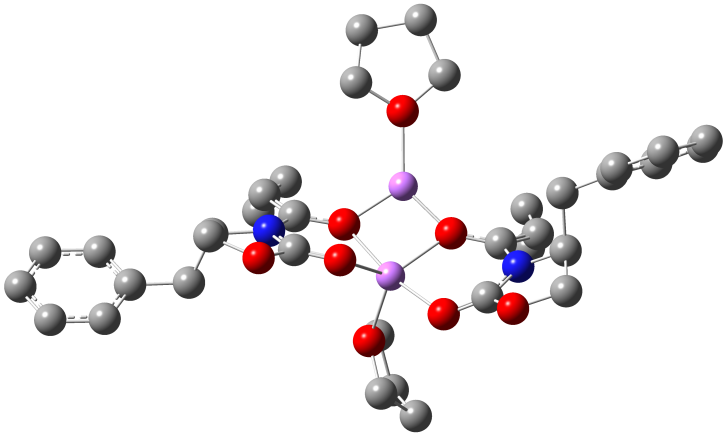
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.88616886	-1.14971633	-1.22897677
O	0.00000000	0.00000000	1.91162270	C	-1.99809927	-0.95943783	-1.86873565
C	1.07650503	0.00000000	2.49616371	N	-2.51823779	0.40964975	-1.81843405
O	1.17414804	0.53154391	3.74655589	C	-3.91575027	0.76605672	-2.09954620
C	2.47221623	0.22620475	4.28342433	C	-3.79515749	2.29279965	-2.20504143
H	2.37749019	-0.63801045	4.95081554	H	-3.64440625	2.62536254	-3.23865879
H	2.82311856	1.08718070	4.85468655	H	-4.64297575	2.82744744	-1.77378392
C	3.33607467	-0.08603226	3.05241961	O	-2.61736312	2.61368468	-1.44568655
H	3.99743436	-0.92875122	3.26395474	C	-1.84202513	1.49765101	-1.33836235
N	2.29437080	-0.47063487	2.08946597	O	-0.71640516	1.58069585	-0.85856681
C	2.58239826	-1.06114282	0.78089944	H	-4.23103416	0.34703039	-3.05761746
C	3.71263647	-1.81505561	0.68403554	C	-4.86730025	0.28354451	-0.97835904
H	4.30436450	-2.00487104	1.57418438	H	-4.68362323	-0.78674802	-0.83670963
C	4.25048548	-2.37752270	-0.60272213	H	-4.58610083	0.78761512	-0.04560095
H	3.54937031	-2.17181157	-1.41796302	C	-6.32395267	0.53714793	-1.29736409
H	4.33158532	-3.47576939	-0.53892027	C	-7.03210333	1.58012449	-0.68508830
C	5.63696188	-1.82024741	-0.97540419	C	-8.36837949	1.82759928	-1.00714585
H	5.59247958	-0.73515229	-1.12528422	C	-9.01972776	1.03312156	-1.95085503
H	6.36759639	-2.01291533	-0.17932350	C	-8.32795230	-0.01312660	-2.56595082
H	6.02202302	-2.27756395	-1.89630127	C	-6.99428832	-0.25745487	-2.24036615
O	1.73177157	-0.78184606	-0.16026783	H	-6.46700898	-1.08280326	-2.71477681
Li	0.87352612	-1.77883512	-1.57088312	H	-8.82975154	-0.64331630	-3.29573537

H -10.05997796 1.22276020 -2.20151224
H -8.89997716 2.63877179 -0.51642687
H -6.53530981 2.19619987 0.06147687
C -2.72122154 -1.88229445 -2.56131389
C -2.35890141 -3.34112811 -2.63741239
H -1.37457453 -3.49840753 -2.18450789
H -3.06868819 -3.94243211 -2.04323381
C -2.35803371 -3.89535865 -4.07281077
H -3.33282206 -3.74981393 -4.55612121
H -1.60809824 -3.38901360 -4.69230570
H -2.14174858 -4.97154566 -4.08732346
H -3.63118345 -1.58613033 -3.07304500
O 1.07615739 -3.74412215 -1.44166706
C 0.87534208 -4.33726439 -0.13474960
C 1.05877267 -5.84025868 -0.34526462
C 2.11508294 -5.87846412 -1.46131618
C 1.70970021 -4.68548925 -2.33304927
H 0.98426479 -4.97398022 -3.10454477
H 2.55738013 -4.18896852 -2.81415412
H 2.12398446 -6.81891026 -2.02059136
H 3.11557522 -5.72069365 -1.04235218
H 0.12286538 -6.29800072 -0.68685271
H 1.37615478 -6.35324112 0.56757235
H 1.62355527 -3.92293224 0.55170964
H -0.12316252 -4.05266417 0.20723894
C 4.17294101 1.11038022 2.54097066
H 4.53434793 0.84395798 1.54179727
H 3.50963353 1.97679393 2.42922350
C 5.33372317 1.44479330 3.45121267
C 6.47859345 0.63323004 3.46699094
C 7.54245106 0.91113605 4.32447792
C 7.48148060 2.01054684 5.18428862
C 6.35206807 2.82937085 5.17553348
C 5.28841429 2.54692804 4.31561173
H 4.41663374 3.19784436 4.30573171
H 6.29830194 3.69202979 5.83456202
H 8.31101407 2.22973949 5.85117564
H 8.42243018 0.27307038 4.31776002
H 6.53814345 -0.21736084 2.79081755
C 2.45363641 0.02638542 -3.26917087
O 1.60064499 -1.14003945 -3.33972033
C 0.68815211 -1.00184154 -4.46059109
C 0.90398216 0.41299667 -5.03097570
C 1.62458271 1.14776552 -3.88668535
H 2.23941239 1.98307548 -4.23633258
H 0.90950382 1.52806490 -3.14951668
H 1.54233631 0.37610533 -5.92134909
H -0.03929156 0.88748283 -5.31723639
H 0.90982171 -1.78617453 -5.19387716
H -0.32608546 -1.15091552 -4.07862324
H 2.70055079 0.17393075 -2.21662740
H 3.37226928 -0.16225066 -3.84404853

Table 62. Geometric coordinates and thermally corrected MP2 energies for **6** trans disolvated spirocyclic dimer with two THF





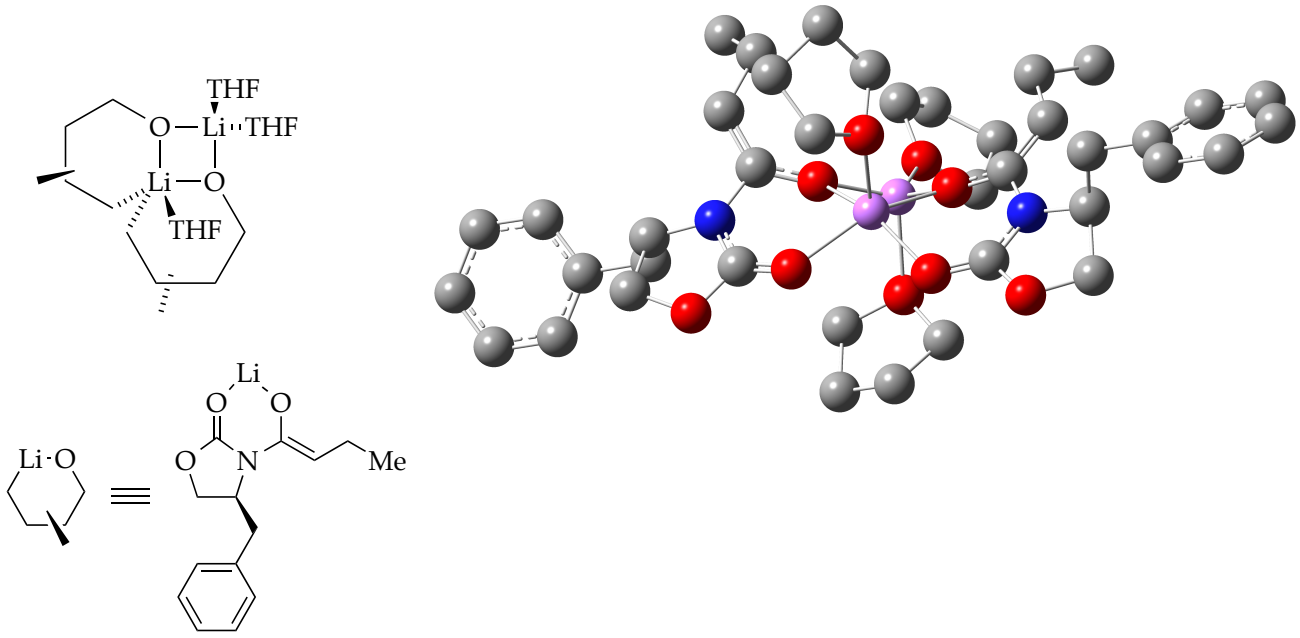


G = -2126.589252 Hartree
G_{MP2} = -1330201.148 kcal/mol
ΔG_{MP2} = 4.206354087 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.18273783	1.76295453	-2.94736720
Li	0.00000000	0.00000000	2.63669680	H	8.51859193	2.46671796	-3.36016691
O	1.43090494	0.00000000	1.53605375	H	10.19982909	2.35060230	-1.52926426
C	2.64817438	0.44005453	1.54807440	H	9.51811921	1.51743344	0.71426012
N	2.94365946	1.45339536	0.54659440	H	7.18335642	0.81296718	1.12142579
C	2.03098225	1.98636927	-0.33092135	C	3.64518206	0.06028397	2.40000878
O	0.85003855	1.73074005	-0.49944863	H	4.62791281	0.51505387	2.33246023
O	2.64215616	2.93824240	-1.09988435	C	3.48616822	-1.04532800	3.40935719
C	3.95849311	3.18331657	-0.58087033	H	3.62121051	-0.66642541	4.43739408
H	3.92406399	4.07175172	0.06108394	H	2.46197111	-1.43319146	3.35855464
H	4.63387768	3.36774451	-1.41796475	C	4.47488702	-2.20645881	3.19946560
C	4.29545362	1.91327008	0.21025024	H	5.51349206	-1.85372956	3.24068147
H	4.84967460	2.16384955	1.11802727	H	4.35722581	-2.98190553	3.96759174
C	5.07447174	0.85543132	-0.61061495	H	4.32459151	-2.67087452	2.21777515
H	5.03298535	-0.08479958	-0.05099209	O	-1.31642631	-0.43099399	1.48242747
H	4.54010459	0.69415420	-1.55482647	C	-2.55524297	-0.81078152	1.38486376
C	6.50853290	1.25401892	-0.87924427	N	-3.31705280	-0.15937432	0.32539228
C	7.47002323	1.18805141	0.14097330	C	-4.68167298	0.34582839	0.49233202
C	8.78817095	1.58093463	-0.08870677	C	-4.98847303	0.78062915	-0.95210617
C	9.17217273	2.04708829	-1.34834918	H	-5.52209816	0.00187711	-1.50901231
C	8.22888524	2.11305964	-2.37403346	H	-5.54828016	1.71557911	-1.01532938
C	6.90957867	1.71993422	-2.13885374	O	-3.70081243	0.97638712	-1.56090310

C	-2.76050804	0.30554808	-0.83201672	O	0.03408254	0.81405692	4.38352872
O	-1.61768646	0.17838449	-1.24277305	C	-0.92290953	0.74472557	5.46902677
H	-5.35728631	-0.45699862	0.79881994	C	-0.37334894	1.65320057	6.58225194
C	-4.74739532	1.48900734	1.53274287	C	1.12079421	1.76744073	6.23209308
H	-4.28758410	1.10835684	2.45225511	C	1.08275373	1.75724709	4.70777205
H	-4.12787488	2.32090924	1.17658355	H	1.99778250	1.41158088	4.22058890
C	-6.15931165	1.95773749	1.80509314	H	0.81464546	2.74570690	4.30765040
C	-6.63584143	3.16950321	1.28707538	H	1.67605813	0.89768027	6.60173749
C	-7.94968535	3.58307371	1.51831763	H	1.58755320	2.67057787	6.63630589
C	-8.81143440	2.78702898	2.27319856	H	-0.55227684	1.23782598	7.57811558
C	-8.34927701	1.57781461	2.79843096	H	-0.84771468	2.64010935	6.54084466
C	-7.03617964	1.16959472	2.56650020	H	-1.90244012	1.06534283	5.09968511
H	-6.68074703	0.23135631	2.98810473	H	-0.99300165	-0.30244441	5.78162864
H	-9.01128006	0.95430258	3.39392401	O	0.83834633	-1.58755661	-0.99738177
H	-9.83376447	3.10716027	2.45554364	C	0.99166578	-2.76393916	-0.16727700
H	-8.29688516	4.52886508	1.11047418	C	0.78774095	-3.96853931	-1.09543528
H	-5.96704077	3.80082386	0.70578689	C	-0.11197965	-3.38611124	-2.19715814
C	-3.21842968	-1.70766395	2.16001577	C	0.44337935	-1.96872056	-2.33071186
C	-2.59583483	-2.43955399	3.31656723	H	-0.28377977	-1.23409912	-2.68031456
H	-1.65087764	-1.95383882	3.59293562	H	1.32633991	-1.94845264	-2.98620909
H	-3.24593679	-2.37172619	4.20364218	H	-1.15537037	-3.35200633	-1.86214628
C	-2.32233870	-3.92848574	3.03154208	H	-0.06999783	-3.94781153	-3.13575879
H	-1.90061357	-4.43696631	3.90851525	H	0.34124739	-4.82185137	-0.57559097
H	-3.24590528	-4.45103246	2.75360260	H	1.74428499	-4.29552252	-1.52094795
H	-1.61848207	-4.03882307	2.19866799	H	1.97940521	-2.73223740	0.30152020
H	-4.23900329	-1.97454377	1.89857953	H	0.23110540	-2.72024262	0.62091477

Table 63. Geometric coordinates and thermally corrected MP2 energies for **6** spirocyclic dimer with three THF

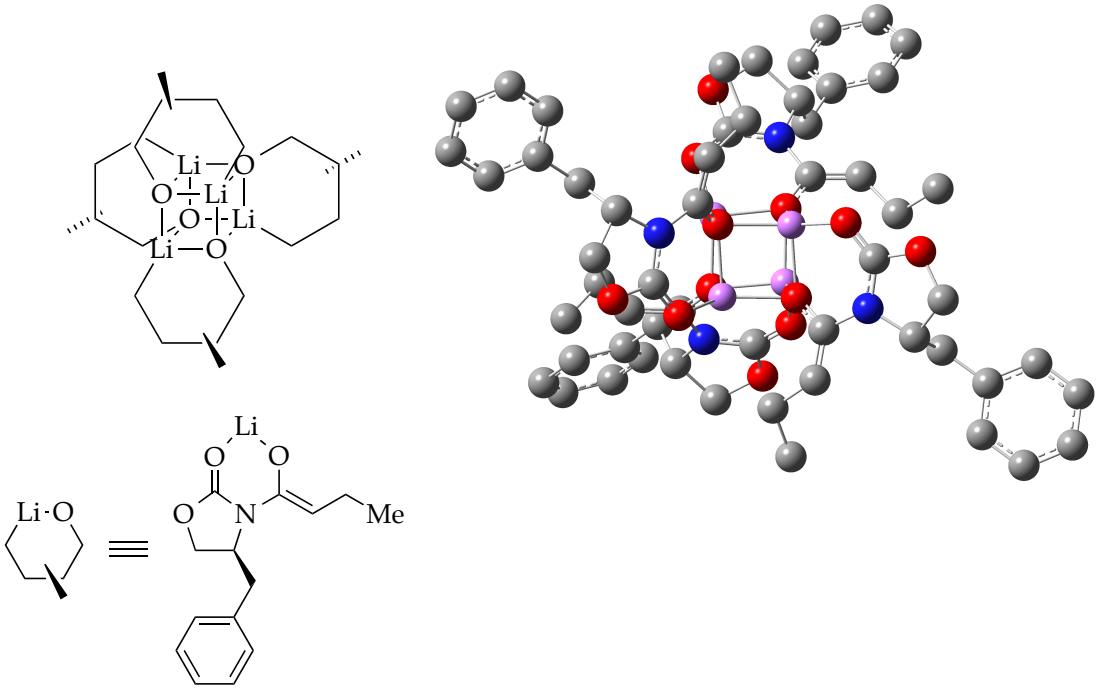


G = - 2358.93525 Hartree
G_{MP2} = - 1475523.693 kcal/mol
ΔG_{MP2} = -0.920884578 kcal/mol Li vs. **6** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	8.48191775	0.64486255	-4.27464102
Li	0.00000000	0.00000000	2.64404150	H	10.22924292	0.09821046	-2.58906335
O	1.42685657	0.00000000	1.43175902	H	9.55109319	-0.63490582	-0.30973369
C	2.69099910	-0.08648300	1.16659564	H	7.15726575	-0.81467429	0.27694190
N	3.13858440	0.76870104	0.07122899	C	3.62461421	-0.85475878	1.79600961
C	2.31128396	1.47697311	-0.76160653	H	4.65635059	-0.84015029	1.46202782
O	1.09574303	1.45772183	-0.86974136	C	3.31635085	-1.75383307	2.96148104
O	3.06325474	2.29121484	-1.56624137	H	3.33404981	-2.81501043	2.65708915
C	4.42740400	2.25248328	-1.11257916	H	2.29682978	-1.55770110	3.31050770
H	4.60494678	3.10945266	-0.45159584	C	4.30243161	-1.58341655	4.13020420
H	5.08315212	2.32161368	-1.98206116	H	4.08222216	-2.27861055	4.95154263
C	4.52985221	0.91735776	-0.36610735	H	5.33420991	-1.77563464	3.80852521
H	5.18771178	0.99642487	0.50304199	H	4.27246348	-0.56085668	4.52652287
C	4.98353419	-0.25203318	-1.27845701	O	-1.28164588	-0.75805988	1.50894099
H	4.77110032	-1.18758201	-0.75155639	C	-2.38715753	-1.34690015	1.18872769
H	4.35730605	-0.24273782	-2.17889710	N	-3.29383050	-0.54755415	0.35511721
C	6.44633293	-0.17289758	-1.65649744	C	-4.74897259	-0.50511379	0.51987638
C	7.44379879	-0.48350624	-0.71922164	C	-5.13773922	0.38203474	-0.67844572
C	8.79498663	-0.38564698	-1.04985717	H	-5.45018262	-0.21225379	-1.54459780
C	9.17654972	0.02437988	-2.32958617	H	-5.91716738	1.10963248	-0.44431818
C	8.19655918	0.33174442	-3.27363566	O	-3.93581869	1.09202590	-1.02350340
C	6.84461187	0.23359767	-2.93738765	C	-2.86397859	0.41882319	-0.50454670
H	6.08641134	0.46481852	-3.68269347	O	-1.72316123	0.70761354	-0.83489637

H	-5.17865151	-1.50391629	0.40420269
C	-5.16643706	0.06464461	1.89610927
H	-4.62562354	-0.50848390	2.65776446
H	-4.82491323	1.10498260	1.96200202
C	-6.65733390	-0.01733415	2.13703830
C	-7.47635425	1.11516021	2.03613258
C	-8.85641568	1.02371206	2.23048228
C	-9.44084881	-0.20710470	2.52970982
C	-8.63606116	-1.34396035	2.63741919
C	-7.25853168	-1.24791752	2.44363731
H	-6.63642219	-2.13539590	2.54123584
H	-9.08148490	-2.30570189	2.87853327
H	-10.51412191	-0.28041259	2.68320212
H	-9.47252348	1.91565852	2.15144631
H	-7.02739171	2.08115096	1.81419633
C	-2.82085092	-2.59332134	1.52241659
C	-2.08357255	-3.52509045	2.44243882
H	-1.77278405	-4.43660086	1.90493637
H	-1.15868859	-3.04109526	2.77581558
C	-2.91215217	-3.95797597	3.66540409
H	-3.83989191	-4.45660922	3.35659640
H	-2.35801328	-4.65900855	4.30340609
H	-3.19690190	-3.09059705	4.27398861
H	-3.75993360	-2.95195184	1.10847377
O	-0.46173907	1.98838671	2.96549211
C	-1.86788729	2.32619928	2.97796390
C	-2.04209644	3.55021079	2.05432729
C	-0.71475019	3.60260825	1.27474999
C	0.27078432	3.03067644	2.28918318
H	0.58515780	3.78960550	3.02242670
H	1.14893577	2.55996831	1.84577762
H	-0.44994925	4.61579244	0.95591635
H	-0.75280759	2.96103684	0.38997402
H	-2.17963533	4.46175828	2.64747606
H	-2.90870940	3.44794260	1.39411569
H	-2.40604887	1.44462753	2.62028670
H	-2.17672024	2.53603921	4.00980688
O	0.21450421	-0.47842068	4.58629646
C	-0.09693307	-1.68795882	5.30702048
C	0.17083317	-1.36318031	6.77661261
C	1.35882512	-0.39399607	6.67057749
C	1.01936006	0.40323548	5.40703068
H	1.90015786	0.69985571	4.83009714
H	0.42680584	1.29777277	5.62753722
H	2.29215708	-0.95108920	6.53237933
H	1.47408414	0.24924830	7.54818069
H	0.39040487	-2.25570503	7.37011649
H	-0.69717247	-0.86157632	7.22100429
H	-1.13502173	-1.95116528	5.09162471
H	0.55386926	-2.49740370	4.94941087
O	0.50156167	-1.62026944	-1.12049062
C	0.78945454	-2.82958611	-0.37179027
C	0.25861125	-3.99254304	-1.22168393
C	-0.83236028	-3.31458507	-2.06690662
C	-0.20226541	-1.94813565	-2.33276588
H	-0.91776053	-1.14517312	-2.52436002
H	0.51161517	-1.99415440	-3.16861306
H	-1.74777052	-3.19764545	-1.47539727
H	-1.07280196	-3.85822343	-2.98626361
H	-0.12138511	-4.81320582	-0.60565180
H	1.04720622	-4.39384408	-1.86999089
H	1.86762451	-2.87544287	-0.18989343
H	0.27304961	-2.74896186	0.58829053

Table 64. Geometric coordinates and thermally corrected MP2 energies for **6** S_4 tetramer

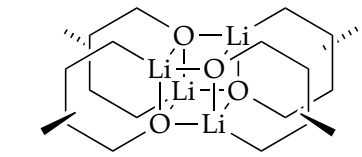


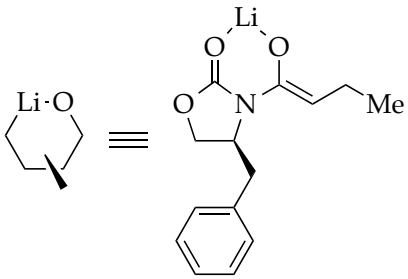
G = - 3323.810652 Hartree
G_{MP2} = - 2079166.49 kcal/mol
ΔG_{MP2} = 0.867684937 kcal/mol Li vs. **6** D_{2d} tetramer

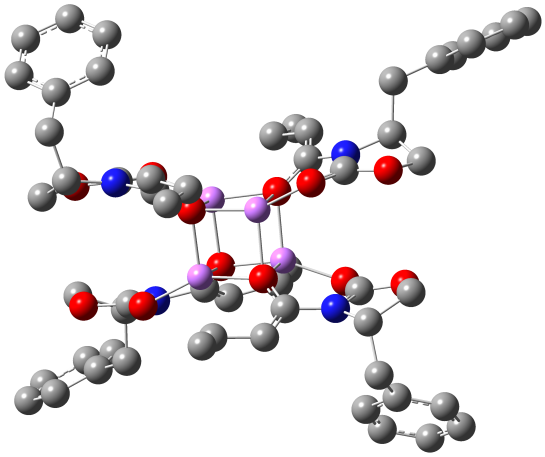
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.94213511	-4.68435329	-0.99585664
O	0.00000000	0.00000000	1.89041750	N	-1.16282136	-3.61274388	-1.40101251
C	1.03901107	0.00000000	2.54440496	C	-1.47938923	-2.24543547	-1.01907917
O	1.02139463	0.38480264	3.84700012	O	-0.55716310	-1.35486810	-1.31393585
C	2.30005966	0.09502010	4.44063498	Li	-0.31207464	0.04738266	-2.63429328
H	2.21126307	-0.83531077	5.01213236	O	-1.60364761	1.03446440	-3.56095477
H	2.56014277	0.91105288	5.11640863	C	-1.91576903	2.18189301	-3.25903491
C	3.26241121	-0.04392567	3.24979762	O	-2.90292226	2.80987864	-3.95211912
H	3.93197254	-0.89219485	3.40825960	C	-3.22333628	4.04508670	-3.28671687
N	2.30827350	-0.33682390	2.16987644	H	-4.09118466	3.87679359	-2.63920648
C	2.71439402	-0.76696649	0.84109527	H	-3.47005255	4.79129539	-4.04301241
O	1.91241571	-0.39964658	-0.13484599	C	-1.95744974	4.37284329	-2.48895341
Li	1.36285492	-1.67509213	-1.52903981	H	-2.21356674	4.81304949	-1.52300426
O	1.18298699	-3.55688509	-1.51823002	N	-1.41456119	3.01781176	-2.29714471
C	0.09110637	-4.11004652	-1.61338108	C	-0.40075404	2.69672044	-1.30271572
O	0.02087506	-5.41402667	-1.98734793	O	0.04907774	1.46212082	-1.33967223
C	-1.33005263	-5.88027320	-1.81712537	Li	1.92726838	0.91711451	-1.56156213
H	-1.38406311	-6.44372202	-0.87924344	O	3.38835094	1.70336368	-2.42656579
H	-1.57521714	-6.54058538	-2.65025418	C	3.77699873	1.35653670	-3.53734448
C	-2.18351049	-4.60218095	-1.77734033	O	4.88035714	1.94425932	-4.07249499

C	5.25089171	1.23355895	-5.26780698
H	6.03345544	0.50972046	-5.01402957
H	5.63763543	1.95220909	-5.99144385
C	3.95134706	0.55386227	-5.70997481
H	4.15469508	-0.43826729	-6.11834298
N	3.26749765	0.43394847	-4.41166676
C	2.13797655	-0.45577646	-4.18281567
O	1.57943316	-0.35845481	-2.99685468
C	1.76336020	-1.29758212	-5.17812580
H	2.30787086	-1.30443144	-6.11531826
C	0.63163761	-2.28351766	-5.07565892
H	0.12568317	-2.17420301	-4.10985538
H	-0.12647784	-2.06283190	-5.84392035
C	1.08965261	-3.74357166	-5.24517058
H	1.77653700	-4.03286016	-4.44299626
H	0.23675609	-4.43458798	-5.22722867
H	1.60816488	-3.88566575	-6.20188444
C	3.13019722	1.39449211	-6.71957684
H	2.12189904	0.97076419	-6.76534692
H	3.03405894	2.41135274	-6.31948625
C	3.75535665	1.43067815	-8.09713205
C	3.67427359	0.31508509	-8.94452260
H	3.12793198	-0.56725604	-8.61735333
C	4.27062151	0.32719644	-10.20489802
H	4.19208377	-0.54583797	-10.84749246
C	4.96028625	1.45993014	-10.64368868
C	5.04474807	2.57848649	-9.81434071
C	4.44695320	2.56147276	-8.55223414
H	4.50623591	3.44286017	-7.91689875
H	5.57199349	3.46791124	-10.14929673
H	5.42282959	1.47154226	-11.62688129
C	-0.01410267	3.66459643	-0.43477005
H	-0.46519079	4.64890169	-0.48509765
C	1.00479064	3.47048804	0.65497526
H	1.42449878	2.45978093	0.59987333
H	1.85003020	4.16052488	0.50302974
C	0.42948146	3.70397087	2.06379330
H	-0.35483713	2.97445179	2.29100720
H	1.20786772	3.61597745	2.83296770
H	-0.00667137	4.70728050	2.15035220
C	-0.96846322	5.28818875	-3.25333977
H	-0.00479856	5.24503380	-2.73584886
H	-0.81546103	4.86592799	-4.25414359
C	-1.45353926	6.71780740	-3.35669660
C	-1.98889658	7.21939707	-4.55081443
H	-2.02492503	6.57961500	-5.43024045
C	-2.45961275	8.53180924	-4.63184792
H	-2.86630841	8.90186230	-5.56935485
C	-2.40255158	9.36581504	-3.51502336
C	-1.86774275	8.88067050	-2.31924971
C	-1.39783265	7.57004880	-2.24324300
H	-0.97080030	7.20583875	-1.31101563
H	-1.81115957	9.52573878	-1.44634071
H	-2.76628187	10.38792410	-3.57621498
C	-2.67260618	-2.00252397	-0.42737430
H	-3.32136734	-2.83559447	-0.17400721
C	-3.17476685	-0.62948512	-0.06850120
H	-3.12680154	-0.47473798	1.02094033
H	-2.52212465	0.13143840	-0.51379824
C	-4.61856192	-0.38105211	-0.53685330
H	-4.69293905	-0.44127148	-1.62899810
H	-5.30541074	-1.12566272	-0.11430488
H	-4.97282388	0.60874759	-0.22358523
C	-2.86417533	-4.24227009	-3.11853884
H	-3.23549061	-3.21551337	-3.02779702
H	-2.10350652	-4.24458437	-3.90865280
C	-3.99478918	-5.18425093	-3.46916048
C	-5.22450840	-5.09758886	-2.79869336
H	-5.37078578	-4.32205121	-2.04955114
C	-6.26386261	-5.97981897	-3.09155865
H	-7.21044230	-5.89262400	-2.56454172
C	-6.09264053	-6.96716011	-4.06489795
C	-4.87753628	-7.06125321	-4.74364134
C	-3.83866419	-6.17646270	-4.44628561
H	-2.89880332	-6.24777374	-4.98984311
H	-4.73712031	-7.82015397	-5.50893756
H	-6.90304388	-7.65315986	-4.29611886
C	3.86339857	-1.47199809	0.71619272
H	4.40374180	-1.77309856	1.60864078
C	4.45619277	-1.89672231	-0.60077194
H	4.31950824	-2.97894678	-0.75320258
H	3.92350480	-1.40311140	-1.42285934
C	5.95497271	-1.57021543	-0.71333193
H	6.12698479	-0.48917345	-0.65252595
H	6.52526128	-2.04461447	0.09566271
H	6.36945820	-1.92999378	-1.66312224
C	4.09867658	1.22162896	2.94863810
H	4.55476204	1.08110471	1.96244535
H	3.41994303	2.07990655	2.87395215
C	5.16372132	1.47792871	3.99196484
C	6.32661867	0.69325456	4.02665203
H	6.47327386	-0.07772151	3.27289010
C	7.30135670	0.89978102	5.00214683
H	8.19738891	0.28459907	5.00851718
C	7.13138458	1.89940915	5.96308361
C	5.98306056	2.69105517	5.93713648
C	5.00861261	2.47997685	4.95916510
H	4.12231397	3.11075786	4.93752509
H	5.84531951	3.47731221	6.67480346
H	7.89185753	2.06326888	6.72179660

Table 65. Geometric coordinates and thermally corrected MP2 energies for **6** D_{2d} tetramer







G = - 3323.803718 Hartree
G_{MP2} = - 2079169.961 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **6** tetramer

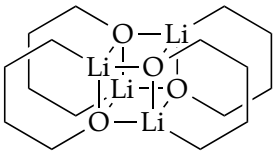
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	0.20623812	3.04334315	-5.07420755
O	0.00000000	0.00000000	1.89606150	C	-1.17196529	2.98962765	-5.51680026
C	1.05872974	0.00000000	2.51655724	H	-1.31665228	2.05574199	-6.06816275
O	1.13935282	-0.60632017	3.72982399	H	-1.35343423	3.84722458	-6.16563436
C	2.51596600	-0.60470732	4.16232353	C	-1.96828020	3.02579054	-4.20801765
H	2.94042296	-1.59087178	3.95064096	H	-2.86781239	2.40840902	-4.26022077
H	2.52515513	-0.41139920	5.23622264	N	-0.99398175	2.38858026	-3.30952956
C	3.17920584	0.50745228	3.33229682	C	-1.33616793	1.63903994	-2.11386966
H	4.16944382	0.20556421	2.97929316	C	-2.54988688	1.82900054	-1.54494206
N	2.26402940	0.54933700	2.18345240	H	-3.21209586	2.59315041	-1.93680444
C	2.63495844	0.97134542	0.84438330	C	-3.05793934	1.04426554	-0.36386659
C	3.68879748	1.80541919	0.68039442	H	-2.51380417	0.09448808	-0.28225470
H	4.19052783	2.21496455	1.54908226	H	-2.86493419	1.58259312	0.57888667
C	4.23080331	2.21671987	-0.66371973	C	-4.56244576	0.74615390	-0.45377824
H	3.80017144	3.17977338	-0.98447458	H	-5.14536715	1.67379935	-0.52156850
H	3.93246691	1.48661982	-1.42749309	H	-4.79190589	0.14396400	-1.34053193
C	5.76208925	2.34250564	-0.67285814	H	-4.91225163	0.19947840	0.42973038
H	6.10266831	3.07764785	0.06746809	O	-0.41417782	0.78706319	-1.72393503
H	6.23715025	1.38436843	-0.43205164	Li	-0.02671083	-1.00978836	-2.49757812
H	6.12735786	2.66690750	-1.65426398	O	-0.32175009	-1.06019622	-4.37001753
O	1.90894628	0.44047400	-0.11502547	C	0.56563543	-0.72226740	-5.14736859
Li	1.52568693	1.01337243	-1.92772842	O	0.24886030	-0.15636294	-6.34133401
O	1.35426419	2.35462433	-3.27000996	C	1.46154218	0.29138364	-6.98247615
C	0.26635600	2.55669429	-3.80291494	H	1.55897864	1.36798474	-6.81240779

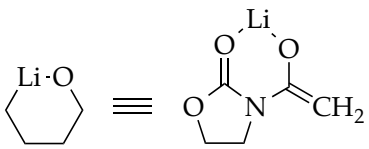
H	1.36764448	0.08386911	-8.04963710
C	2.57931195	-0.51219229	-6.29646375
H	3.45357647	0.11296298	-6.09356631
N	1.92151395	-0.82741278	-5.02090536
C	2.61570062	-1.06557089	-3.76790048
C	3.89943692	-1.49511740	-3.79230665
H	4.36774508	-1.73685326	-4.73904118
C	4.74879298	-1.66620457	-2.55977723
H	4.71216782	-2.70679680	-2.19691540
H	4.35126446	-1.05038014	-1.74229435
C	6.21863353	-1.28541419	-2.79459700
H	6.66083050	-1.89168454	-3.59547711
H	6.31086454	-0.23260195	-3.08577740
H	6.81822321	-1.44268229	-1.89041641
O	1.91292173	-0.78229656	-2.69306807
Li	2.03143837	-1.40127781	-0.85896577
O	2.53004235	-2.68521015	0.45759135
C	1.66956611	-3.22516575	1.14780296
O	1.97429804	-3.66868813	2.39962024
C	0.74430544	-4.06757378	3.05251307
H	0.38272341	-3.22135495	3.64432779
H	0.96382299	-4.91829814	3.69863051
C	-0.18705782	-4.40420911	1.88306830
H	-1.22170778	-4.12254634	2.09095450
N	0.36528777	-3.50240026	0.86120231
C	-0.38950901	-2.94387880	-0.24635144
C	-1.54208598	-3.54484099	-0.62483232
C	-2.45989333	-3.00761958	-1.69162455
H	-2.28924930	-1.93167660	-1.82632685
H	-2.24193421	-3.47055886	-2.66837793
C	-3.94387870	-3.23602817	-1.36610627
H	-4.16019820	-4.30462294	-1.23872637
H	-4.22580791	-2.72685669	-0.43718896
H	-4.58871095	-2.86148931	-2.16965717
H	-1.84077735	-4.47577916	-0.15565620
O	0.12114425	-1.84315452	-0.75198455
C	-0.09990232	-5.89561587	1.46736773
H	-0.56670326	-6.01162899	0.48431919
H	0.95887071	-6.15462783	1.34441740
C	-0.75044694	-6.82142879	2.47337791
C	0.01990776	-7.63172825	3.31801293
C	-0.58446903	-8.46770328	4.25961924
C	-1.97435906	-8.50493160	4.37189417
C	-2.75514330	-7.70439389	3.53462773
C	-2.14764688	-6.87228898	2.59502917
H	-2.76579639	-6.25981510	1.94163315
H	-3.83900794	-7.73149985	3.61034149
H	-2.44719487	-9.15558835	5.10252843
H	0.03208703	-9.09152242	4.90148348
H	1.10418193	-7.61693930	3.22867403
C	3.03398426	-1.74705416	-7.12462820
H	3.45745508	-1.35408040	-8.05846350
H	3.85688676	-2.23848770	-6.59787700
C	1.95399343	-2.76101481	-7.43425284
C	1.33574312	-2.80122078	-8.69122375
C	0.33297392	-3.73173878	-8.96870438
C	-0.06605355	-4.64150551	-7.98922924
C	0.54993488	-4.62047722	-6.73603396
C	1.55372698	-3.69123787	-6.46234756
H	2.03682055	-3.68805242	-5.48841038
H	0.25284663	-5.33169173	-5.96995344
H	-0.84637551	-5.36710951	-8.20247869
H	-0.13219893	-3.74747146	-9.95092494
H	1.65065915	-2.10502081	-9.46627506
C	-2.32206957	4.47073372	-3.77020777
H	-2.64173711	4.44980412	-2.72372653
H	-1.40574714	5.07260634	-3.80633107
C	-3.39323730	5.09803460	-4.63708849
C	-4.72760319	4.67452572	-4.53876212
C	-5.71704149	5.22976417	-5.34932549
C	-5.38987518	6.22318923	-6.27537745
C	-4.06833124	6.65683865	-6.38145326
C	-3.08018193	6.09695944	-5.56853114
H	-2.05372413	6.44871623	-5.64917122
H	-3.80418516	7.43396507	-7.09390308
H	-6.16088997	6.65819419	-6.90550625
H	-6.74512252	4.89009248	-5.25496832
H	-4.99523904	3.90785495	-3.81436815
C	3.31722858	1.84549111	4.11207398
H	3.98763929	1.64269649	4.95778493
H	3.83551495	2.56936820	3.47683246
C	2.02225567	2.44759574	4.61295642
C	1.62983471	2.31308164	5.95151465
C	0.42956149	2.86153850	6.40642628
C	-0.39829016	3.55797140	5.52556808
C	-0.01380803	3.70989209	4.19159746
C	1.18758233	3.16309463	3.74031017
H	1.48604535	3.29502483	2.70326931
H	-0.64724686	4.25928240	3.50029935
H	-1.33322979	3.98609869	5.87695705
H	0.14484428	2.74766001	7.44919103
H	2.27620056	1.78403012	6.64928748

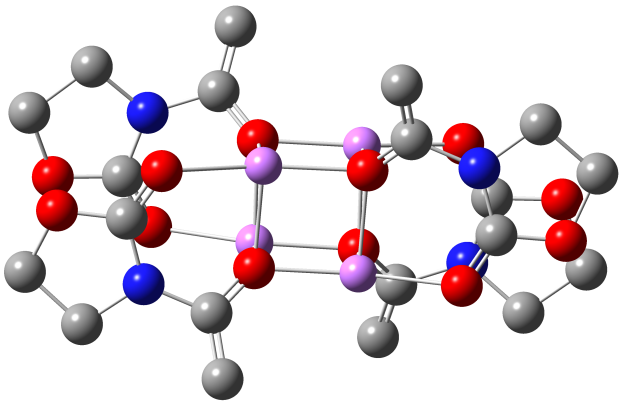
Part 7: Tetramer Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 66. Geometric coordinates and thermally corrected MP2 energies for **30** D_{2d} tetramer





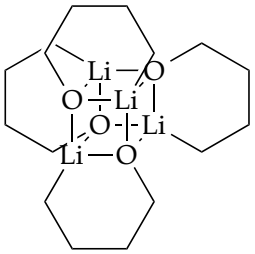


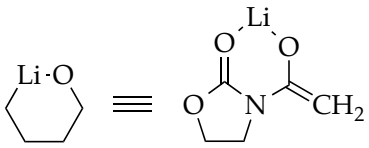
G = -1928.469207 Hartree
G_{MP2} = -1206550.771 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **30** D_{2d} tetramer

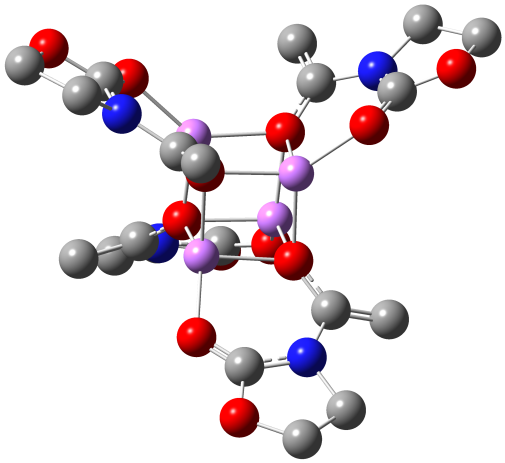
Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-11.05478252	1.71672864	-5.19443396
H	0.00000000	0.00000000	1.10595930	C	-9.57695876	2.67191073	-3.81917142
H	1.02202664	0.00000000	-0.40665553	H	-9.86791047	3.23971948	-2.90805047
O	-0.56412657	1.30157169	-0.38312248	H	-9.40319163	3.40328548	-4.63679727
C	-1.79319532	1.12101945	-1.01570045	O	-7.80476399	-0.43212379	-3.75403705
N	-2.04772055	-0.23815300	-1.17507871	Li	-6.21050266	-0.34902967	-2.28740655
C	-3.26087572	-0.87191989	-1.71885907	O	-7.06192467	-0.53656660	-0.35532703
O	-4.31565077	-0.17921553	-1.46609798	C	-7.93259389	-1.46601550	-0.17004969
Li	-4.59357363	1.89869133	-1.42880622	N	-9.26265464	-1.07600193	-0.66793067
O	-2.43738597	2.10350997	-1.33594294	C	-9.81521768	0.20066306	-0.71636327
O	-6.51056335	1.72405411	-2.19531182	O	-11.06065314	0.15417154	-1.34094803
C	-7.13208530	2.51074027	-3.00222690	C	-11.32502390	-1.20434177	-1.83455680
N	-8.33934144	1.87826991	-3.56041889	H	-11.33738553	-1.11339469	-2.93668261
C	-8.54879025	0.52884980	-3.83009303	H	-12.31678524	-1.46553194	-1.43692638
O	-9.85710764	0.33121984	-4.26897234	C	-10.17243478	-2.07497461	-1.30267942
C	-10.60728951	1.59264586	-4.19730105	H	-9.64021518	-2.62059463	-2.11275686
H	-11.37752652	1.42637855	-3.42128328	H	-10.51034533	-2.82126035	-0.55267875

O	-9.40254931	1.27230325	-0.31123401
Li	-7.25427903	1.54658516	-0.21811117
O	-5.33950714	1.74166882	0.54939135
C	-4.90231414	2.57819528	1.42422949
N	-3.58053372	2.18639888	1.94227921
C	-3.07344397	0.89994397	2.10177577
O	-1.75078126	0.96302914	2.53765193
C	-1.30131257	2.36136971	2.57898971
H	-0.51928784	2.43604798	1.80056704
H	-0.88522791	2.49869414	3.58791945
C	-2.54918500	3.21150520	2.27993807
H	-2.39901225	3.90380003	1.42239716
H	-2.87560345	3.81500110	3.15336476
O	-3.58490457	-0.19296250	1.93810172
Li	-5.16928787	-0.34624590	0.46672184
C	-5.48822363	3.71084633	1.84282257
H	-6.43164725	4.04675637	1.45600802
H	-5.09890176	4.36303453	2.59695033
C	-7.73579855	-2.68204074	0.36281142
H	-8.49954116	-3.41438052	0.52415137
H	-6.77119244	-3.01341206	0.69782239
C	-6.81708552	3.77546081	-3.32259511
H	-5.96775136	4.28019487	-2.90260934
H	-7.34977766	4.38374101	-4.02394110
C	-3.18519274	-2.05190111	-2.35389545
H	-4.05397544	-2.56085944	-2.72631315
H	-2.27841648	-2.57898417	-2.56742315
C	-0.93354243	-1.05842859	-0.61448607
H	-1.32477903	-1.77383100	0.14202721
H	-0.44343498	-1.64619564	-1.41944030

Table 67. Geometric coordinates and thermally corrected MP2 energies for **30** S_4 tetramer





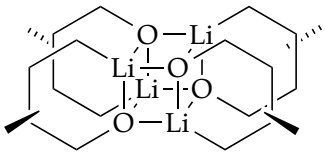


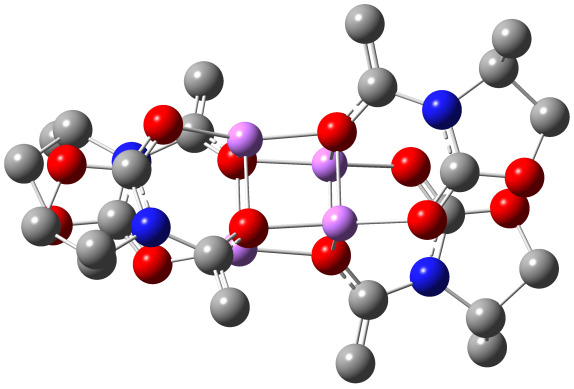
G = -1928.471624 Hartree
G_{MP2} = -1206544.781 kcal/mol
ΔG_{MP2} = 1.497452719 kcal/mol Li vs. **30** D_{2d} tetramer

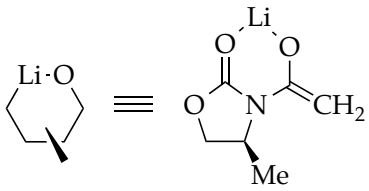
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-3.28863090	2.86182952	-3.30493357
O	0.00000000	0.00000000	1.89154310	C	-3.71239726	3.88909530	-2.38986970
C	1.03981492	0.00000000	2.53944564	H	-4.51473301	3.48329620	-1.76414957
N	2.32240599	-0.26420911	2.14124019	H	-4.09462088	4.72932306	-2.97188085
C	3.20653179	-0.33871641	3.30062953	C	-2.45393877	4.21810349	-1.57895150
C	2.36422671	0.37781159	4.36209901	N	-1.66732322	3.00373516	-1.77374500
H	2.40006766	-0.09322606	5.34579393	C	-0.43019853	2.76188224	-1.06324984
H	2.62717029	1.43715767	4.45472323	O	0.05861571	1.55233313	-1.19531325
O	1.01532639	0.28793187	3.86753003	Li	1.94566055	1.07556623	-1.46641297
H	3.41416570	-1.38422228	3.56388482	O	3.46315652	1.88394312	-2.25528817
H	4.15512468	0.16406923	3.09700008	C	3.97881910	1.43816708	-3.27330935
C	2.74332841	-0.67912158	0.82041987	O	5.21667068	1.85507979	-3.64915740
O	1.91338952	-0.37475700	-0.14804186	C	5.66166672	1.07665591	-4.77531836
Li	1.40396223	-1.52483637	-1.65786882	H	6.36627797	0.31979787	-4.41389802
O	1.24772885	-3.38355837	-1.97278153	H	6.17066085	1.74394671	-5.47278718
C	0.16287365	-3.91896519	-2.16621587	C	4.37873437	0.45392817	-5.33733732
O	0.10535188	-5.18058498	-2.66856264	H	4.51099065	-0.58310909	-5.65538285
C	-1.26471575	-5.52093660	-2.95011900	N	3.49618795	0.53038710	-4.17687070
H	-1.42718019	-6.55870174	-2.65437542	C	2.18690237	-0.08553521	-4.15962108
H	-1.43054795	-5.41820221	-4.02802539	O	1.59523134	-0.09942992	-2.98954532
C	-2.08186906	-4.50976672	-2.13809004	C	1.70632722	-0.61249828	-5.30872768
H	-2.41059708	-4.91411622	-1.17169117	H	2.22377895	-0.54921887	-6.25620586
N	-1.10200280	-3.44478900	-1.94559774	H	0.74593794	-1.11350932	-5.29238713
C	-1.45055991	-2.17173598	-1.35256342	C	0.09015536	3.76085708	-0.31466095
O	-0.51821264	-1.25245144	-1.42321190	H	-0.33852895	4.75229160	-0.26187440
Li	-0.30065411	0.27519856	-2.63170630	H	0.99254601	3.57199345	0.25424780
O	-1.66204973	1.32577721	-3.42000198	H	-2.65954633	4.38011484	-0.51802465
C	-2.13256079	2.30606249	-2.85551480	H	-1.91909833	5.09386229	-1.96944465

C	-2.68466920	-2.02442380	-0.81927627
H	-3.40884802	-2.82545934	-0.76098061
H	-2.96681301	-1.06059776	-0.41299702
H	-2.95733785	-4.13772763	-2.67588696
C	3.93837992	-1.29850213	0.68874943
H	4.57426676	-1.55209389	1.52589280
H	4.27864263	-1.57245193	-0.30261167
H	3.96586932	1.02763756	-6.17751151

Table 68. Geometric coordinates and thermally corrected MP2 energies for **31** D_{2d} tetramer





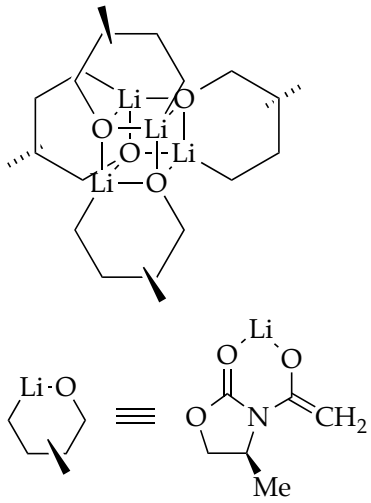


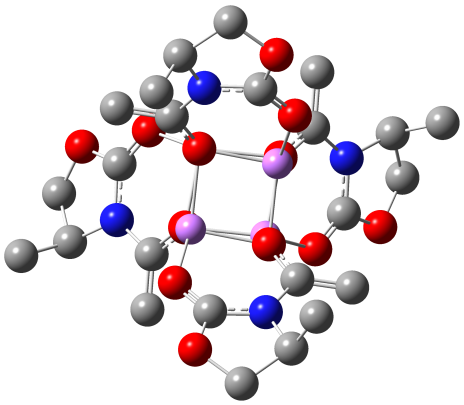
G = -2085.622761 Hartree
G_{MP2} = -1304802.017 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **31** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.28351768	-1.09491846	-4.38407154
O	0.00000000	0.00000000	1.90900000	C	0.63253600	-0.80584742	-5.14776364
C	1.05635845	0.00000000	2.53354127	O	0.35649622	-0.32723874	-6.39378352
O	1.10250978	-0.51236596	3.79575238	C	1.59247026	0.12144461	-6.99627256
C	2.48572129	-0.57721434	4.21343985	H	1.68279304	1.19884822	-6.82562301
H	2.85559641	-1.58716176	4.01027393	H	1.54116578	-0.09203161	-8.06554571
H	2.52309319	-0.36583172	5.28370527	C	2.67199454	-0.68194833	-6.25811532
C	3.17870188	0.48599809	3.35028208	H	3.56720707	-0.08098188	-6.07997869
H	4.17490093	0.16225707	3.03870509	N	1.98298536	-0.89750367	-4.97511887
N	2.28729635	0.46995314	2.17877832	C	2.66351832	-1.09178999	-3.71202641
C	2.70364549	0.82498534	0.83829806	C	3.97717857	-1.41149459	-3.70937317
C	3.85794700	1.50634887	0.66151043	H	4.54749892	-1.60068445	-4.60776731
H	4.46836991	1.86855610	1.47659016	H	4.49476244	-1.48298780	-2.76007064
H	4.19793071	1.70350881	-0.34830196	O	1.91823974	-0.87568663	-2.65474040
O	1.91314611	0.38381838	-0.11063748	Li	2.00624586	-1.47849633	-0.81577169
Li	1.57168746	0.94948705	-1.93172163	O	2.42313420	-2.73493297	0.55939616
O	1.41927131	2.24469060	-3.32554094	C	1.53258181	-3.23642191	1.23869891
C	0.33804566	2.45719754	-3.86574149	O	1.80686153	-3.69180088	2.49378596
O	0.29562307	2.94662433	-5.13716112	C	0.55898947	-4.03525100	3.13925840
C	-1.07472414	2.90638280	-5.59792650	H	0.23996747	-3.17843277	3.74107518
H	-1.21534531	1.98222558	-6.16735916	H	0.73880966	-4.90288462	3.77676439
H	-1.23956735	3.77624154	-6.23644738	C	-0.39293940	-4.31671990	1.96870733
C	-1.89705758	2.92775048	-4.30220392	H	-1.40221278	-3.95286197	2.17670699
H	-2.77897788	2.28670685	-4.37680679	N	0.21884844	-3.45631925	0.94263982
N	-0.93006265	2.29872024	-3.38753131	C	-0.50906805	-2.87254711	-0.16443855
C	-1.30157864	1.55382257	-2.20289185	C	-1.72857782	-3.35974650	-0.48614892
C	-2.55312341	1.67890067	-1.70685284	H	-2.17568516	-4.21712357	-0.00330128
H	-3.28836760	2.36301613	-2.10628442	H	-2.29622509	-2.86971127	-1.26834478
H	-2.84406930	1.06304414	-0.86408285	O	0.09020195	-1.85318055	-0.73155816
O	-0.36415888	0.75966347	-1.74418263	C	-0.41376351	-5.79598656	1.56573678
Li	-0.02109779	-1.05646188	-2.49358397	H	-0.95151834	-5.94472703	0.62662875

H	0.60783913	-6.17134671	1.43671666
H	-0.90390483	-6.39157579	2.34480383
C	3.02303647	-1.99391072	-6.96988469
H	3.55925944	-1.78426393	-7.90284851
H	3.65317980	-2.62975742	-6.34390883
H	2.11183741	-2.55182335	-7.21415181
C	-2.28387292	4.34724721	-3.87041193
H	-2.70730588	4.35505569	-2.86349772
H	-1.40440153	5.00124881	-3.87546665
H	-3.02591782	4.76226710	-4.56253761
C	3.23480931	1.85760695	4.03339160
H	3.93150488	1.82863106	4.87937439
H	3.56482644	2.63422123	3.33971672
H	2.24483462	2.13684390	4.41179874

Table 69. Geometric coordinates and thermally corrected MP2 energies for **31** S_4 tetramer



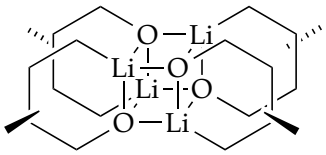


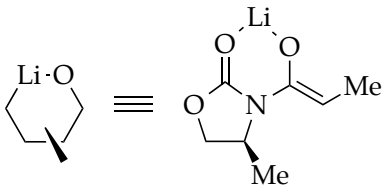
G = -2085.626801 Hartree
G_{MP2} = -1304797.245 kcal/mol
ΔG_{MP2} = 1.192916208 kcal/mol Li vs. **31** D_{2d} tetramer

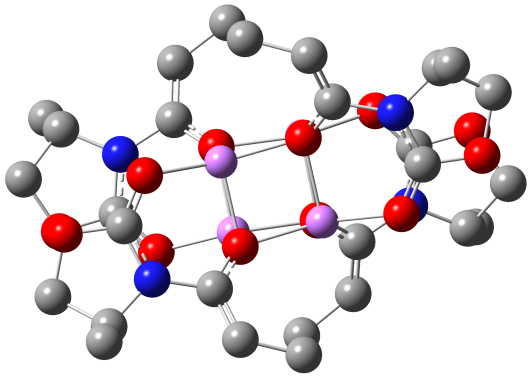
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-0.56809705	-3.79245680	-1.15423257
O	0.00000000	0.00000000	1.88604670	C	-1.14799657	-2.46533035	-1.09668517
C	1.02125812	0.00000000	2.56359129	O	-0.30581729	-1.47717727	-1.27848147
N	2.33694388	-0.04401345	2.18762438	Li	-0.30571620	-0.07739318	-2.64573932
C	3.21079484	0.15810051	3.35568398	O	-1.65748695	0.76843613	-3.65189755
C	2.22747277	-0.16672659	4.49106972	C	-2.10802606	1.87560323	-3.38021248
H	2.28801032	-1.21322269	4.81066801	O	-3.09805880	2.40425337	-4.14838538
H	2.33639403	0.48713147	5.35867992	C	-3.60078617	3.59277062	-3.51407709
O	0.92824622	0.05954824	3.91902863	H	-4.51561948	3.33430546	-2.96879431
H	4.02189922	-0.57428127	3.33470537	H	-3.83289965	4.32216140	-4.29267280
C	3.77301819	1.58124992	3.42306627	C	-2.46528084	4.03701796	-2.57974611
H	4.33595249	1.81636855	2.51667484	H	-2.86913649	4.38174555	-1.62431369
H	2.96039128	2.30932937	3.52703712	N	-1.77331618	2.75194825	-2.38287269
H	4.44121544	1.68300987	4.28618467	C	-0.81330191	2.52863574	-1.32002272
C	2.84529479	-0.16139785	0.83534491	O	-0.16763772	1.38947680	-1.37850168
O	1.94075395	-0.09515490	-0.11132469	Li	1.78305742	1.16971706	-1.59592028
Li	1.62993926	-1.48783218	-1.48024248	O	3.02459700	2.18771004	-2.58452365
O	1.74104931	-3.36647700	-1.35566325	C	3.42874728	1.86514318	-3.69593297
C	0.76303121	-4.09757690	-1.25074252	O	4.34120914	2.64815440	-4.33157037
O	0.93231280	-5.44670327	-1.22602180	C	4.81425196	1.96162779	-5.50313570
C	-0.31652880	-6.07233579	-0.88631929	H	5.77245398	1.48675137	-5.26354976
H	-0.30043684	-6.32148959	0.18074472	H	4.95960476	2.69938779	-6.29476781
H	-0.40997460	-6.98784839	-1.47389456	C	3.71303175	0.93767411	-5.81703522
C	-1.38141688	-5.01804063	-1.22692787	H	4.15287767	-0.01567559	-6.12108381
H	-2.15080062	-4.99103623	-0.45102149	N	3.10563977	0.79255883	-4.48324597

C	2.22364059	-0.30347461	-4.13405955
O	1.63934149	-0.20181505	-2.96519430
C	2.06871216	-1.33032716	-5.00246657
H	2.56831334	-1.39612834	-5.95825900
H	1.41345349	-2.14571211	-4.72128430
C	2.70934074	1.42803361	-6.86550680
H	1.86234540	0.74226017	-6.94188515
H	2.32998855	2.42011892	-6.59525657
H	3.19310416	1.49820613	-7.84676444
C	-0.65352749	3.47332049	-0.36367444
H	-1.20419220	4.40241994	-0.33182449
H	0.06103736	3.28581516	0.42848710
C	-1.55360472	5.10262677	-3.19656377
H	-0.67611976	5.27285361	-2.56842061
H	-1.21417243	4.78555179	-4.18924967
H	-2.09745447	6.04854513	-3.30278335
C	-2.47577670	-2.33331225	-0.86902473
H	-3.14706376	-3.16424418	-0.70537496
H	-2.89619911	-1.33536374	-0.84132284
C	-2.01617946	-5.21473065	-2.60691978
H	-2.64362107	-4.35917528	-2.86781249
H	-1.24015196	-5.32401700	-3.37315006
H	-2.63695493	-6.11829473	-2.61191128
C	4.17489634	-0.32423495	0.64066140
H	4.89937532	-0.39270829	1.43959647
H	4.54065096	-0.39785127	-0.37630874

Table 70. Geometric coordinates and thermally corrected MP2 energies for **32** D_{2d} tetramer





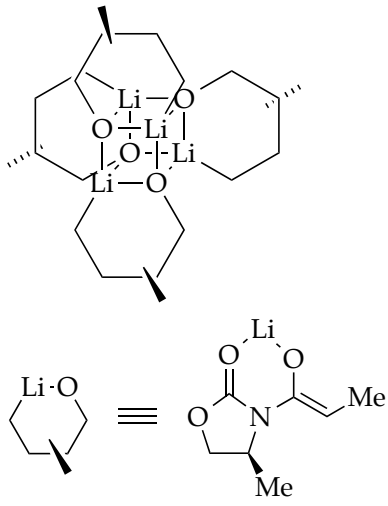


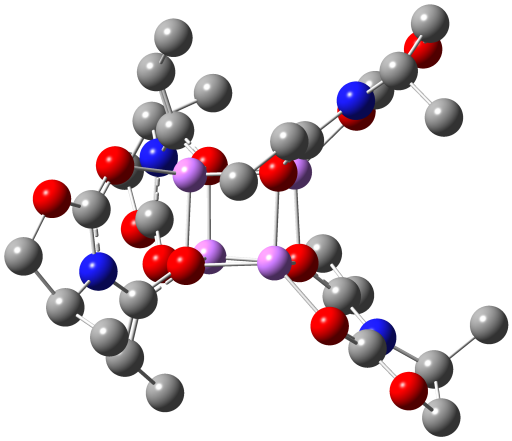
G = -2242.774368 Hartree
G_{MP2} = -1403050.978 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **32** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.13516196	2.63845855	-1.96842429
O	0.00000000	0.00000000	1.91217630	C	-2.96052700	1.12421525	-0.35195400
C	1.06284457	0.00000000	2.52768217	H	-2.58079416	0.09535320	-0.32948661
O	1.13346388	-0.55852210	3.77016533	H	-2.65443954	1.60266859	0.59152182
C	2.52442931	-0.61482956	4.16380616	H	-4.05523232	1.06216424	-0.33417256
H	2.90998879	-1.60656140	3.90836564	O	-0.38018135	0.77310291	-1.74134500
H	2.57409102	-0.45173754	5.24209363	Li	-0.02514328	-1.03183944	-2.50734002
C	3.17911762	0.50320637	3.34059220	O	-0.28543428	-1.06965154	-4.40134605
H	4.18215254	0.22664597	3.00606680	C	0.63977385	-0.78076027	-5.15567857
N	2.27643232	0.50942876	2.17734908	O	0.37947852	-0.24986095	-6.38494374
C	2.65817859	0.91389679	0.83741374	C	1.63043349	0.19032753	-6.96309600
C	3.73837835	1.71097750	0.66867158	H	1.75029664	1.25551717	-6.74300638
H	4.25288876	2.11142070	1.53366273	H	1.57700058	0.02662874	-8.04111151
C	4.25586076	2.10610511	-0.68816000	C	2.68071161	-0.67990865	-6.25888876
H	3.78522985	3.02312860	-1.07586992	H	3.60011072	-0.12396878	-6.05861601
H	5.33571089	2.29433838	-0.65610950	N	1.98386154	-0.91853232	-4.98394875
H	4.08974302	1.31876659	-1.43366027	C	2.64322797	-1.17171086	-3.71671760
O	1.91724383	0.39800101	-0.11859540	C	3.91744126	-1.62668966	-3.71239476
Li	1.56205157	0.95690182	-1.94517098	H	4.40155110	-1.88203759	-4.64712575
O	1.41015913	2.25632511	-3.33969418	C	4.70532854	-1.83213552	-2.44672058
C	0.32322453	2.46143436	-3.87358557	H	4.57100628	-2.83702789	-2.01672599
O	0.26711859	2.89688680	-5.16505446	H	5.77942891	-1.70746555	-2.62920522
C	-1.11123704	2.84575399	-5.60153374	H	4.42615138	-1.10945974	-1.67014733
H	-1.26856340	1.89475548	-6.11949288	O	1.92384038	-0.86800999	-2.65873110
H	-1.27838312	3.68331867	-6.28146884	Li	1.99360418	-1.46838797	-0.81222716
C	-1.90891305	2.94486533	-4.29379464	O	2.40731832	-2.72973515	0.56403908
H	-2.80621633	2.32136665	-4.31753850	C	1.50623530	-3.22374292	1.23674995
N	-0.93592763	2.34010907	-3.36877728	O	1.75210685	-3.63154482	2.51499278
C	-1.28300366	1.63874630	-2.14714292	C	0.48851321	-3.96429663	3.13595653
C	-2.48390562	1.87076923	-1.56866242	H	0.14025195	-3.08673454	3.68915875

H	0.65964420	-4.80123633	3.81566974
C	-0.41865391	-4.31124136	1.94727419
H	-1.44389028	-3.96714274	2.10523941
N	0.20779925	-3.47408398	0.91054330
C	-0.48665802	-2.92408843	-0.23837254
C	-1.63973853	-3.49817498	-0.65246759
C	-2.46930702	-2.94144271	-1.77796816
H	-2.40322290	-1.84782063	-1.83164757
H	-2.17170827	-3.33226202	-2.76358851
H	-3.52856061	-3.19228690	-1.64527249
H	-1.98613052	-4.41082314	-0.18302688
O	0.06997005	-1.84636799	-0.74609194
C	-0.38544526	-5.80782234	1.61123136
H	-0.89266333	-6.02158200	0.66793226
H	0.65031361	-6.15606658	1.52675996
H	-0.87742479	-6.38116493	2.40581470
C	2.97538134	-1.97152248	-7.03265385
H	3.50745611	-1.73808563	-7.96245087
H	3.58871031	-2.66132568	-6.44889578
H	2.04065717	-2.48250357	-7.29033372
C	-2.25562174	4.39586004	-3.93577035
H	-2.66928975	4.47571865	-2.92815894
H	-1.35951103	5.02486947	-3.98616173
H	-2.99325697	4.79054491	-4.64446441
C	3.19829179	1.84039275	4.09250912
H	3.89609548	1.78564150	4.93642435
H	3.50567419	2.66403002	3.44450475
H	2.20125625	2.07062647	4.48509341

Table 71. Geometric coordinates and thermally corrected MP2 energies for **32** S_4 tetramer



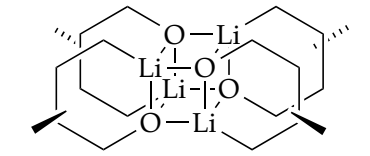


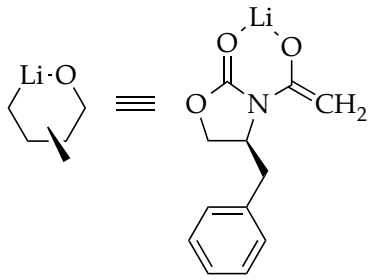
G = -2242.778425 Hartree
G_{MP2} = -1403048.226 kcal/mol
ΔG_{MP2} = 0.687774412 kcal/mol Li vs. **32** D_{2d} tetramer

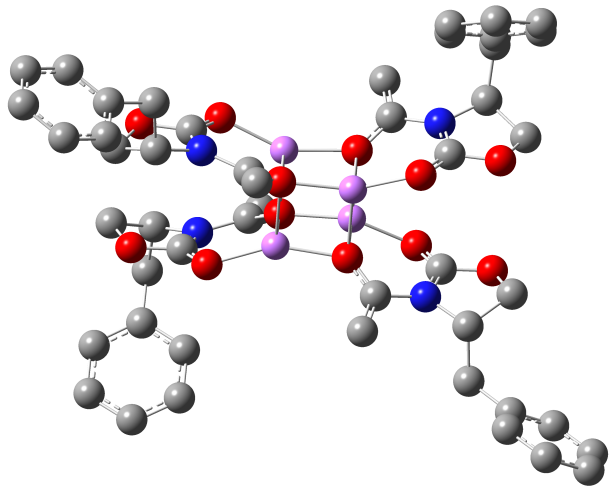
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-1.40266416	-3.53626594	-1.41202023
O	0.00000000	0.00000000	1.89315970	C	-1.62887059	-2.16084236	-0.99521638
C	1.05016387	0.00000000	2.52878083	O	-0.66488082	-1.31770463	-1.30011483
N	2.29665845	-0.40263649	2.15254185	Li	-0.34123866	0.06592755	-2.62309378
C	3.28497380	-0.10980914	3.20316476	O	-1.53845420	1.15479353	-3.56649753
C	2.34896954	0.16687645	4.39589480	C	-1.69703212	2.34637724	-3.31963274
H	2.23687277	-0.70604510	5.04852205	O	-2.51920106	3.08598465	-4.11376605
H	2.65535319	1.02863887	4.99292789	C	-2.71190113	4.37649972	-3.51290057
O	1.06986265	0.45958184	3.80874341	H	-3.66558885	4.36993745	-2.97272071
H	3.88876196	-0.99877123	3.40431767	H	-2.74804567	5.12276642	-4.30917951
C	4.19532286	1.06362415	2.83515862	C	-1.50861116	4.54409211	-2.57385145
H	4.72976661	0.85023995	1.90546382	H	-1.82487646	5.00696275	-1.63590317
H	3.61123661	1.98068470	2.69974184	N	-1.16226082	3.13095466	-2.33656150
H	4.93248159	1.23358320	3.62867315	C	-0.26047285	2.70408641	-1.27443170
C	2.65591046	-0.91532420	0.83923528	O	0.14356908	1.45540351	-1.34680851
O	1.88377595	-0.51429457	-0.14874488	Li	1.97187871	0.77205016	-1.60029300
Li	1.22905134	-1.76619206	-1.51725679	O	3.44540300	1.47493122	-2.51879942
O	0.94061620	-3.63656855	-1.46678329	C	3.73750367	1.14907777	-3.66529602
C	-0.18264340	-4.11056838	-1.60986240	O	4.77050607	1.77669063	-4.29190445
O	-0.32952098	-5.39486945	-2.03283255	C	5.05652739	1.09122793	-5.52151178
C	-1.71208244	-5.77299870	-1.92291171	H	5.90540045	0.41806064	-5.35532142
H	-1.82994762	-6.39123022	-1.02604142	H	5.32258069	1.83586232	-6.27451573
H	-1.97614058	-6.36035396	-2.80509141	C	3.76195876	0.33162281	-5.84539066
C	-2.48576823	-4.44376006	-1.82392455	H	3.99604996	-0.66421097	-6.22949583
H	-3.23689120	-4.51019192	-1.03229555	N	3.18008898	0.21758631	-4.49570792

C	2.07427963	-0.67851652	-4.18306614
O	1.50730267	-0.48624169	-3.01291024
C	1.71984952	-1.61257609	-5.09885934
H	2.27617226	-1.70429794	-6.02365166
C	0.57880069	-2.57237980	-4.90904762
H	-0.06606457	-2.26930789	-4.07859201
H	-0.04559951	-2.62734747	-5.81151006
H	0.92329073	-3.59529411	-4.69587733
C	2.84236659	1.07999170	-6.81538879
H	1.87232929	0.58263713	-6.88763924
H	2.68117792	2.10845391	-6.47249783
H	3.29402255	1.11500643	-7.81371148
C	0.08853863	3.60291189	-0.32203118
H	-0.32773700	4.60266689	-0.34083185
C	1.03413931	3.29536709	0.80513337
H	1.58229279	2.36539748	0.62612214
H	1.77389548	4.09810235	0.93048959
H	0.51498389	3.18571555	1.76893923
C	-0.35230444	5.33070890	-3.19898539
H	0.53389500	5.28436732	-2.56176086
H	-0.09622988	4.91763508	-4.18137382
H	-0.63650774	6.38151298	-3.32900657
C	-2.79035780	-1.85822430	-0.37287750
H	-3.48104795	-2.65441472	-0.11617999
C	-3.17049046	-0.45898146	0.02725084
H	-2.92787928	-0.23909893	1.07764470
H	-2.65462588	0.28573962	-0.59011439
H	-4.24889886	-0.29401315	-0.09302742
C	-3.14741780	-4.00448684	-3.13173594
H	-3.55941760	-2.99711207	-3.02710314
H	-2.42144671	-4.00149319	-3.95237806
H	-3.96388758	-4.68873900	-3.39083056
C	3.74070114	-1.71535274	0.73379555
H	4.25993833	-2.03100668	1.63247291
C	4.25643616	-2.23530880	-0.58003353
H	3.89155331	-3.24834053	-0.80623268
H	3.95544805	-1.58644063	-1.41083988
H	5.35297623	-2.28267162	-0.58193210

Table 72. Geometric coordinates and thermally corrected MP2 energies for **24** D_{2d} tetramer





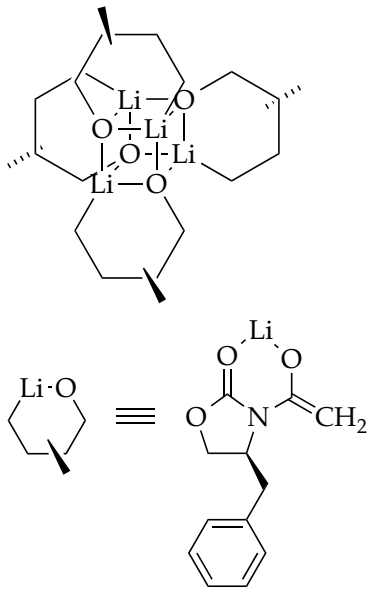


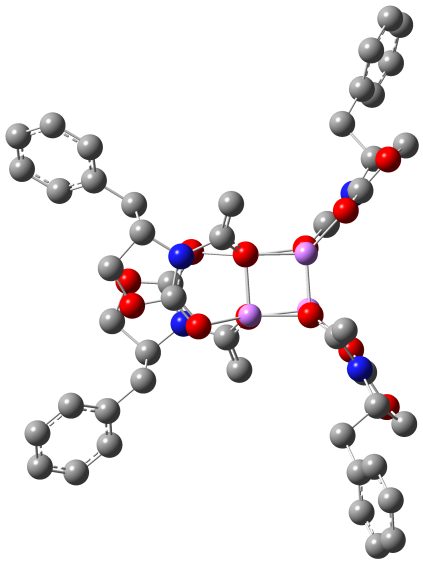
G = -3009.509144 Hartree
G_{MP2} = -1882679.921 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **24** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.19756726	2.41135716	-2.22000977
O	0.00000000	0.00000000	1.89704380	H	-2.81134074	1.12753598	-0.94311307
C	1.04095165	0.00000000	2.54500686	O	-0.31822504	0.75729309	-1.75097017
O	1.04865719	-0.47476380	3.81720989	Li	-0.04655814	-1.08668465	-2.47689859
C	2.40749723	-0.50812811	4.29955868	O	-0.29154775	-1.11280999	-4.35787463
H	2.77393490	-1.53608592	4.21474419	C	0.63359608	-0.90313802	-5.13478068
H	2.39674679	-0.19607035	5.34493882	O	0.37706829	-0.45490369	-6.39066460
C	3.16952994	0.45618941	3.37602114	C	1.62467109	-0.14358024	-7.04395288
H	4.14324455	0.04382480	3.09693553	H	1.77488741	0.93947515	-6.99301863
N	2.29263195	0.43124330	2.19841434	H	1.54477858	-0.46530021	-8.08338961
C	2.74237815	0.70872883	0.85091585	C	2.68495370	-0.91356383	-6.23993225
C	3.94639849	1.29421539	0.65535734	H	3.57806405	-0.30211736	-6.08327857
H	4.59575838	1.61704364	1.45597408	N	1.98196172	-1.05710654	-4.95871054
H	4.29542990	1.43625943	-0.36065784	C	2.65011805	-1.21537908	-3.68452942
O	1.92529140	0.30712733	-0.09259582	C	3.96518188	-1.53222619	-3.65418302
Li	1.62515067	0.86199921	-1.92063305	H	4.55889651	-1.72248792	-4.53632713
O	1.54245685	2.16700447	-3.30681455	H	4.46448128	-1.58380449	-2.69380663
C	0.48281755	2.40217284	-3.87971401	O	1.89576518	-0.98136239	-2.63795620
O	0.48624859	2.88050803	-5.15372330	Li	1.95748605	-1.56165948	-0.79428333
C	-0.87421737	2.87820260	-5.64914535	O	2.33040307	-2.83571592	0.57286486
H	-1.03002365	1.95265595	-6.21183251	C	1.42683847	-3.28023971	1.27452168
H	-1.00020626	3.74412422	-6.30004235	O	1.69514259	-3.72960488	2.53070642
C	-1.72396371	2.93452855	-4.37468960	C	0.44016315	-4.00621762	3.19766130
H	-2.63013045	2.33203376	-4.46933867	H	0.16748109	-3.12636785	3.78845821
N	-0.80303026	2.28218496	-3.43274680	H	0.58395805	-4.87024422	3.84738508
C	-1.22392972	1.56344526	-2.24890053	C	-0.53612206	-4.25726131	2.04296610
C	-2.48576373	1.72213879	-1.78844380	H	-1.52861392	-3.85723688	2.26214041

N	0.09775652	-3.43911373	0.99905061
C	-0.61396761	-2.84116458	-0.11051576
C	-1.86299281	-3.26763040	-0.40630039
H	-2.35235611	-4.08494886	0.10404319
H	-2.41255657	-2.76636044	-1.19423828
O	0.03019097	-1.86973027	-0.71009188
C	-0.62720823	-5.75083183	1.64114988
H	-1.13116859	-5.81563900	0.67147230
H	0.39213002	-6.12797194	1.49286095
C	-1.34964112	-6.59167753	2.67227451
C	-0.65048801	-7.47653142	3.50410269
C	-1.31718445	-8.23377344	4.46987576
C	-2.69898693	-8.11586988	4.61980927
C	-3.40940466	-7.23976131	3.79566780
C	-2.73995218	-6.48689619	2.83159313
H	-3.30505543	-5.81537730	2.18831904
H	-4.48710541	-7.14613532	3.90050277
H	-3.22041482	-8.70489009	5.36941677
H	-0.75581007	-8.91765072	5.10110671
H	0.42590632	-7.58257739	3.38567478
C	3.11121466	-2.25852541	-6.88998734
H	3.62142007	-2.00495252	-7.82862910
H	3.85929847	-2.72792940	-6.24455817
C	1.98945075	-3.23799811	-7.15933309
C	1.43283653	-3.36915678	-8.43891700
C	0.38776110	-4.26273455	-8.67911908
C	-0.11645361	-5.04378172	-7.63881063
C	0.43775340	-4.93325281	-6.36177017
C	1.48446905	-4.04173025	-6.12542494
H	1.92155006	-3.97271336	-5.13239893
H	0.05929192	-5.54548356	-5.54762023
H	-0.93022690	-5.74000575	-7.82283711
H	-0.02820317	-4.35081379	-9.67941131
H	1.83005374	-2.77539071	-9.26008038
C	-2.07397031	4.38106466	-3.94395384
H	-2.45074565	4.35196124	-2.91650891
H	-1.14613438	4.96584961	-3.92338423
C	-3.08384690	5.03717261	-4.86146204
C	-4.42982202	4.64059773	-4.84130534
C	-5.36121797	5.22274303	-5.70038481
C	-4.96313997	6.21705300	-6.59724124
C	-3.62937841	6.62453943	-6.62542461
C	-2.69951496	6.03756037	-5.76436391
H	-1.66331425	6.36888984	-5.78450413
H	-3.31046148	7.40228417	-7.31439958
H	-5.68897595	6.67306034	-7.26504512
H	-6.39953661	4.90346839	-5.66642922
H	-4.75339270	3.87431836	-4.13973700
C	3.38415196	1.86949710	3.98404312
H	4.05308532	1.74167061	4.84534751
H	3.92721526	2.47659563	3.25393117
C	2.12611325	2.59517589	4.40947923
C	1.72439680	2.62412715	5.75191810
C	0.55495302	3.28153911	6.13736918
C	-0.23207202	3.92488952	5.18175444
C	0.16330778	3.91563645	3.84243291
C	1.33440749	3.26063168	3.46062177
H	1.64424075	3.27127449	2.41860753
H	-0.43718638	4.42347210	3.09249343
H	-1.14316545	4.43716548	5.47891473
H	0.26252014	3.29406614	7.18412352
H	2.34009505	2.13837807	6.50664296

Table 73. Geometric coordinates and thermally corrected MP2 energies for **24** S_4 tetramer



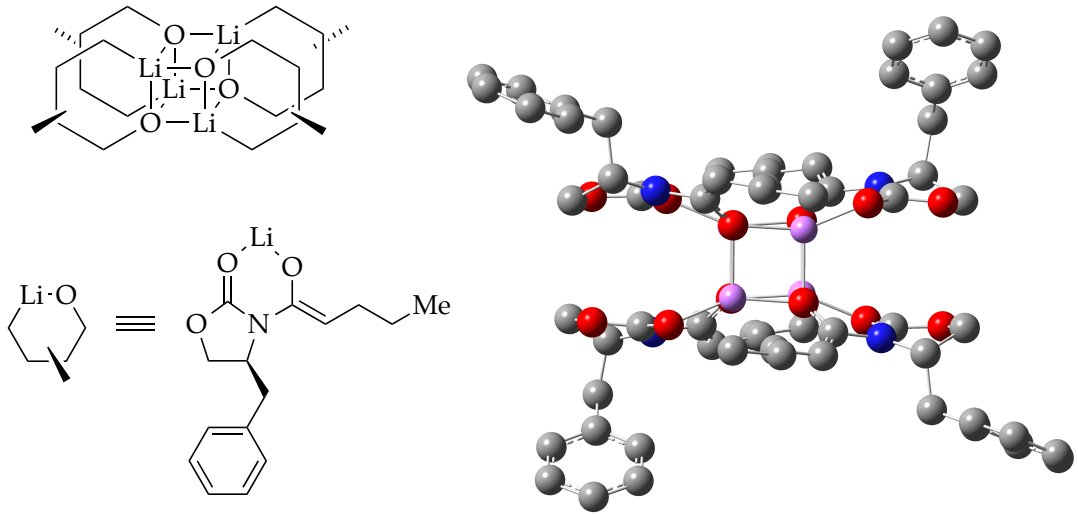


G = -3009.519077 Hartree
G_{MP2} = -1882679.503 kcal/mol
ΔG_{MP2} = 0.104548176 kcal/mol Li vs. **24** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.85268827	-0.09754369	0.84872769
O	0.00000000	0.00000000	1.88639640	O	1.95055258	-0.04354120	-0.10187270
C	1.01709881	0.00000000	2.57016047	Li	1.67549316	-1.43487189	-1.47184171
N	2.33692266	-0.01675945	2.19950735	O	1.77388013	-3.32202874	-1.51741610
C	3.19615701	0.18865187	3.37582080	C	0.78754718	-4.03609348	-1.66449011
C	2.22055227	-0.19546729	4.49544723	O	0.93925558	-5.33828751	-2.01769864
H	2.29862803	-1.25308318	4.77055220	C	-0.32910011	-6.00928290	-1.90248401
H	2.31742443	0.42186286	5.38936174	H	-0.34390927	-6.55599939	-0.95338794
O	0.91848164	0.03061181	3.92430436	H	-0.42293413	-6.71506621	-2.72895229
H	4.03968761	-0.50475034	3.34850626	C	-1.37115062	-4.88077074	-1.94095652
C	3.70856913	1.64672603	3.46709656	H	-2.15440554	-5.06643845	-1.20268746
H	4.19613118	1.88714620	2.51656553	N	-0.54091188	-3.73927543	-1.52806709
H	2.84059043	2.31058828	3.56325913	C	-1.09354942	-2.44457794	-1.17577725
C	4.66263526	1.85846936	4.62247551	O	-0.28489807	-1.42504548	-1.34269401
C	5.97842694	1.37507592	4.55695668	Li	-0.24472243	0.00165345	-2.67200001
H	6.32147770	0.87655957	3.65260633	O	-1.19738571	1.06575781	-3.94162593
C	6.85598285	1.53816382	5.62829088	C	-1.26877744	2.28387438	-3.79003705
H	7.87236965	1.16008429	5.55556208	O	-1.38812599	3.10572326	-4.86563429
C	6.43334597	2.19204462	6.78811392	C	-1.63964788	4.45163515	-4.40931940
C	5.13006303	2.68346222	6.86514469	H	-2.69814086	4.67338840	-4.57809686
C	4.25397690	2.51647229	5.79039009	H	-1.02872669	5.13510902	-5.00115148
H	3.24299682	2.91371051	5.85353757	C	-1.27145671	4.45226303	-2.91029842
H	4.79371708	3.20122188	7.75959310	H	-2.06693487	4.92903379	-2.33063576
H	7.11743262	2.32210794	7.62229450	N	-1.24849282	3.00772321	-2.64080695

C	-0.99912666	2.43820687	-1.32494954
O	-0.16049272	1.42978161	-1.31334993
Li	1.78319165	1.24756956	-1.57462964
O	2.61362888	2.52088523	-2.74195029
C	2.66197522	2.31715948	-3.95337857
O	2.73134225	3.35978627	-4.82315462
C	2.97725293	2.85200538	-6.15167135
H	4.03045689	3.02880195	-6.39220056
H	2.34896399	3.40402525	-6.85245105
C	2.63486609	1.34954501	-6.08252177
H	3.42562304	0.76342568	-6.55881559
N	2.65718573	1.13798392	-4.62841116
C	2.47720255	-0.16300127	-4.00192980
O	1.69841165	-0.16151946	-2.94674831
C	3.08546651	-1.22857632	-4.56367163
H	3.76342119	-1.13025489	-5.40248509
H	2.91991492	-2.21764769	-4.15269896
C	1.27235839	0.97102668	-6.70485089
H	1.07704657	-0.07620141	-6.44785426
H	0.48577983	1.56793513	-6.23139012
C	1.25027335	1.16107026	-8.20575998
C	1.97830157	0.30661090	-9.04797522
H	2.53765609	-0.52158265	-8.61720670
C	1.98071640	0.49385849	-10.42983605
H	2.54750371	-0.18175158	-11.06529001
C	1.25056627	1.54103638	-10.99715393
C	0.51636392	2.39388526	-10.17260851
C	0.51813906	2.20422270	-8.78885209
H	-0.07021407	2.86067343	-8.15134517
H	-0.06343808	3.20523877	-10.60506609
H	1.24931425	1.68580308	-12.07415565
C	-1.61096405	3.00338663	-0.26354892
H	-2.33864007	3.79791254	-0.37490420
H	-1.39246405	2.64556510	0.73591311
C	0.07749012	5.12723760	-2.57611457
H	0.27756259	4.94425949	-1.51425818
H	0.87365083	4.63052654	-3.13991186
C	0.07141295	6.61198623	-2.86694936
C	0.80038670	7.13444725	-3.94407546
H	1.40505219	6.46294534	-4.54989629
C	0.77742861	8.50124354	-4.23027719
H	1.35499954	8.88699332	-5.06641849
C	0.02183088	9.36930955	-3.44165969
C	-0.70491899	8.86283545	-2.36144739
C	-0.67805256	7.49766274	-2.07759159
H	-1.23555217	7.11525593	-1.22472951
H	-1.28818724	9.53303811	-1.73523736
H	0.00401739	10.43340332	-3.66142414
C	-2.37145997	-2.37817592	-0.73837408
H	-2.98798893	-3.25023288	-0.56760549
H	-2.79938744	-1.40787365	-0.51608901
C	-2.00883113	-4.65206158	-3.33163563
H	-2.54831909	-3.69954739	-3.29115124
H	-1.20340580	-4.53989865	-4.06792574
C	-2.94237412	-5.77149197	-3.73718808
C	-4.21029481	-5.88833477	-3.14729550
H	-4.53244350	-5.14559849	-2.42017142
C	-5.06727676	-6.93278100	-3.49248288
H	-6.04717209	-7.00270057	-3.02748690
C	-4.67199226	-7.88124749	-4.43885765
C	-3.41682148	-7.77401869	-5.03803414
C	-2.56081659	-6.72744181	-4.68807990
H	-1.58896324	-6.64334460	-5.17008415
H	-3.10292992	-8.50161087	-5.78190172
H	-5.34063058	-8.69347543	-4.71081448
C	4.18723054	-0.21886481	0.65405302
H	4.91019429	-0.28739204	1.45438001
H	4.55760344	-0.27232270	-0.36278781

Table 74. Geometric coordinates and thermally corrected MP2 energies for **28** D_{2d} tetramer

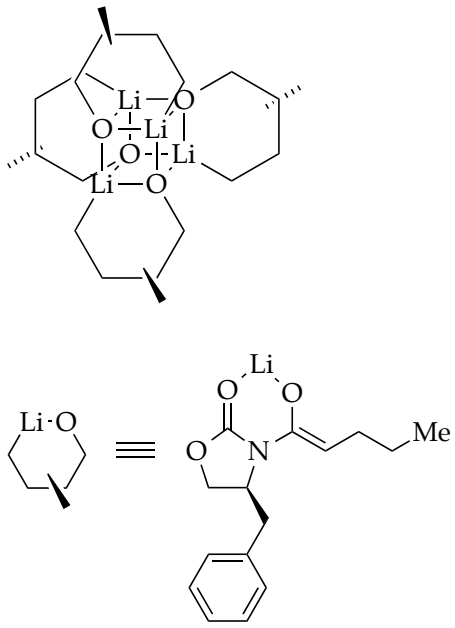


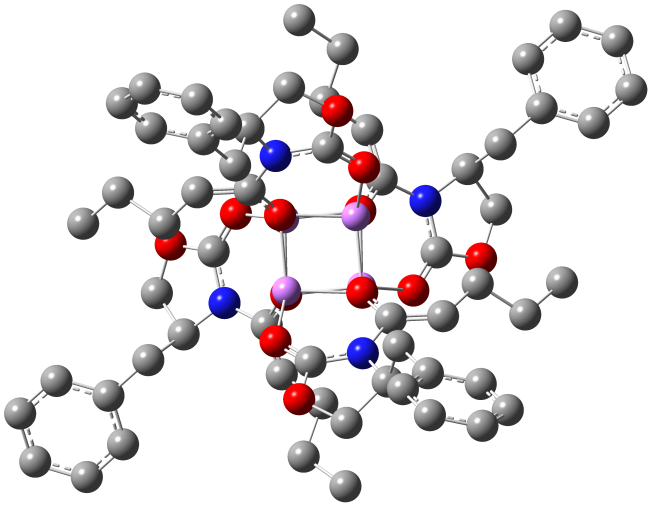
G = -3480.950722 Hartree
G_{MP2} = -2177412.233 kcal/mol
ΔG_{MP2} = 0.0 kcal/mol Li vs. **28** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.99135361	3.04479937	-4.18209556
O	0.00000000	0.00000000	1.89850500	H	-2.89099121	2.42684470	-4.22640039
C	1.06047699	0.00000000	2.51615129	N	-1.00800804	2.40677204	-3.29425534
O	1.15143216	-0.62286899	3.71999847	C	-1.33553426	1.65786037	-2.09462216
C	2.53029117	-0.61687776	4.14590138	C	-2.53577809	1.85534310	-1.50099652
H	2.96036837	-1.59706125	3.91893277	H	-3.20032501	2.62634535	-1.87457533
H	2.54310005	-0.43781539	5.22224062	C	-3.01454226	1.07109170	-0.30709504
C	3.18202062	0.51155543	3.32810054	H	-2.54558221	0.07683330	-0.29619079
H	4.17171572	0.22086377	2.96421595	H	-2.70774553	1.55596385	0.63582364
N	2.25913459	0.56494534	2.18597889	C	-4.54189499	0.89368773	-0.28057399
C	2.61566041	1.00878706	0.85049913	H	-5.01942627	1.88433097	-0.30666412
C	3.64102701	1.87779742	0.68960864	H	-4.85914361	0.37803503	-1.19759886
H	4.12994061	2.30140447	1.55866141	O	-0.41445592	0.79722539	-1.72206478
C	4.15656517	2.31374904	-0.65720096	Li	-0.01717204	-0.99122070	-2.50387320
H	3.63835476	3.22391379	-1.00562422	O	-0.30638702	-1.04379684	-4.37947437
H	3.94126115	1.54196778	-1.40995019	C	0.57930943	-0.68883471	-5.15124621
C	5.66906741	2.59303716	-0.66135735	O	0.26132653	-0.10752732	-6.33719111
H	5.89737211	3.35029585	0.10288836	C	1.47247028	0.35896984	-6.96820333
H	6.20362889	1.68243635	-0.35748230	H	1.56034731	1.43366413	-6.78231889
O	1.90656969	0.46296359	-0.11313429	H	1.38319281	0.16588646	-8.03847565
Li	1.52552135	1.03847186	-1.92706141	C	2.59525646	-0.44566491	-6.29084692
O	1.33999545	2.37603783	-3.27460494	H	3.46305441	0.18391518	-6.07413131
C	0.24754577	2.57813023	-3.79811903	N	1.93535042	-0.78765968	-5.02333903
O	0.17535450	3.06799547	-5.06754509	C	2.62402838	-1.04065918	-3.77060131
C	-1.20667861	3.01161811	-5.49816698	C	3.90101591	-1.48931534	-3.79205011
H	-1.35383841	2.07813213	-6.04952981	H	4.36902516	-1.73817153	-4.73691763
H	-1.39563218	3.86959401	-6.14433184	C	4.73572992	-1.67878548	-2.55227517

H	4.63095555	-2.70336087	-2.15527999
H	4.37961399	-1.01225574	-1.75382111
C	6.23143285	-1.40687465	-2.78605846
H	6.59270077	-2.05556867	-3.59742653
H	6.35795541	-0.37493055	-3.14154511
O	1.92400687	-0.75208829	-2.69541744
Li	2.04992681	-1.37407541	-0.86137887
O	2.55346362	-2.65339497	0.46116782
C	1.69489916	-3.21172852	1.13901697
O	1.99353931	-3.66039099	2.39047486
C	0.76253663	-4.08103619	3.02789175
H	0.38272496	-3.24378892	3.62103273
H	0.98766220	-4.93245931	3.67113095
C	-0.15113119	-4.42413799	1.84622421
H	-1.19251421	-4.16049638	2.04418867
N	0.39807057	-3.50629495	0.83713262
C	-0.35025989	-2.95363175	-0.27726248
C	-1.48026516	-3.57635171	-0.68628037
C	-2.38012768	-3.04364551	-1.77075930
H	-2.29635066	-1.94891473	-1.82649497
H	-2.07144521	-3.41733482	-2.76241646
C	-3.85777806	-3.41262342	-1.55763580
H	-3.94842197	-4.50655412	-1.48557312
H	-4.19081444	-3.01462374	-0.58905196
H	-1.76652413	-4.52090186	-0.23737676
O	0.14179429	-1.83511772	-0.76169980
C	-0.03545379	-5.91141970	1.42238189
H	-0.48838357	-6.02896917	0.43311136
H	1.02866628	-6.15309384	1.31075323
C	-0.68364670	-6.85346953	2.41474000
C	0.08871697	-7.65682693	3.26412068
C	-0.51420253	-8.50785080	4.19310388
C	-1.90462869	-8.56734917	4.28774543
C	-2.68734805	-7.77396990	3.44548553
C	-2.08129491	-6.92678823	2.51852426
H	-2.70069500	-6.31995348	1.86104801
H	-3.77151574	-7.81840768	3.50743145
H	-2.37629645	-9.22972369	5.00853738
H	0.10399637	-9.12592354	4.83893621
H	1.17365027	-7.62467563	3.18846392
C	3.06454724	-1.66111596	-7.13926615
H	3.48195494	-1.24735849	-8.06683870
H	3.89473082	-2.15059198	-6.62216461
C	1.99679276	-2.68298124	-7.46491304
C	1.38157769	-2.71277791	-8.72365143
C	0.39027657	-3.65091076	-9.01633421
C	-0.00010506	-4.57885076	-8.05054042
C	0.61290459	-4.56800111	-6.79573925
C	1.60514710	-3.63101839	-6.50676992
H	2.08560521	-3.63533747	-5.53153050
H	0.32249681	-5.29322053	-6.04028830
H	-0.77142980	-5.31047993	-8.27564134
H	-0.07268600	-3.65827431	-9.99969687
H	1.68990466	-2.00215200	-9.48818114
C	-2.34224277	4.48917228	-3.73972306
H	-2.65135598	4.46768286	-2.69014782
H	-1.42702533	5.09213916	-3.78475916
C	-3.42297338	5.11559254	-4.59529732
C	-4.75574618	4.69054091	-4.48297966
C	-5.75427236	5.24479710	-5.28298917
C	-5.43798696	6.23872206	-6.21227733
C	-4.11813080	6.67391994	-6.33214570
C	-3.12084104	6.11502264	-5.52976711
H	-2.09571016	6.46801185	-5.62111366
H	-3.86237033	7.45147319	-7.04718265
H	-6.21607621	6.67294835	-6.83418911
H	-6.78092369	4.90395931	-5.17787094
H	-5.01478777	3.92340838	-3.75594084
C	3.31832521	1.83737283	4.12872304
H	3.99050915	1.62226228	4.96997853
H	3.83478915	2.57256501	3.50507010
C	2.02280454	2.42807551	4.64160487
C	1.63576078	2.27492177	5.97971589
C	0.43523915	2.81317292	6.44605280
C	-0.39828710	3.51791406	5.57725953
C	-0.01933588	3.68812836	4.24390107
C	1.18221563	3.15138657	3.78112013
H	1.47597689	3.29701675	2.74456416
H	-0.65729684	4.24404369	3.56202799
H	-1.33339348	3.93821751	5.93755798
H	0.15477477	2.68482987	7.48828973
H	2.28653682	1.73920100	6.66823192
C	6.18690621	3.06898418	-2.02157573
H	5.68658468	3.99416906	-2.33378789
H	7.26539083	3.26427957	-1.99553266
H	6.00202779	2.31721820	-2.79917439
C	7.08439850	-1.63258983	-1.53450422
H	6.99585473	-2.66586736	-1.17636614
H	8.14513222	-1.43595270	-1.72976376
H	6.76724489	-0.97331549	-0.71672566
C	-4.77286992	-2.89870005	-2.67249254
H	-4.47463648	-3.30344444	-3.64764351
H	-5.81751915	-3.18193824	-2.49778920
H	-4.73092757	-1.80471909	-2.74459732
C	-5.03661356	0.12265845	0.94629077
H	-4.75288237	0.63262452	1.87532584
H	-6.12792915	0.01753698	0.94195193
H	-4.60405914	-0.88507243	0.97989844

Table 75. Geometric coordinates and thermally corrected MP2 energies for **28** S_4 tetramer





G = -3480.955593 Hartree
G_{MP2} = -2177408.26 kcal/mol
ΔG_{MP2} = 0.993177387 kcal/mol Li vs. **28** D_{2d} tetramer

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-0.45211301	-1.41713026	-1.28809478
O	0.00000000	0.00000000	1.89570250	Li	-0.24704482	-0.06140664	-2.65403890
C	1.02739839	0.00000000	2.56715863	O	-1.50335139	0.82224544	-3.71138223
O	0.97407823	0.32582796	3.88666864	C	-1.87761935	1.97004055	-3.49270637
C	2.24915282	0.04248030	4.49263082	O	-2.82231855	2.52753944	-4.29651246
H	2.17575390	-0.91822081	5.01369722	C	-3.24887923	3.77279648	-3.71553810
H	2.47143272	0.83027218	5.21368739	H	-4.16416226	3.59200264	-3.14056078
C	3.23750564	-0.00812698	3.31662229	H	-3.45619644	4.47782126	-4.52162161
H	3.93047078	-0.84209164	3.44851527	C	-2.07433310	4.18581592	-2.82333965
N	2.31368957	-0.28008504	2.20472810	H	-2.43572694	4.64521489	-1.90109225
C	2.75921248	-0.63106271	0.86655903	N	-1.49075670	2.86527064	-2.53213045
O	1.93392275	-0.29772383	-0.10166314	C	-0.56019406	2.62944394	-1.43426314
Li	1.48613779	-1.63852970	-1.47043173	O	-0.03905228	1.42309242	-1.38549018
O	1.37933666	-3.52844692	-1.36809520	Li	1.87872493	0.99773837	-1.53850736
C	0.31719940	-4.14309958	-1.38977573	O	3.23794188	1.93453271	-2.40569848
O	0.31338479	-5.47999412	-1.64040221	C	3.65995372	1.63120063	-3.51710531
C	-1.00708306	-6.00001890	-1.39702980	O	4.67685830	2.35040672	-4.06300147
H	-1.01444688	-6.46863819	-0.40698717	C	5.13576719	1.67753673	-5.24909029
H	-1.22733239	-6.75194516	-2.15600645	H	6.00623287	1.06579250	-4.98624940
C	-1.92890741	-4.77204973	-1.46575089	H	5.42548975	2.42995902	-5.98375412
H	-2.67165475	-4.81908531	-0.66624536	C	3.93647259	0.82718075	-5.67893465
N	-0.95972892	-3.69726557	-1.20260190	H	4.26926749	-0.13770203	-6.06680655
C	-1.34724078	-2.31942897	-0.95005605	N	3.26782348	0.64320675	-4.37960491

C	2.26560469	-0.38825874	-4.13772832	H	-5.21791147	-1.27272194	-0.41535423
O	1.67899778	-0.34041399	-2.96177930	C	-2.64433384	-4.58212108	-2.82366491
C	2.03434402	-1.29903353	-5.11516375	H	-3.07698582	-3.57557783	-2.82444540
H	2.57502176	-1.23387061	-6.05204451	H	-1.89367605	-4.61368102	-3.62189720
C	1.07465680	-2.45264699	-5.00316683	C	-3.71820101	-5.61999768	-3.06597050
H	0.75615412	-2.57883517	-3.96197686	C	-4.94071747	-5.55201044	-2.38033225
H	0.15624302	-2.25330554	-5.58213176	H	-5.12556750	-4.72491455	-1.69776158
C	1.68806953	-3.77057402	-5.51320465	C	-5.92619374	-6.51916670	-2.57505075
H	2.59240846	-3.99213414	-4.93152356	H	-6.86834792	-6.44546010	-2.03810945
H	2.01811630	-3.63036518	-6.55320849	C	-5.70731025	-7.57465950	-3.46361798
C	3.01669994	1.53309317	-6.70609913	C	-4.49900068	-7.65174307	-4.15649224
H	2.07648454	0.97432933	-6.75294893	C	-3.51388540	-6.68192916	-3.95729869
H	2.77853560	2.53228352	-6.32081869	H	-2.57928823	-6.74177566	-4.51107688
C	3.64289337	1.63696334	-8.07974792	H	-4.32217076	-8.46402231	-4.85668936
C	3.73979729	0.50633164	-8.90533070	H	-6.47593303	-8.32701960	-3.61855753
H	3.32990417	-0.44229365	-8.56451064	C	3.95937153	-1.24288500	0.72550972
C	4.33962798	0.58543793	-10.16163155	H	4.52156942	-1.52552250	1.61005331
H	4.40056953	-0.30119089	-10.78727931	C	4.58649483	-1.57619062	-0.60078709
C	4.85365021	1.80148542	-10.61823381	H	4.60818233	-2.66782184	-0.75263113
C	4.75960019	2.93509707	-9.81077270	H	3.97714361	-1.16586712	-1.41582427
C	4.15948641	2.85086750	-8.55250427	C	6.02293909	-1.03775650	-0.74828520
H	4.07919205	3.74222038	-7.93371653	H	6.00942032	0.05376713	-0.62774204
H	5.14946954	3.88773741	-10.15970490	H	6.64383500	-1.43070620	0.07005014
H	5.31856010	1.86479236	-11.59833455	C	4.03739093	1.29669745	3.09426858
C	-0.32310932	3.64343439	-0.56594336	H	4.52242026	1.21705611	2.11512265
H	-0.80591105	4.60256351	-0.71188917	H	3.33227787	2.13429543	3.04035378
C	0.56595122	3.54636270	0.64422964	C	5.06636682	1.54019724	4.17640038
H	0.81820023	2.49857453	0.84410567	C	6.25015351	0.78756051	4.21457822
H	1.52479349	4.06334452	0.46597505	H	6.44004082	0.05001740	3.43731642
C	-0.08709909	4.16252808	1.89611365	C	7.19208558	0.98430427	5.22379539
H	-1.03320684	3.64330509	2.09750449	H	8.10504558	0.39453947	5.23243564
H	-0.35024360	5.20892733	1.68163981	C	6.96771396	1.94206570	6.21570535
C	-1.06177497	5.12059258	-3.53063494	C	5.79801652	2.70167563	6.18700529
H	-0.15156625	5.14899562	-2.92307240	C	4.85633202	2.50029805	5.17540100
H	-0.79274186	4.66687748	-4.49256366	H	3.95258900	3.10564750	5.15246408
C	-1.60311125	6.51752700	-3.74359358	H	5.61791103	3.45551964	6.94899474
C	-2.02674554	6.94726034	-5.00842240	H	7.70265502	2.09846051	7.00071107
H	-1.93402313	6.27531900	-5.85915927	C	6.66009938	-1.40347493	-2.09255606
C	-2.54963477	8.22889292	-5.19408882	H	7.67950582	-1.00884610	-2.17700379
H	-2.86784444	8.54330558	-6.18462501	H	6.70939234	-2.49125581	-2.22614818
C	-2.65836372	9.10345881	-4.11278043	H	6.07283637	-0.99782982	-2.92672572
C	-2.23649346	8.69009103	-2.84683131	C	-5.11077930	0.88262258	-0.55992856
C	-1.71349931	7.41014304	-2.66639527	H	-6.10123049	0.99869439	-1.01554529
H	-1.37464603	7.10252656	-1.67917129	H	-5.21059132	1.08033643	0.51454305
H	-2.30928387	9.36756913	-2.00008066	H	-4.45657774	1.65986613	-0.97607603
H	-3.06325592	10.10175269	-4.25496797	C	0.72769837	-4.96177826	-5.44318192
C	-2.56847539	-2.07997996	-0.41540046	H	1.17796251	-5.86378469	-5.87442969
H	-3.19390093	-2.91575589	-0.11759154	H	0.46504722	-5.19207651	-4.40372044
C	-3.13677215	-0.70531800	-0.19006526	H	-0.19985326	-4.75689898	-5.99385746
H	-3.20826828	-0.49066178	0.88882008	C	0.80305869	4.10952144	3.14150132
H	-2.46136213	0.05140356	-0.60857851	H	0.33036688	4.61476667	3.99215806
C	-4.53174022	-0.51233104	-0.81606510	H	0.99425909	3.07237741	3.44196235
H	-4.46662517	-0.69533284	-1.89699202	H	1.76967350	4.59756029	2.95972050