Supporting Information

Lithium Phenolates Solvated by Tetrahydrofuran and 1,2-Dimethoxyethane: Structure Determination Using the Method of Continuous Variation

Timothy S. De Vries, Anandarup Goswami, Lara R. Liou, Jocelyn M. Gruver, Emily Jayne and David B**.** Collum*

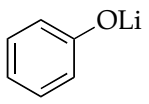
Contribution from the Department of Chemistry and Chemical Biology

Baker Laboratory, Cornell University

Ithaca, New York 14853-1301

X_A = the mole fraction of phenolate subunits **A**

X_B = the mole fraction of phenolate subunits **B**



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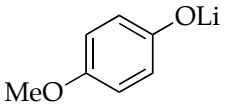

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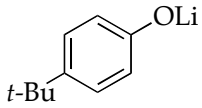

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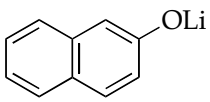

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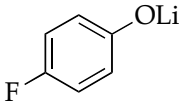

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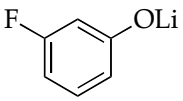

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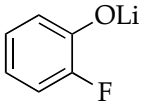

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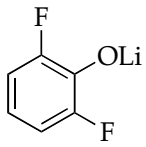

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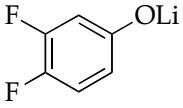

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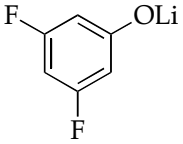

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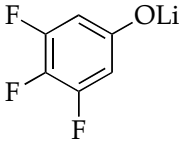

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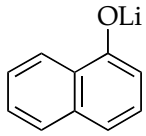

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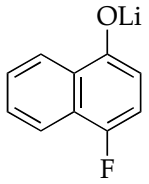

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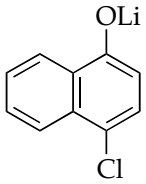

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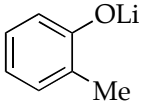

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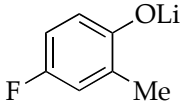

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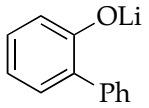

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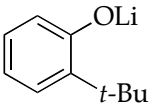

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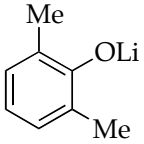

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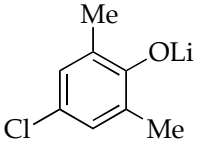

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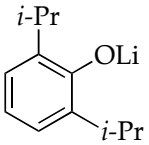

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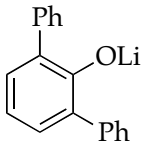

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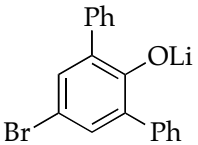

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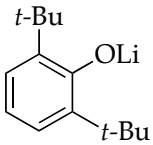

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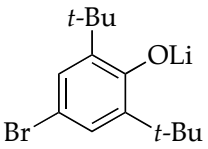

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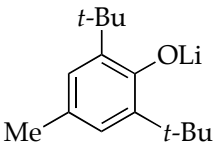

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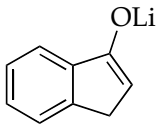


S1

I. Combinations of O-lithiated species in THF, DME and TMEDA: Job plots.

For a full list of Job plots and their corresponding page numbers, please refer to pages S4-S8.

II. Solvent swaps.

For a full list of solvent swaps and their corresponding page numbers, please refer to pages S9-S10.

III. Solvent concentration scans.

For a full list of solvent concentration scans and their corresponding page numbers, please refer to pages S11-S12.

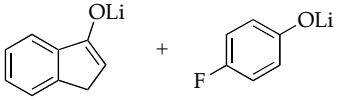
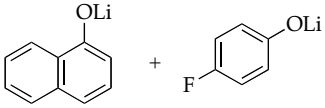
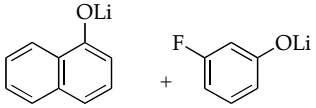
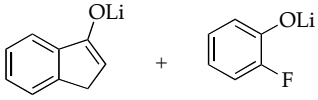
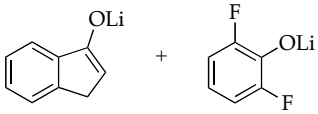
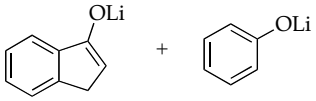
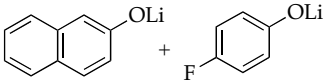
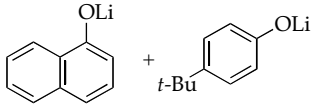
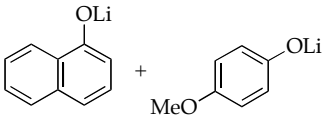
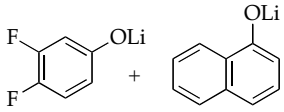
IV. Phenolate concentration scans.

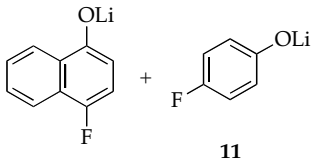
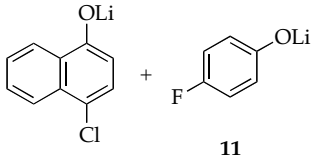
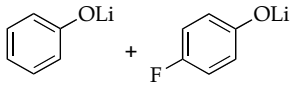
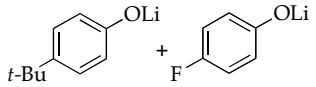
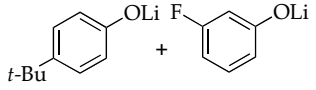
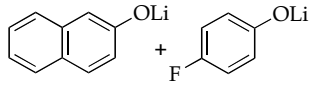
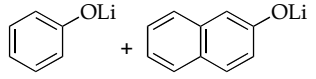
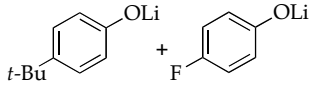
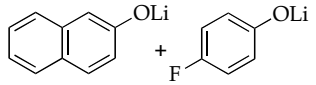
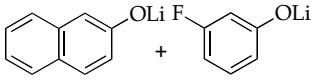
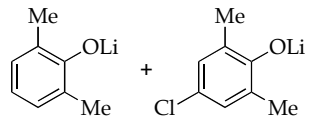
For a full list of phenolate concentration scans and their corresponding page numbers, please refer to page S13.

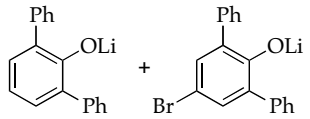
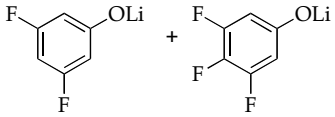
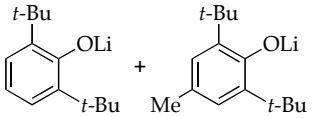
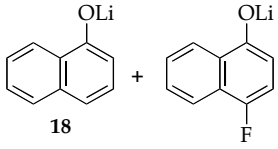
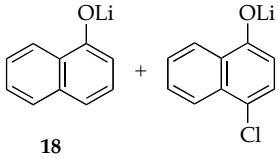
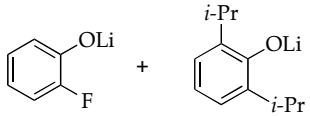
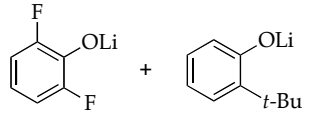
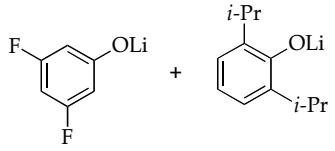
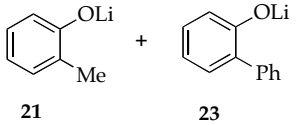
V. ^{19}F NMR spectra.

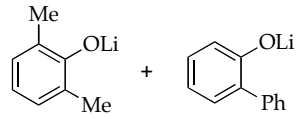
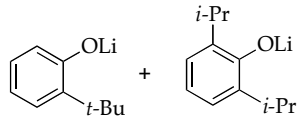
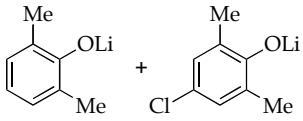
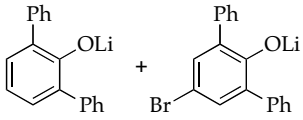
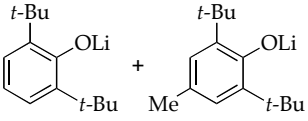
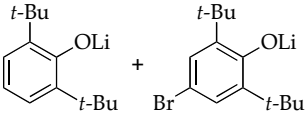
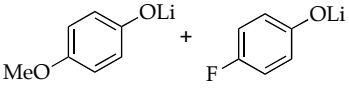
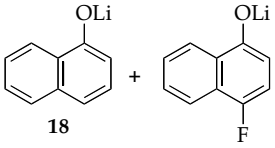
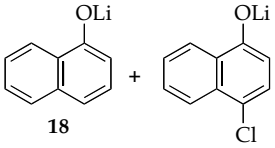
VI. Computational Studies.

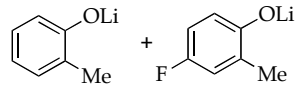
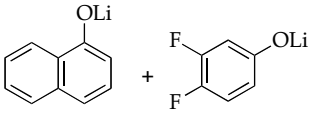
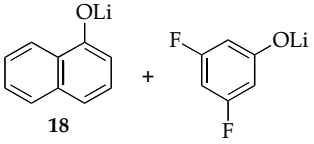
I. Combinations of O-lithiated species in THF, DME and TMEDA: Job plots.

Substrate Combinations	Page	Structure (s)	Solvent
 **S1** **11**	S14	Tetramers	THF
 **18** **11**	S15	Tetramers	THF
 **18** **12**	S16	Tetramers	THF
 **S1** **13**	S17	Tetramers	THF
 **S1** **14**	S18	Tetramers	THF
 **S1** **7**	S19	Tetramers	THF
 **10** **11**	S20	Tetramers	THF
 **18** **9**	S21	Tetramers	THF
 **18** **8**	S22	Tetramers	THF
 **15** **18**	S23	Tetramers	THF

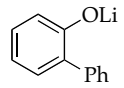
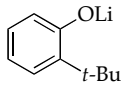
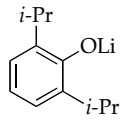
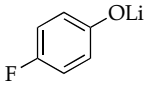
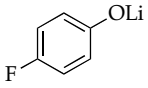
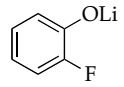
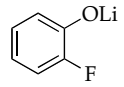
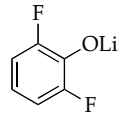
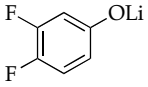
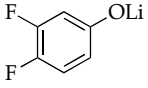
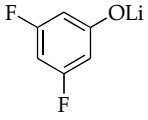
 **19** **11**	S24	Tetramers	THF
 **20** **11**	S25	Tetramers	THF
 **7** **11**	S26	Tetramers	DME
 **9** **11**	S27	Tetramers	DME
 **9** **12**	S28	Tetramers	DME
 **10** **11**	S29	Tetramers	DME
 **7** **10**	S30	Pentamers	DME
 **9** **11**	S31	Pentamers	DME
 **10** **11**	S32	Pentamers	DME
 **10** **12**	S33	Pentamers	DME
 **25** **26**	S34	Dimers	THF

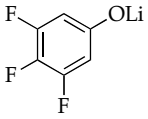
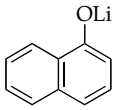
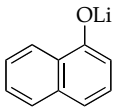
 **28** **29**	S35	Dimers	THF
 **16** **17**	S36	Dimers	THF
 **30** **32**	S37	Dimers	THF
 **18** **19**	S38	Dimers	THF
 **18** **20**	S39	Dimers	THF
 **13** **27**	S40	Dimers	DME
 **14** **24**	S41	Dimers	DME
 **16** **27**	S42	Dimers	DME
 **21** **23**	S43	Dimers	DME

 **25** **23**	S44	Dimers	DME
 **24** **27**	S45	Dimers	DME
 **25** **26**	S46	Dimers	DME
 **28** **29**	S47	Dimers	DME
 **30** **32**	S48	Dimers	DME
 **30** **31**	S49	Monomers	DME
 **8** **11**	S50	Pentamers Tetramers	DME
 **18** **19**	S51	Dimers Trimers	DME
 **18** **20**	S52	Dimers Trimers	DME

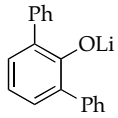
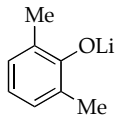
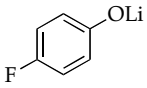
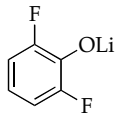
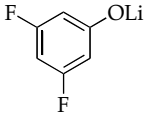
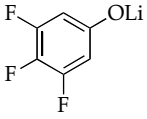
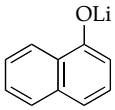
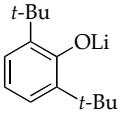
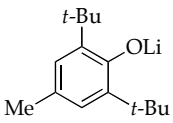
 **21** **22**	S53	Dimers Trimers	DME
 **18** **15**	S54	Dimers	TMEDA
 **18** **16**	S55	Dimers	TMEDA

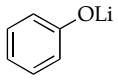
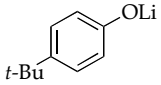
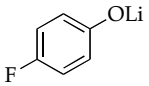
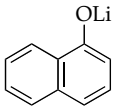
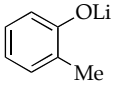
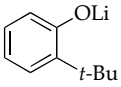
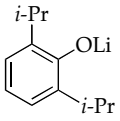
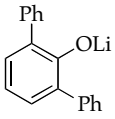
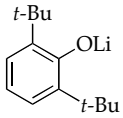
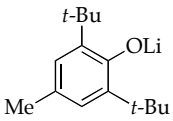
II. Solvent swaps.

Substrate	Solvent 1	Solvent 2	Page no.
 **23**	2.9 M DME/toluene	1.1 M THF/toluene	S56
 **24**	2.9 M DME/toluene	1.1 M THF/toluene	S57
 **27**	2.9 M DME/toluene	1.1 M THF/toluene	S58
 **11**	2.9 M DME/toluene	3.7 M THF/toluene	S59
 **11**	2.9 M DME/toluene	2.0 M TMEDA/toluene	S60
 **13**	2.9 M DME/toluene	1.1 M THF/toluene	S61
 **13**	2.9 M DME/toluene	0.22 M TMEDA/toluene	S62
 **14**	2.9 M DME/toluene	1.1 M THF/toluene	S63
 **15**	2.9 M DME/toluene	1.1 M THF/toluene	S64
 **15**	2.9 M DME/toluene	0.22 M TMEDA/toluene	S65
 **16**	2.9 M DME/toluene	0.18 M TMEDA/toluene	S66

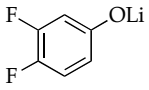
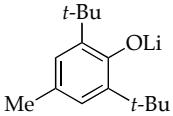
 **17**	2.9 M DME/toluene	3.7 M THF/toluene	S67
 **18**	2.9 M DME/toluene	3.7 M THF/toluene	S68
 **18**	2.9 M DME/toluene	2.0 M TMEDA/toluene	S69

III. Solvent concentration scans.

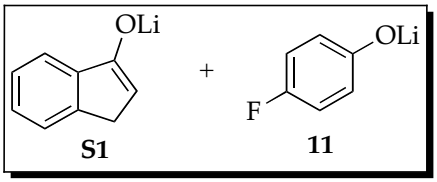
Substrate	Solvent	Lower limit	Upper limit	Page no.
 **28**	THF	1.2 M	12.2 M	S70
 **25**	THF	2.0 M	10.0 M	S71
 **11**	THF	0.12 M	12.2 M	S72
 **14**	THF	2.0 M	10.0 M	S73
 **16**	THF	2.0 M	10.0 M	S74
 **17**	THF	3.0 M	8.0 M	S75
 **18**	THF	2.0 M	12.2 M	S76
 **30**	THF	2.0 M	10.0 M	S77
 **32**	THF	4.0 M	12.2 M	S78

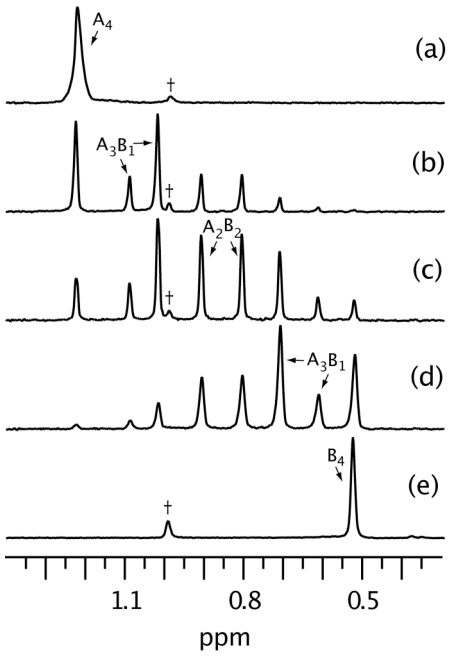
 **7**	DME	0.64 M	2.9 M	S80
 **9**	DME	0.24 M	6.3 M	S81
 **11**	DME	0.22 M	9.6 M	S82
 **18**	DME	0.23 M	2.9 M	S83
 **21**	DME	0.24 M	9.6 M	S84
 **24**	DME	0.24 M	9.6 M	S85
 **27**	DME	0.24 M	9.6 M	S86
 **28**	DME	0.24 M	9.6 M	S87
 **30**	DME	0.21 M	9.6 M	S88
 **32**	DME	0.0 M (neat toluene)	0.87 M	S89

IV. Phenolate concentration scans.

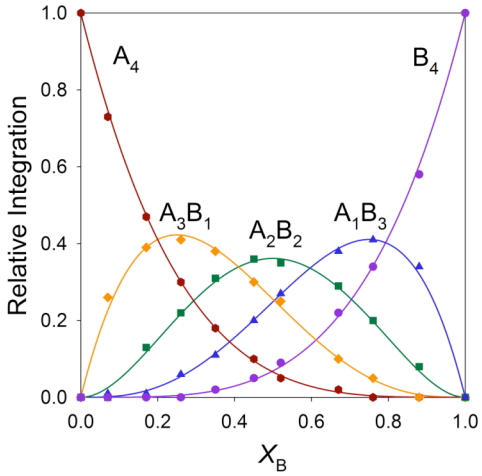
Solvent	Substrate	Lower limit	Upper limit	
DME	 **15**	0.018 N	0.109 N	S90
DME	 **32**	0.011 N	0.229 N	S91

Tetramer Job plots in THF

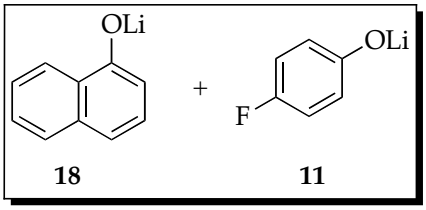


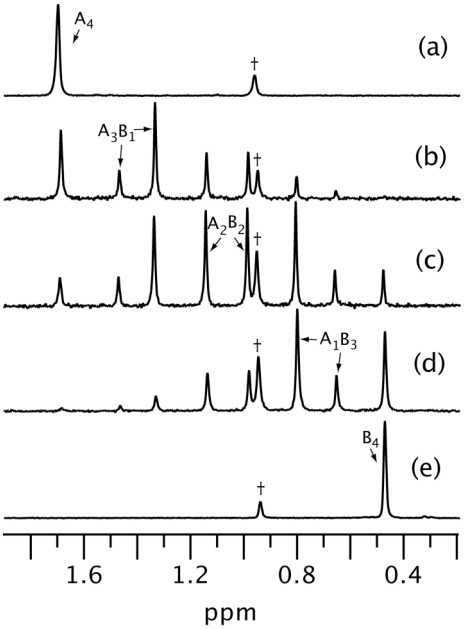


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**S1** (**A**) and [^{6}Li]**11** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.45, 0.67, 1.00 respectively. † denotes excess LiHMDS dimer.

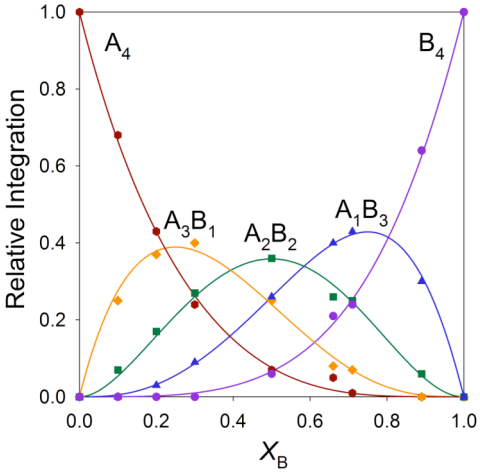


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of [^{6}Li]**S1** (**A**) and [^{6}Li]**11** (**B**) in 1.2 M THF/toluene at -78 °C.

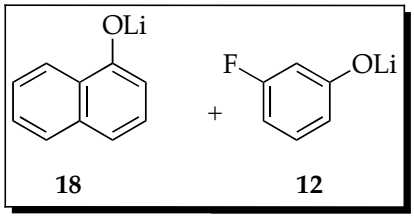


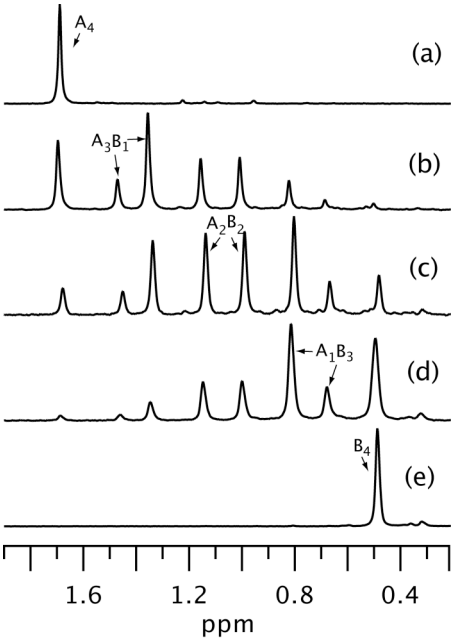


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**11** (**B**) at 1.2 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.71, 1.00 respectively. † denotes excess LiHMDS dimer.

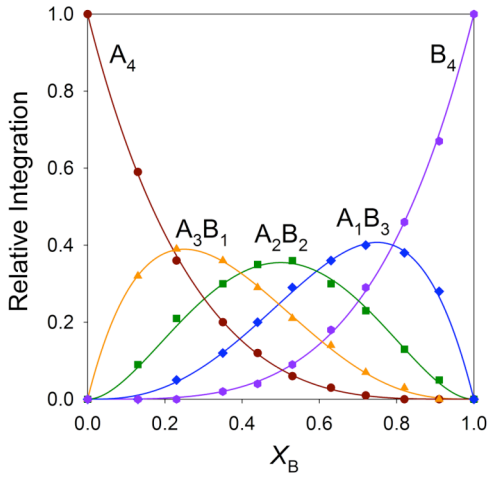


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**11** (**B**) in 1.2 M THF/toluene at -90 °C.

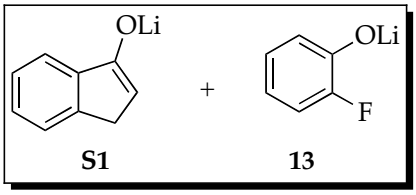


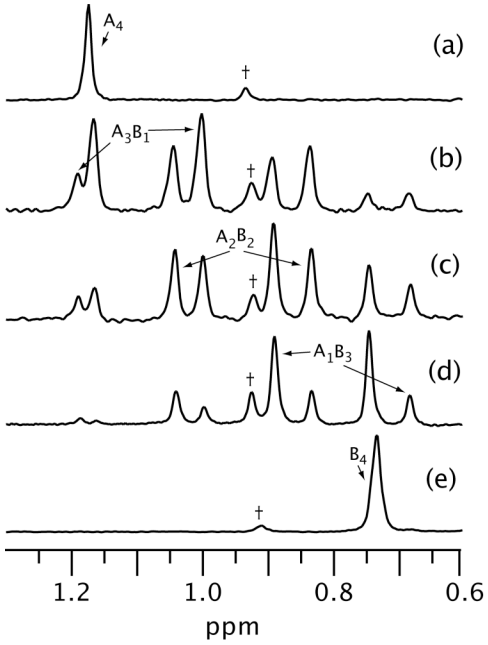


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**12** (**B**) at 1.2 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.72, 1.00 respectively.

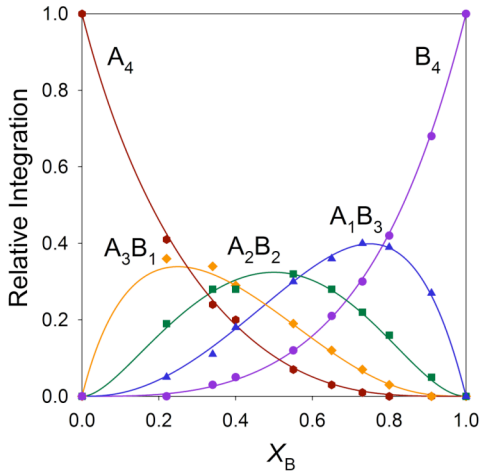


Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**12** (**B**) in 1.2 M THF/toluene at -90 °C.

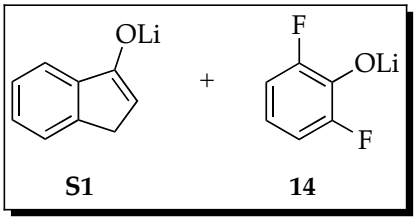


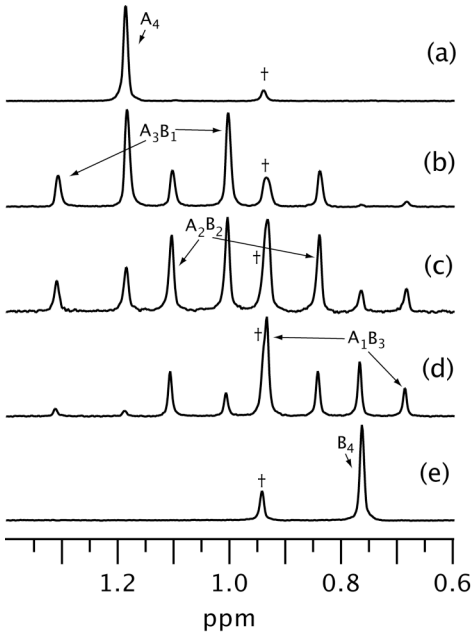


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**S1** (**A**) and [^{6}Li]**13** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.55, 0.73, 1.00 respectively. † denotes excess LiHMDS dimer.

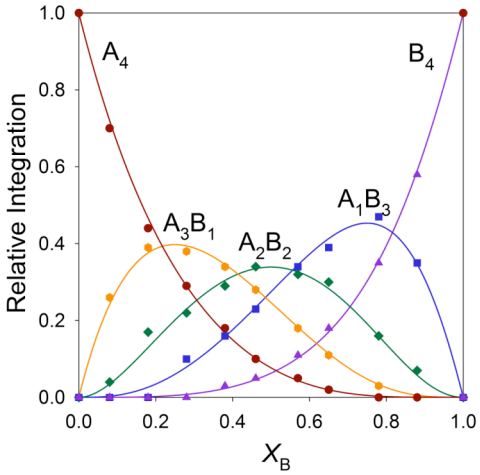


Job plot showing the relative integrations versus mole fractions of **13** for 0.10 M mixtures of [^{6}Li]**S1** (**A**) and [^{6}Li]**13** (**B**) in 1.2 M THF/toluene at -78 °C.

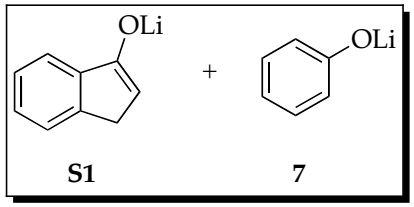


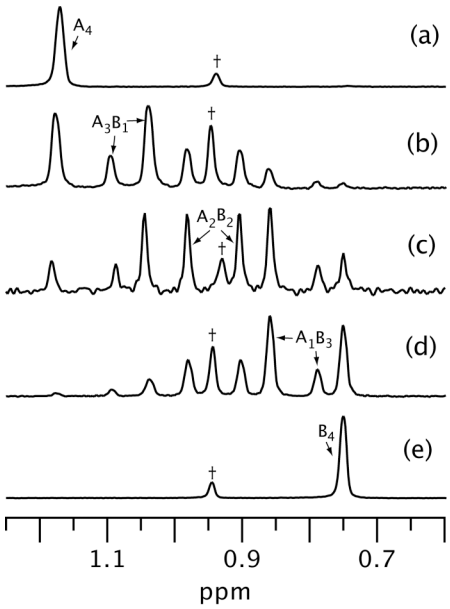


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**S1** (**A**) and [^{6}Li]**14** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.28, 0.46, 0.65, 1.00 respectively. † denotes excess LiHMDS dimer.

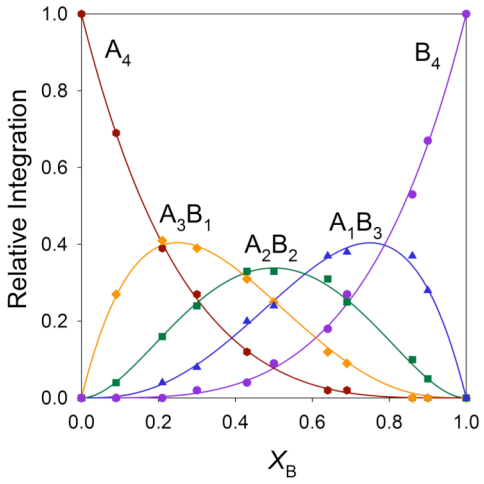


Job plot showing the relative integrations versus mole fractions of **14** for 0.10 M mixtures of enolates [^{6}Li]**S1** (**A**) and [^{6}Li]**14** (**B**) in 1.2 M THF/toluene at -78 °C.

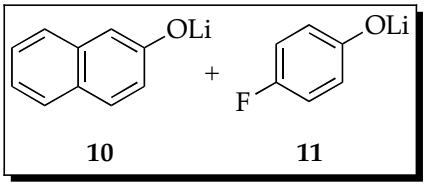


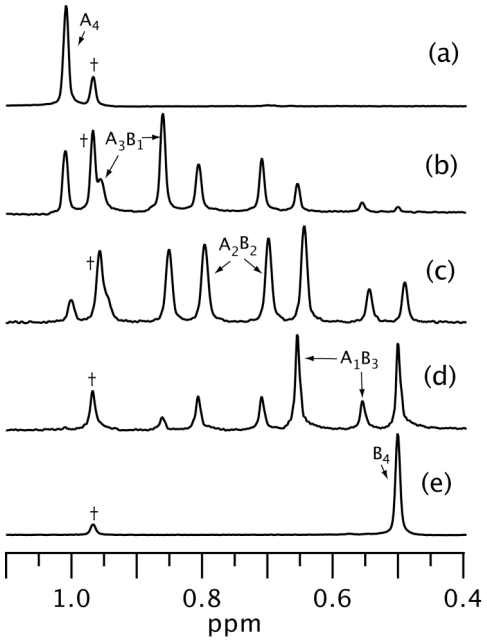


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**S1** (**A**) and [^{6}Li]**7** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.69, 1.00 respectively. † denotes excess LiHMDS dimer.

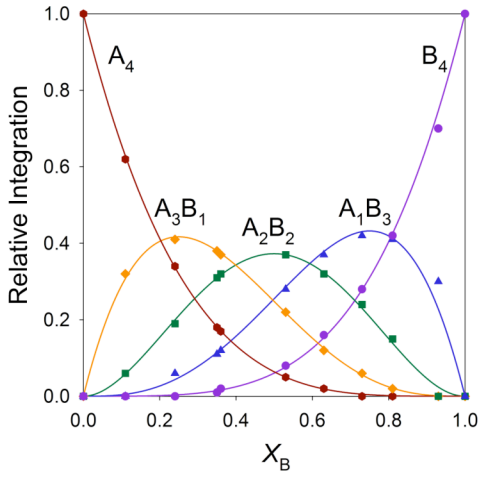


Job plot showing the relative integrations versus mole fractions of **7** for 0.10 M mixtures of [^{6}Li]**S1** (**A**) and [^{6}Li]**7** (**B**) in 1.2 M THF/toluene at -78 °C.

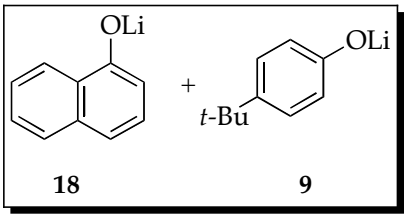


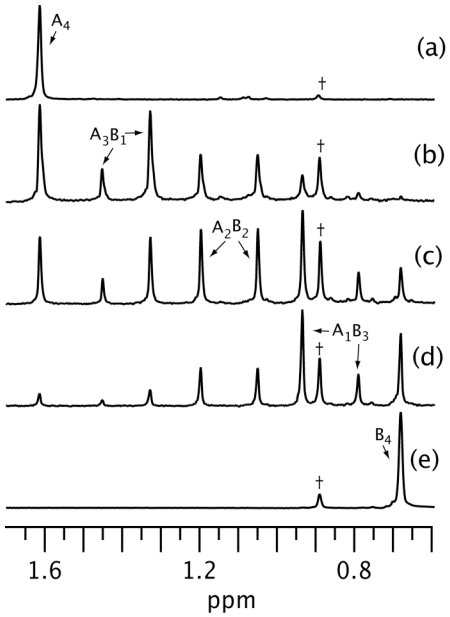


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.73, 1.00 respectively. † denotes excess LiHMDS dimer.

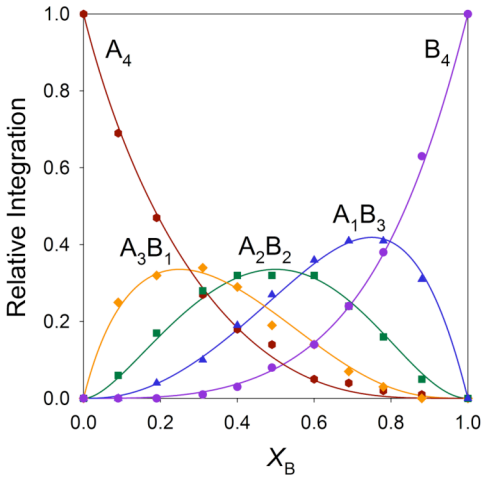


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) in 1.2 M THF/toluene at -78 °C

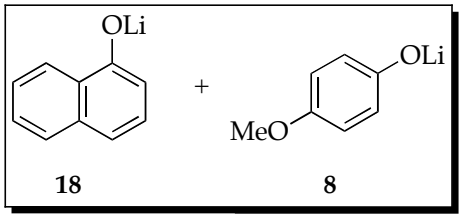


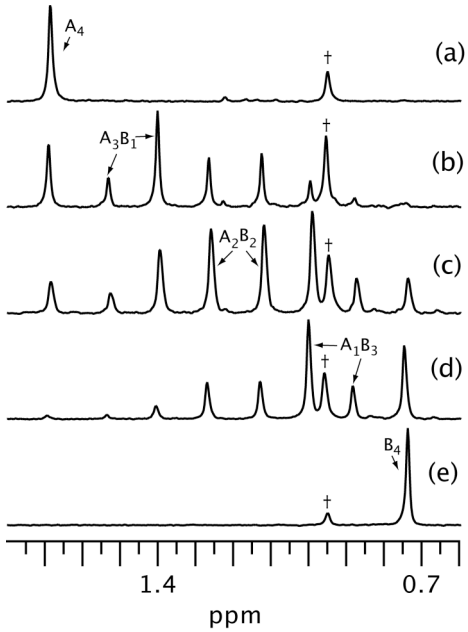


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**9** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.31, 0.49, 0.69, 1.00 respectively. † denotes excess LiHMDS dimer.

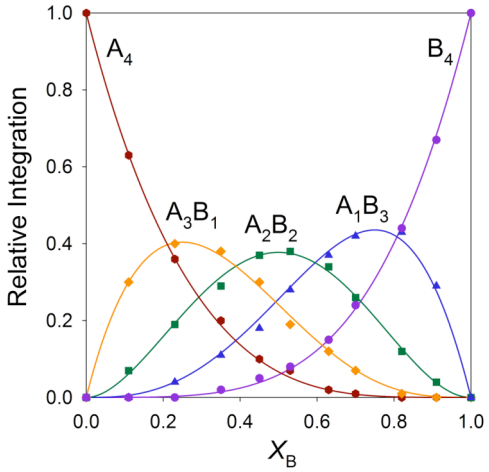


Job plot showing the relative integrations versus mole fractions of **9** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**9** (**B**) in 1.2 M THF/toluene at -78 °C.

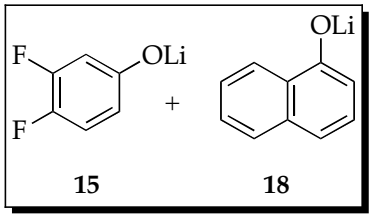


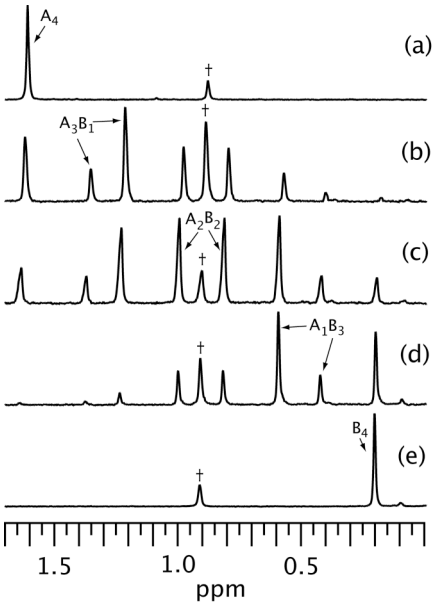


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**8** (**B**) at 1.2 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.70, 1.0 respectively. † denotes excess LiHMDS dimer.

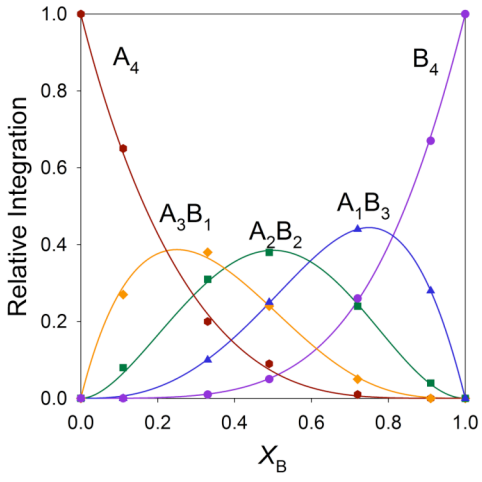


Job plot showing the relative integrations versus mole fractions of **8** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**8** (**B**) in 1.2 M THF/toluene at -90 °C.

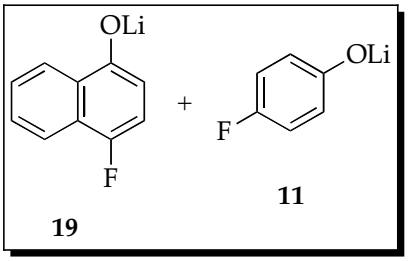


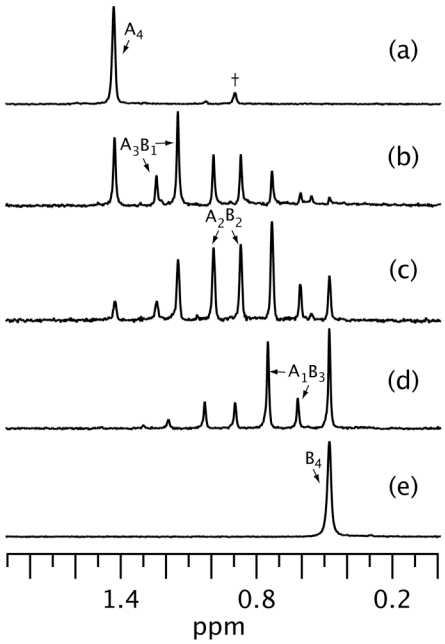


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**15** (**B**) at 1.2 M THF/toluene at -90 ºC. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.49, 0.72, 1.00 respectively. † denotes excess LiHMDS dimer.

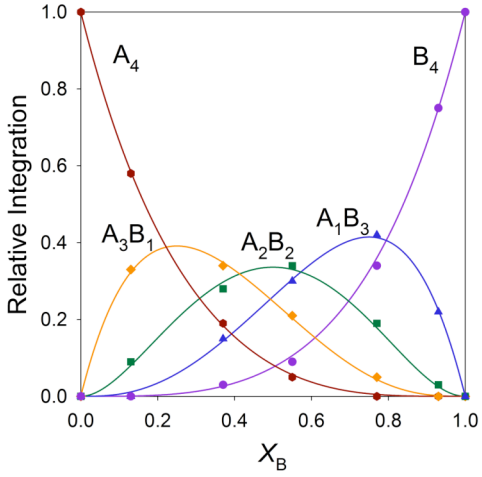


Job plot showing the relative integrations versus mole fractions of **18** for 0.10 M mixtures of phenolates [Li]**18** and [$_{6}$Li]**15** (**B**) in 1.2 M THF/toluene at -90 °C.

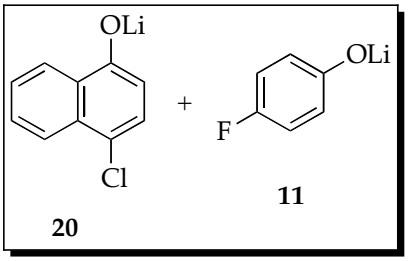


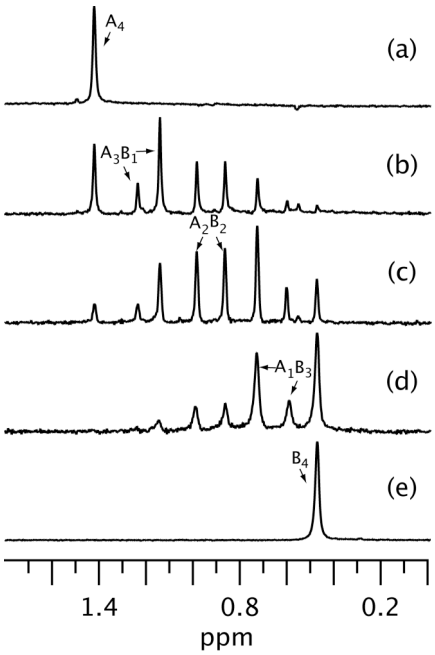


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**19** (**A**) and [^{6}Li]**11** (**B**) at 1.2 M THF/toluene at -90 ºC. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.37, 0.55, 0.77, 1.00 respectively. † denotes excess LiHMDS dimer.

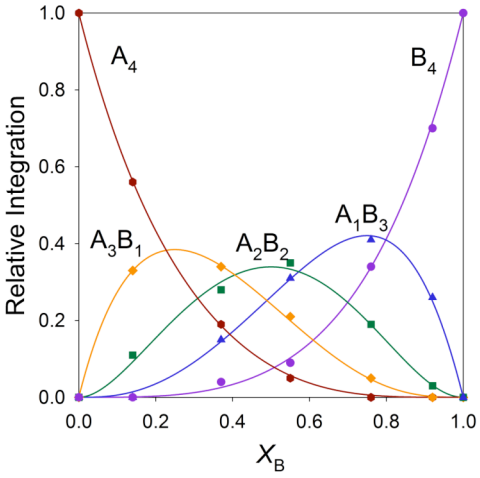


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**19** (**A**) and [^{6}Li]**15** (**B**) in 1.2 M THF/toluene at -90 °C. The non-statistical behavior of the Job plot may stem from low solubility of **19** in 1.2 M THF/toluene at -90 °C.



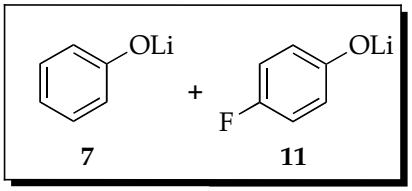


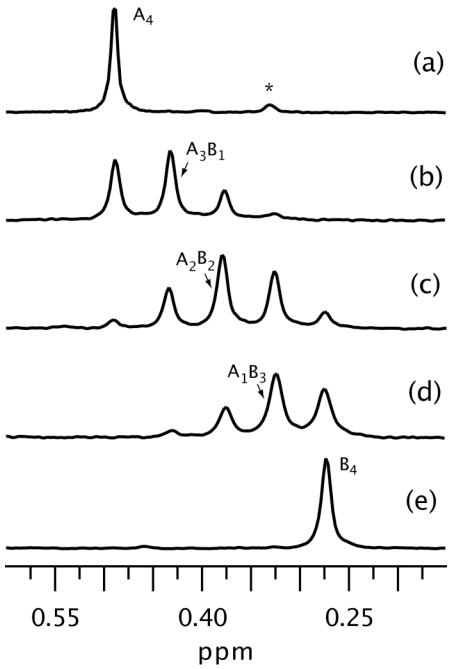
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**20** (**A**) and [^{6}Li]**11** (**B**) at 1.2 M THF/toluene at -90 ºC. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.37, 0.55, 0.76, 1.00 respectively.



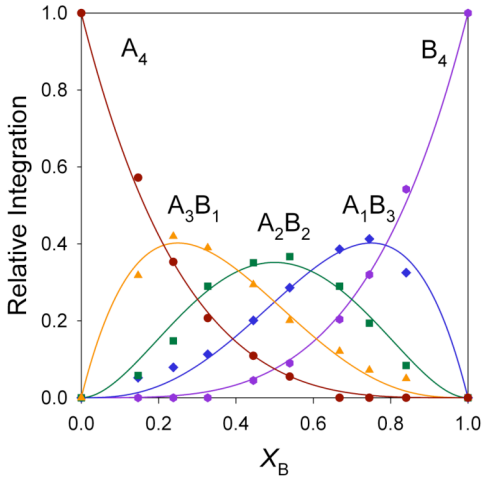
Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**20** (**A**) and [^{6}Li]**11** (**B**) in 1.2 M THF/toluene at -90 °C.

Tetramer Job plots in DME

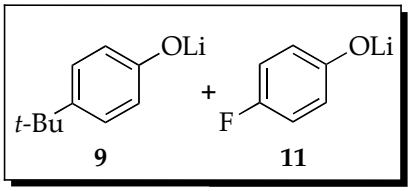


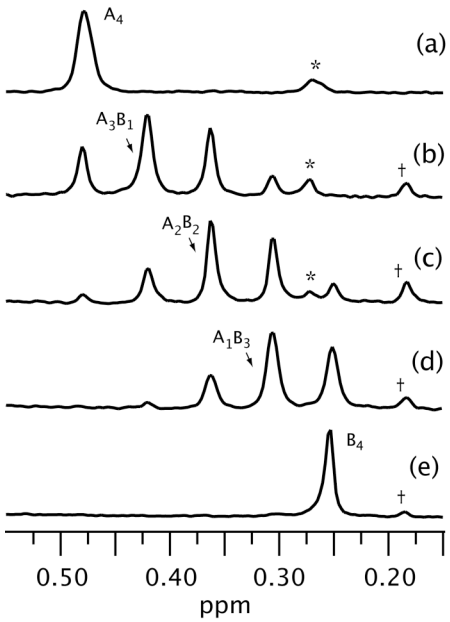


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**7** (**A**) and [^{6}Li]**11** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.54, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate.

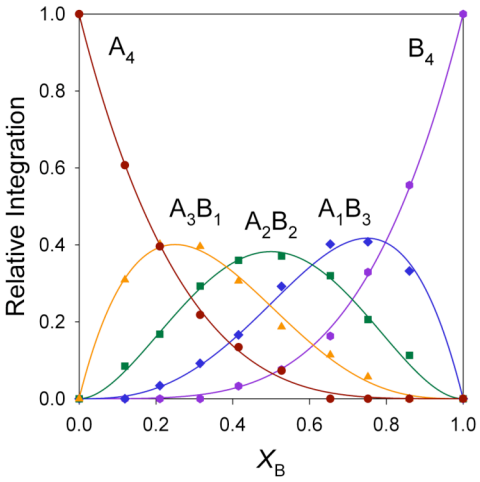


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**7** (**A**) and [^{6}Li]**11** (**B**) in 2.9 M DME/toluene at -90 °C.

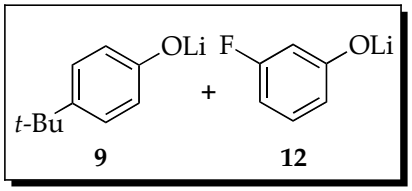


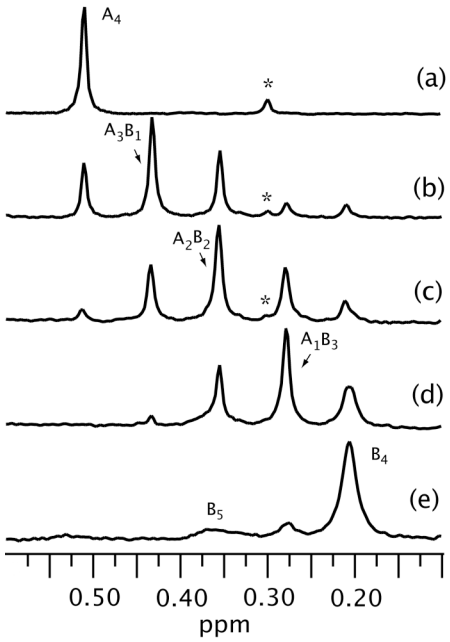


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**9** (**A**) and [^{6}Li]**11** (**B**) at 2.9 M DME/toluene at -70 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.31, 0.53, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

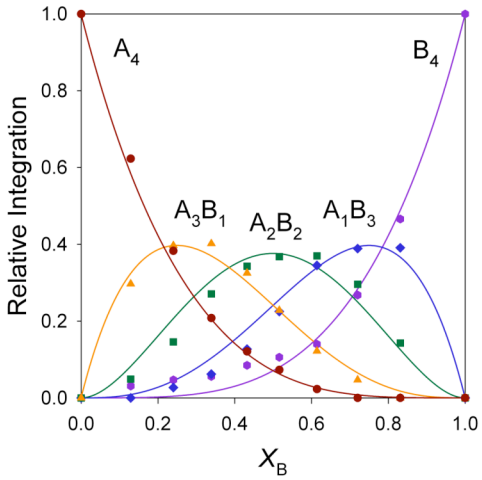


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**9** (**A**) and [^{6}Li]**11** (**B**) in 2.9 M DME/toluene at -70 °C.

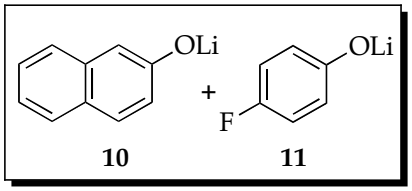


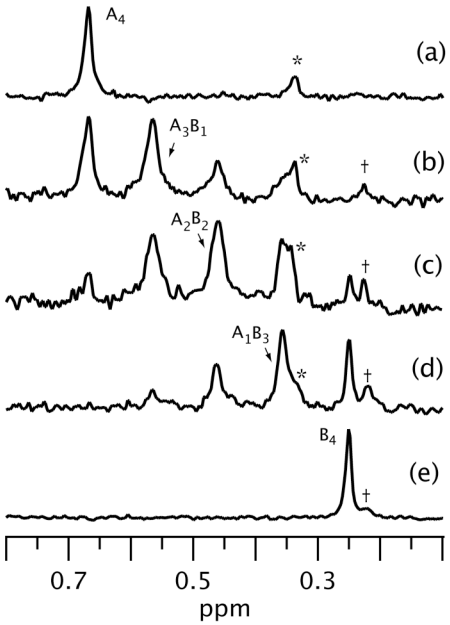


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**9** (**A**) and [^{6}Li]**12** (**B**) at 2.9 M DME/toluene at -70 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.52, 0.72, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate.

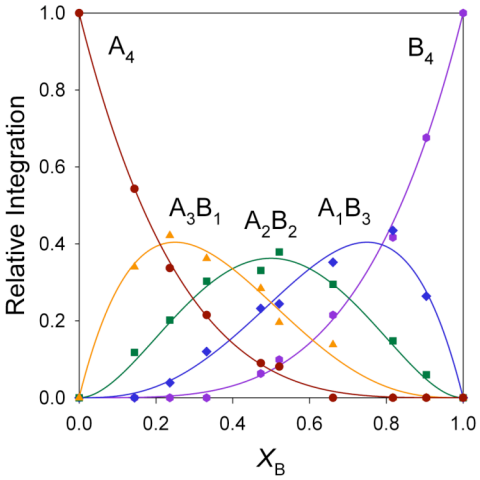


Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates [^{6}Li]**9** (**A**) and [^{6}Li]**12** (**B**) in 2.9 M DME/toluene at -70 °C.



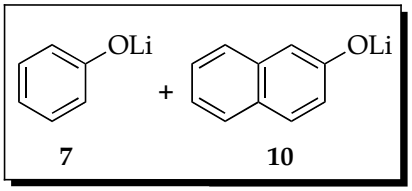


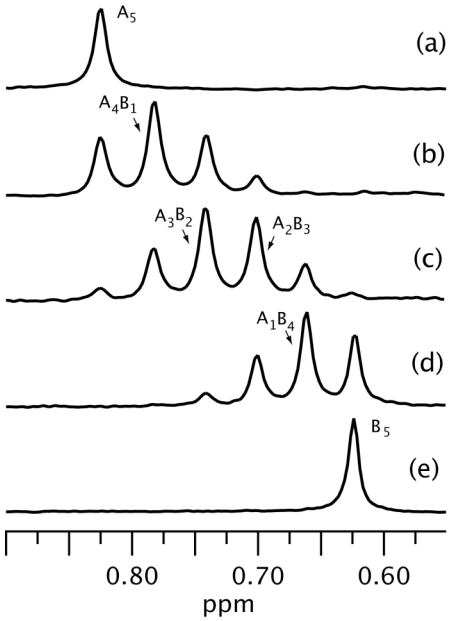
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.47, 0.66, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.



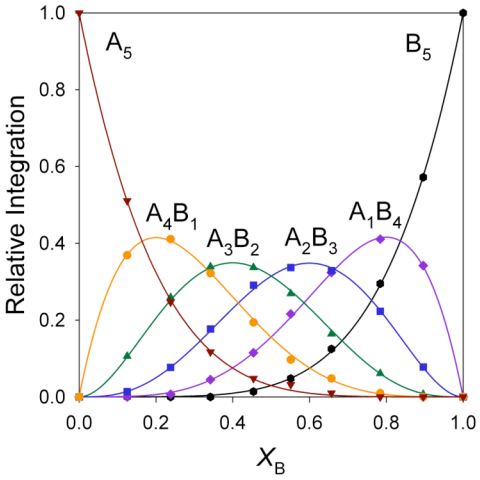
Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) in 2.9 M DME/toluene at -90 °C.

Pentamer Job plots in DME

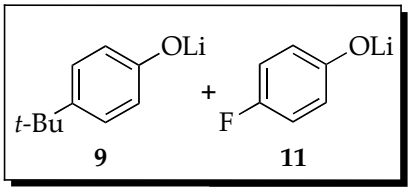


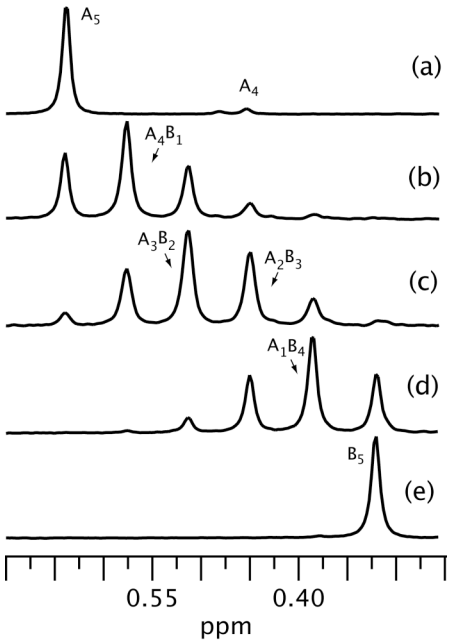


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**7** (**A**) and [^{6}Li]**10** (**B**) at 0.22 M DME/toluene at -30 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.45, 0.78, 1.00 respectively.

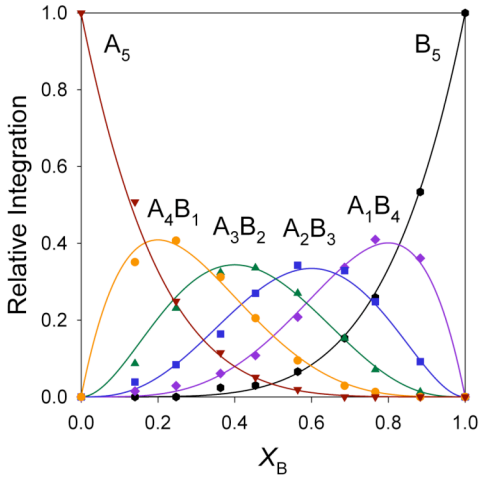


Job plot showing the relative integrations versus mole fractions of **10** for 0.10 M mixtures of phenolates [^{6}Li]**7** (**A**) and [^{6}Li]**10** (**B**) in 0.22 M DME/toluene at -30 °C.

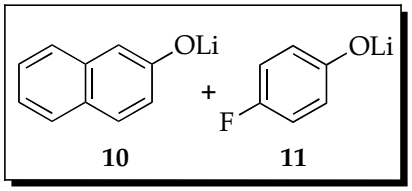


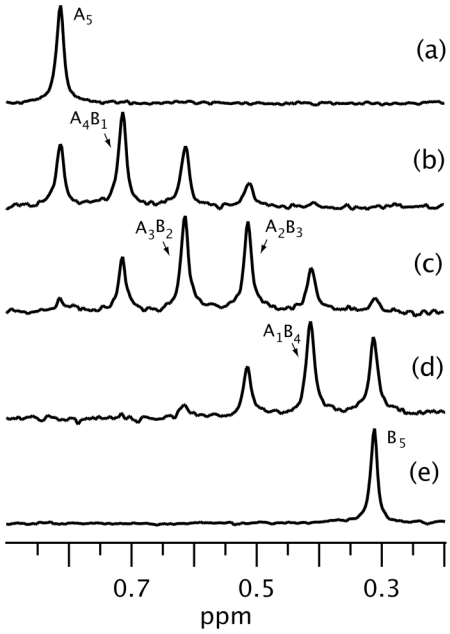


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**9** (**A**) and [^{6}Li]**11** (**B**) at 0.22 M DME/toluene at -30 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.25, 0.45, 0.77, 1.00 respectively.

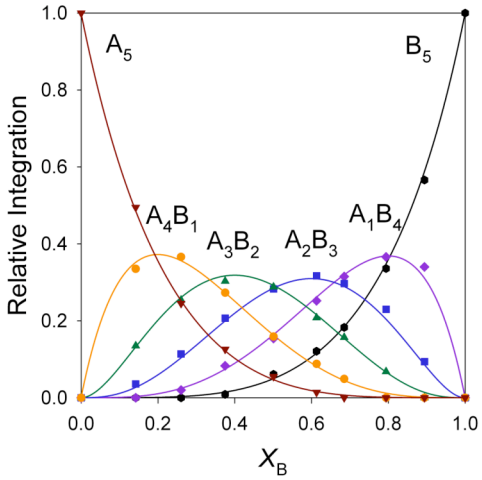


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**9** (**A**) and [^{6}Li]**11** (**B**) in 0.22 M DME/toluene at -30 °C.

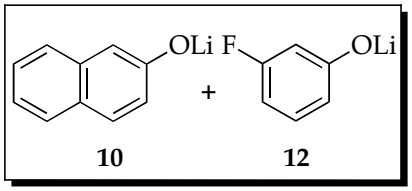


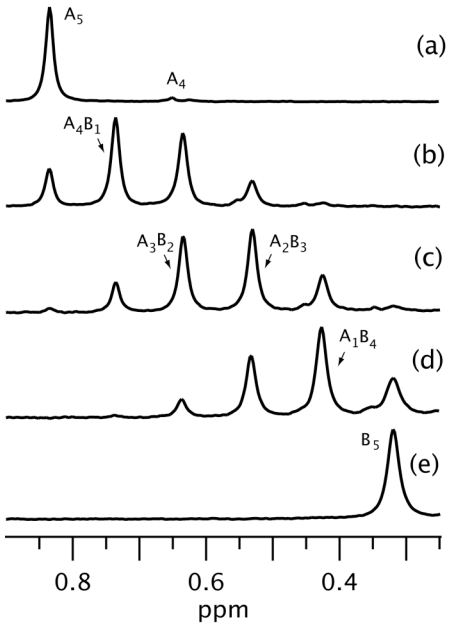


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) at 0.22 M DME/toluene at -30 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.50, 0.79, 1.00 respectively.

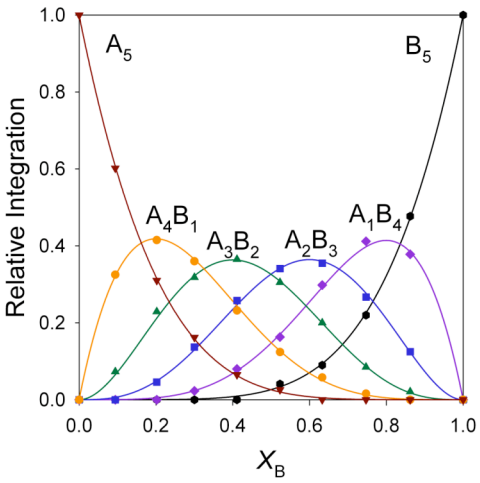


Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^{6}Li]**10** (**A**) and [^{6}Li]**11** (**B**) in 0.22 M DME/toluene at -30 °C.



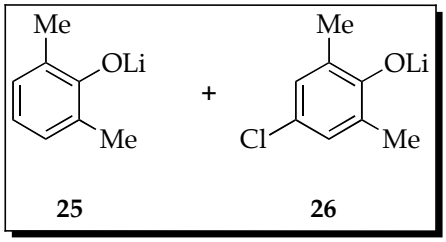


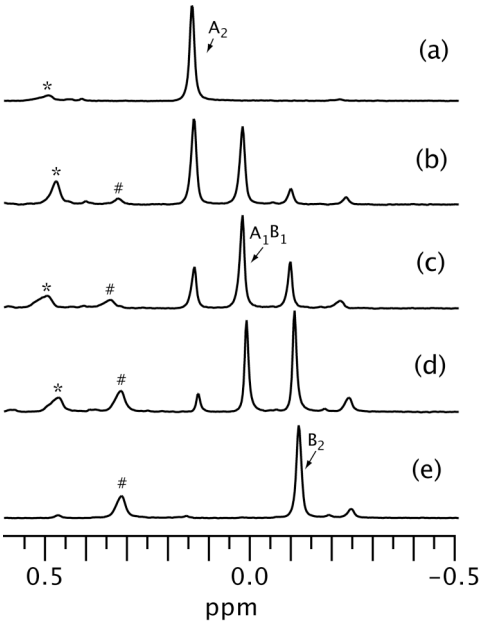
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**10** (**A**) and [^{6}Li]**12** (**B**) at 0.22 M DME/toluene at -30 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.52, 0.75, 1.00 respectively.



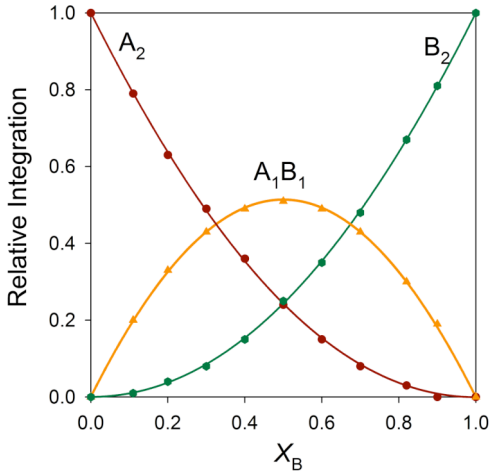
Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates [^{6}Li]**10** (**A**) and [^{6}Li]**12** (**B**) in 0.22 M DME/toluene at -30 °C.

Dimer Job plots in THF

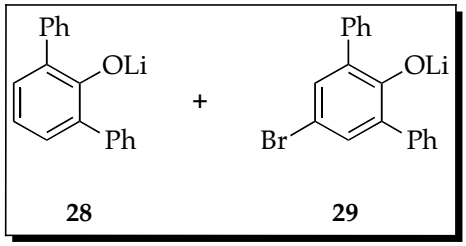


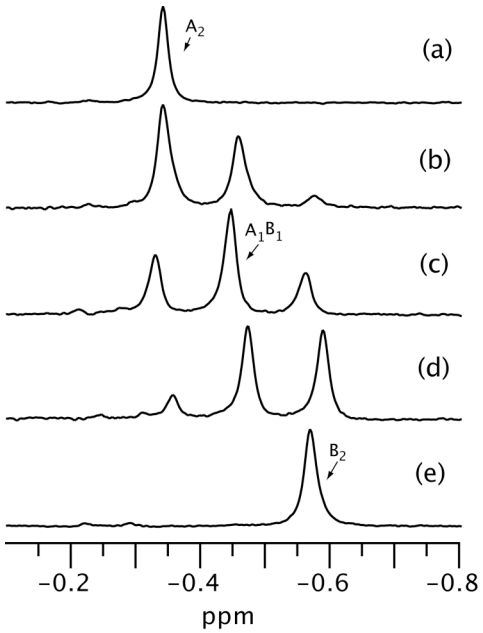


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**25** (**A**) and [^{6}Li]**26** (**B**) at 2.0 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.70, 1.00 respectively. * denotes excess **A.** LiHMDS and # denotes **B.** LiHMDS.

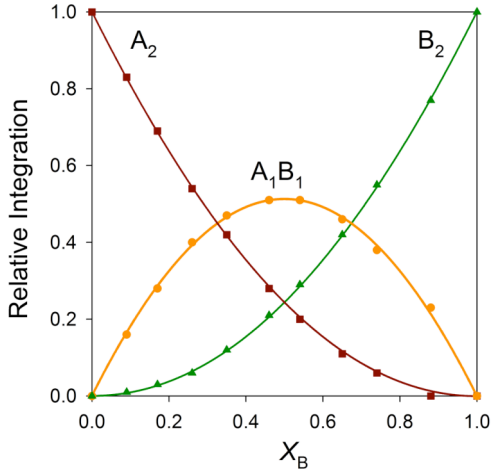


Job plot showing the relative integrations versus mole fractions of **26** for 0.10 M mixtures of phenolates [^{6}Li]**25** (**A**) and [^{6}Li]**26** (**B**) in 2.0 M THF/toluene at -90 °C.

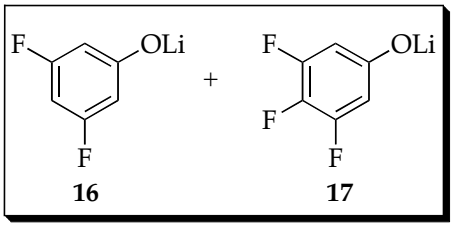


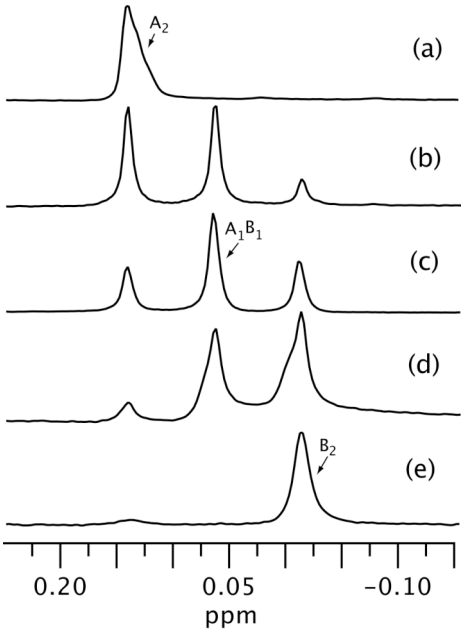


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**28** (**A**) and [^{6}Li]**29** (**B**) at 1.2 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.46, 0.65, 1.00 respectively.

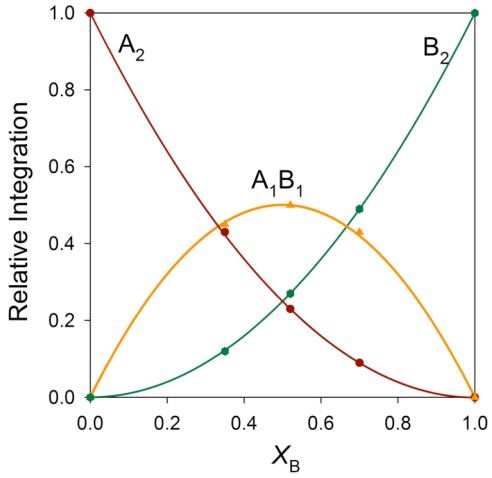


Job plot showing the relative integrations versus mole fractions of **29** for 0.10 M mixtures of phenolates [^{6}Li]**28** (**A**) and [^{6}Li]**29** (**B**) in 1.2 M THF/toluene at -90 °C.

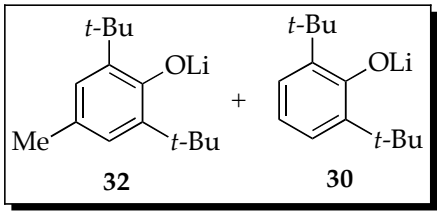


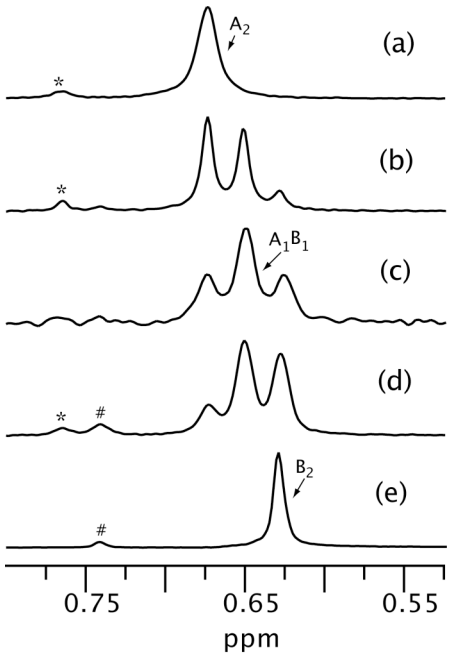


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**16** (**A**) and [^{6}Li]**17** (**B**) at 3.0 M THF/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.52, 0.70, 1.00 respectively.

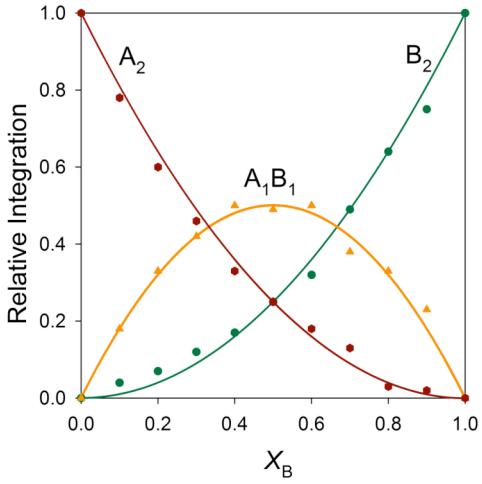


Job plot showing the relative integrations versus mole fractions of **17** for 0.10 M mixtures of penolates [^{6}Li]**16** (**A**) and [^{6}Li]**17** (**B**) in 3.0 M THF/toluene at -90 °C.

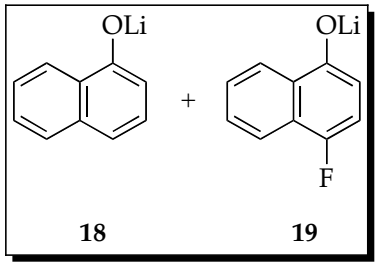


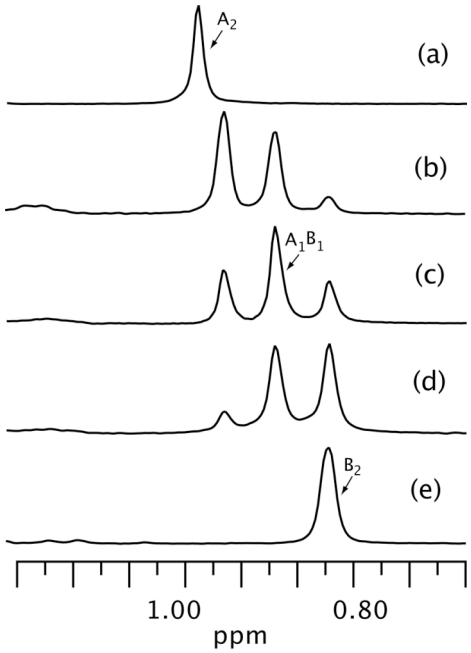


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**32** (**A**) and [^{6}Li]**30** (**B**) at 1.2 M THF/toluene at -78 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.50, 0.73, 1.00 respectively. * denotes excess **A**· LiHMDS and # denotes **B**·LiHMDS mixed aggregates .

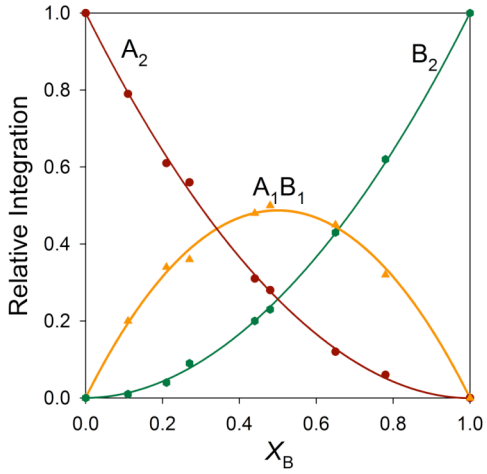


Job plot showing the relative integrations versus mole fractions of **30** for 0.10 M mixtures of phenolates [^{6}Li]**32** (**A**) and [^{6}Li]**32** (**B**) in 1.2 M THF/toluene at -78 °C.

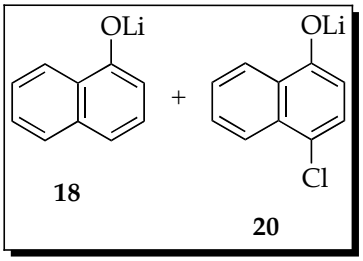


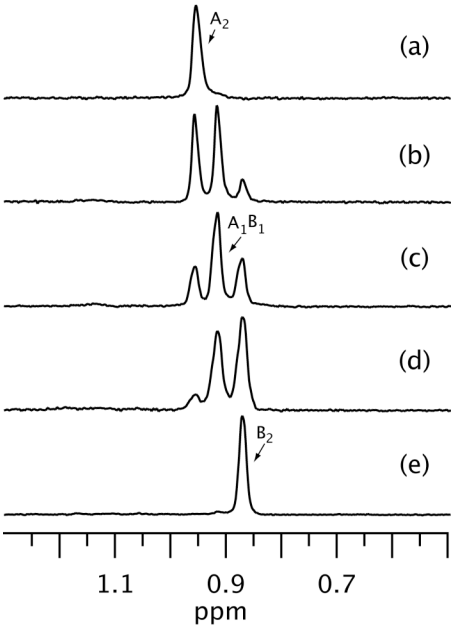


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**19** (**B**) at 12.2 M THF at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.27, 0.48, 0.65, 1.00 respectively.

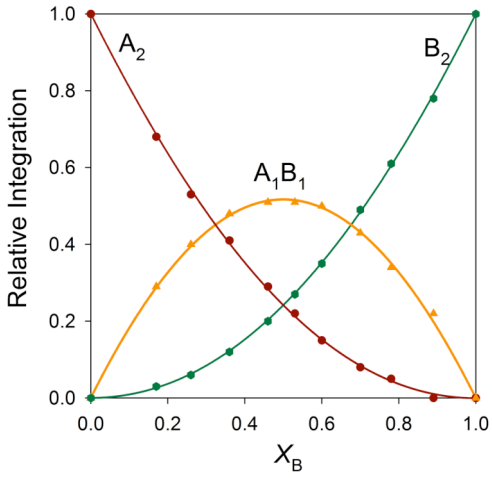


Job plot showing the relative integrations versus mole fractions of **18** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**19** (**B**) in 1.2 M THF/toluene at -90 °C.



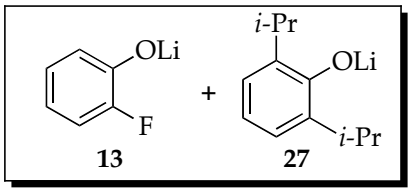


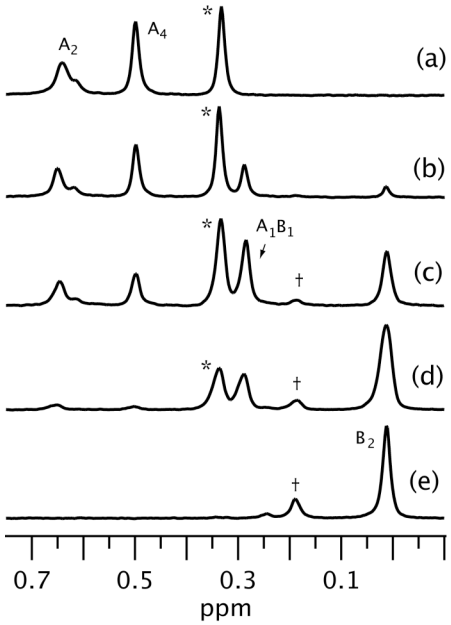
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**20** (**B**) in neat THF (12.2 M) at -90 ºC. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.36, 0.53, 0.70, 1.00 respectively.



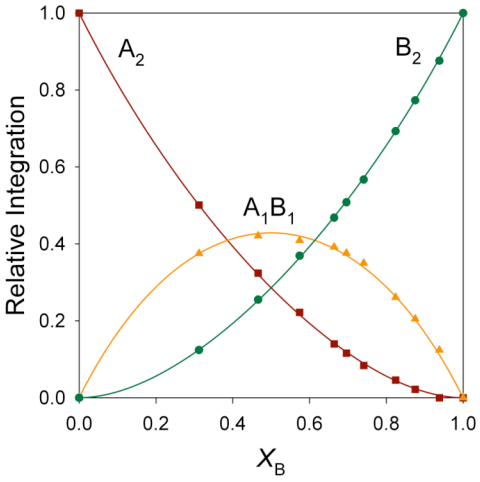
Job plot showing the relative integrations versus mole fractions of **20** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**20** (**B**) in neat THF (12.2 M) at -90 °C.

Dimer Job plots in DME

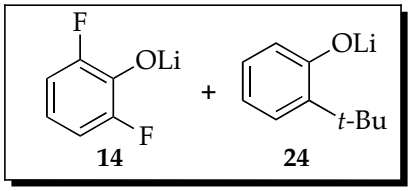


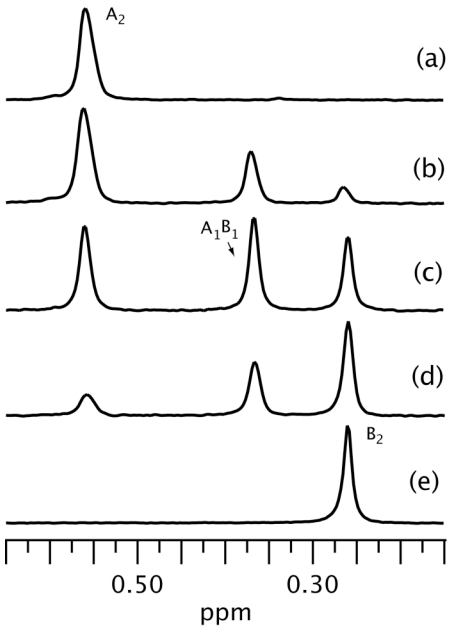


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**13** (**A**) and [^{6}Li]**27** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** within the dimer ensemble in the tubes (a)-(e) are 0.00, 0.31, 0.57, 0.82, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

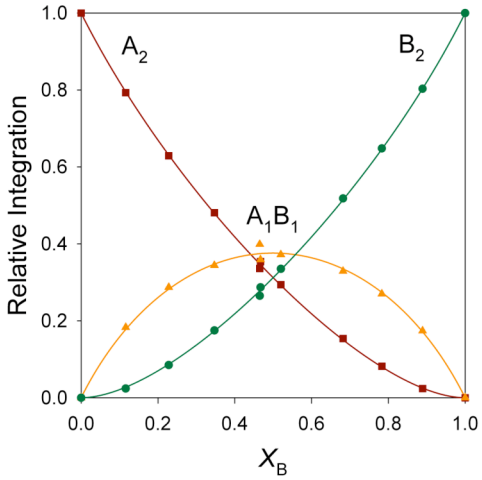


Job plot showing the relative integrations versus mole fractions of **27** (within the dimer ensemble) for 0.10 M mixtures of phenolates [^{6}Li]**13** (**A**) and [^{6}Li]**27** (**B**) in 2.9 M DME/toluene at -90 °C. The data are skewed toward higher X_B because the effective concentration of **13** is reduced by (a) preferential formation of its LiHMDS aggregate and (b) its tetramer homoaggregate.

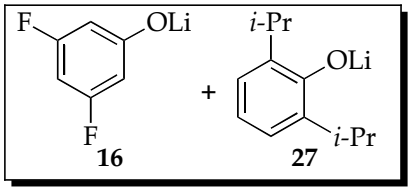


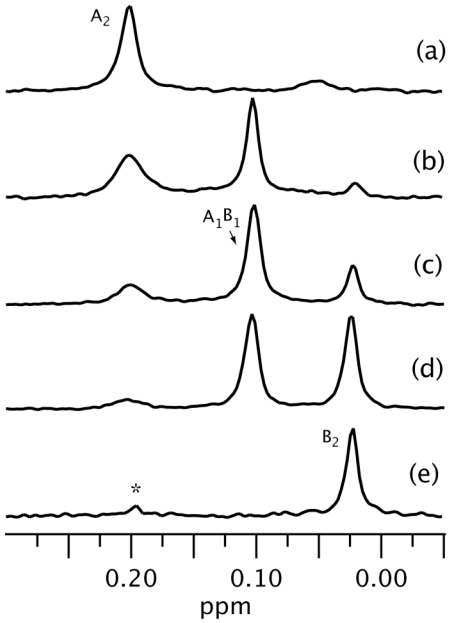


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**14** (**A**) and [^{6}Li]**24** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.23, 0.47, 0.68, 1.00 respectively.

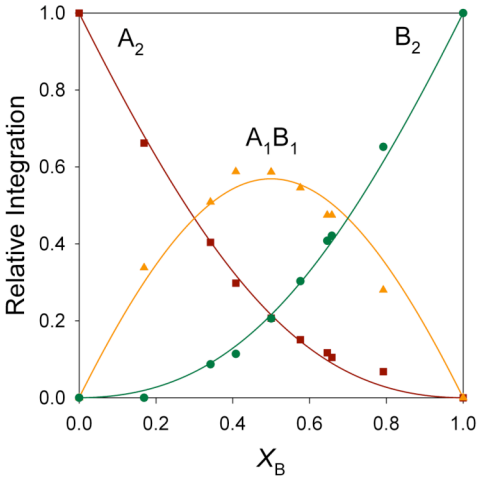


Job plot showing the relative integrations versus mole fractions of **24** for 0.10 M mixtures of phenolates [^{6}Li]**14** (**A**) and [^{6}Li]**24** (**B**) in 2.9 M DME/toluene at -90 °C.

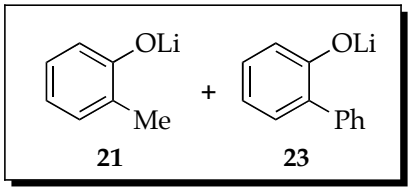


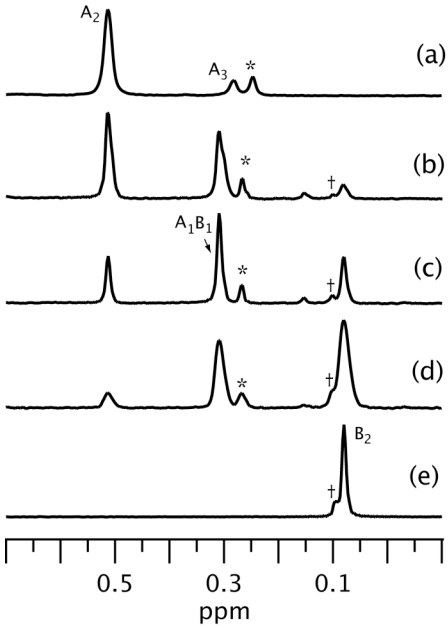


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**16** (**A**) and [^{6}Li]**27** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.50, 0.66, 1.00 respectively. * denotes **B**·LiHMDS mixed aggregate.

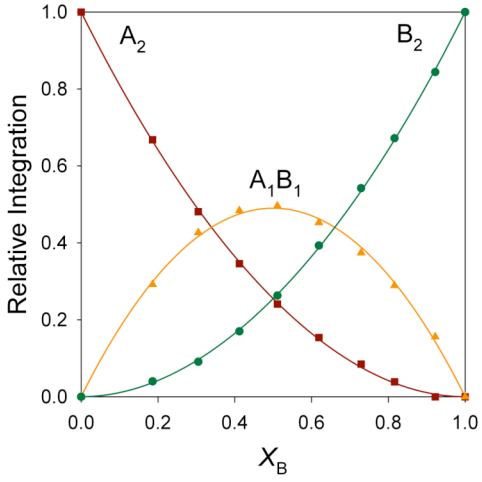


Job plot showing the relative integrations versus mole fractions of **27** for 0.10 M mixtures of phenolates [^{6}Li]**16** (**A**) and [^{6}Li]**27** (**B**) in 2.9 M DME/toluene at -90 °C.

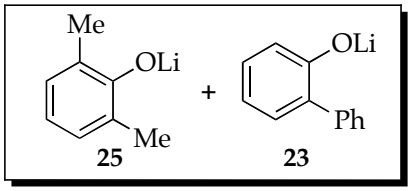


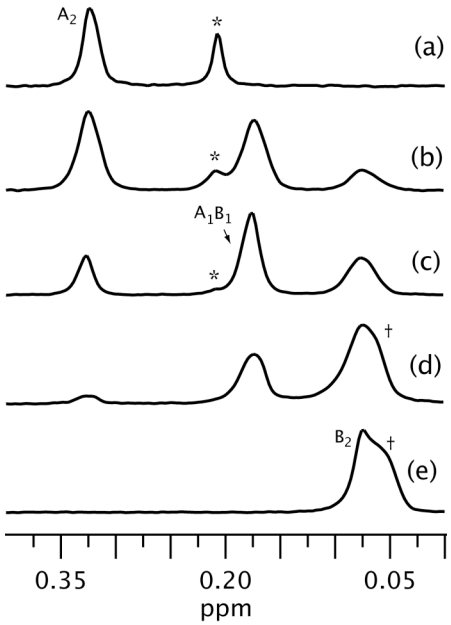


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**21** (**A**) and [^{6}Li]**23** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.51, 0.73, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

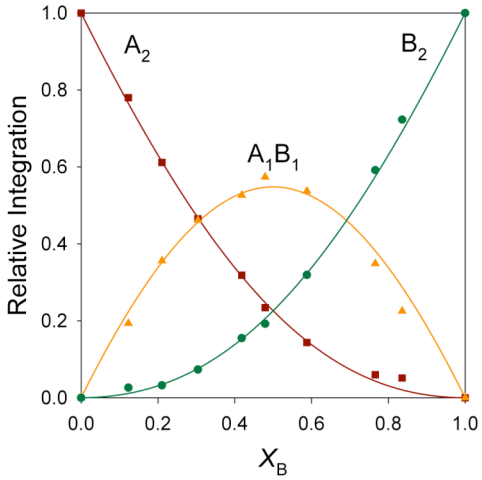


Job plot showing the relative integrations versus mole fractions of **23** for 0.10 M mixtures of phenolates [^{6}Li]**21** (**A**) and [^{6}Li]**23** (**B**) in 2.9 M DME/toluene at -90 °C.

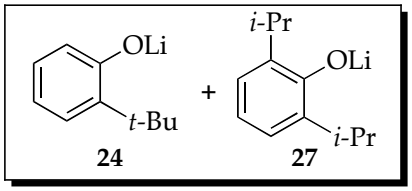


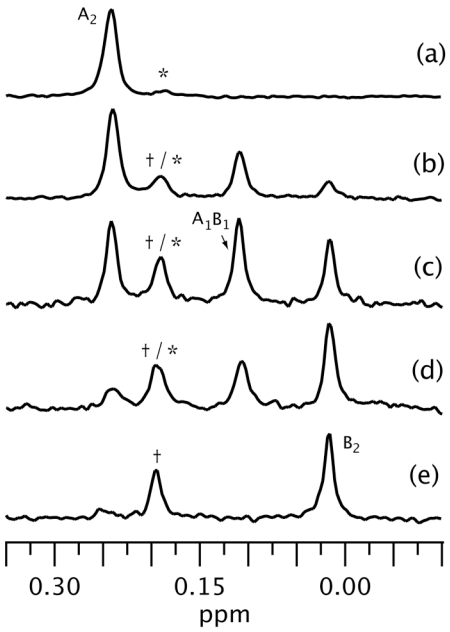


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**25** (**A**) and [^{6}Li]**23** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.48, 0.77, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

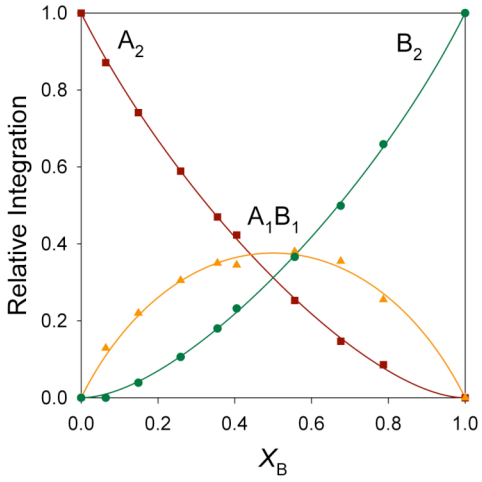


Job plot showing the relative integrations versus mole fractions of **23** for 0.10 M mixtures of phenolates [^{6}Li]**25** (**A**) and [^{6}Li]**23** (**B**) in 2.9 M DME/toluene at -90 °C.

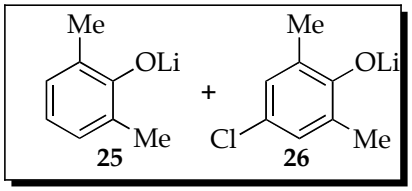


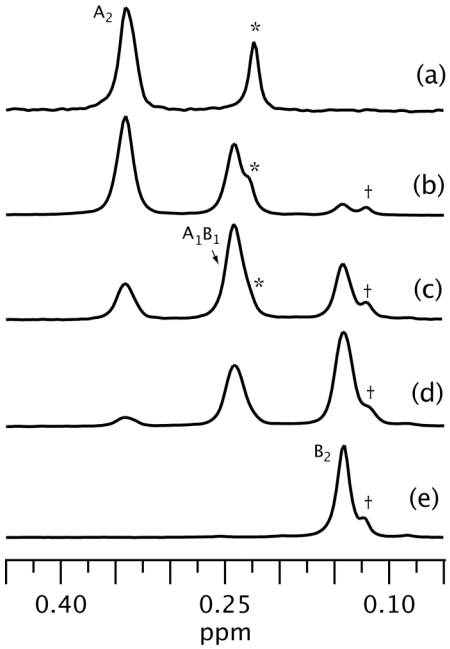


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**24** (**A**) and [^{6}Li]**27** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.40, 0.68, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

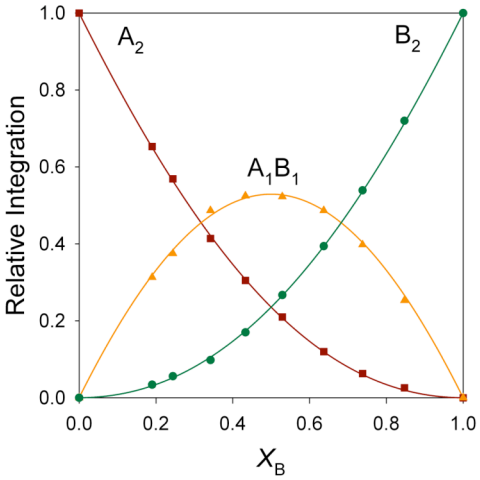


Job plot showing the relative integrations versus mole fractions of **27** for 0.10 M mixtures of phenolates [^{6}Li]**24** (**A**) and [^{6}Li]**27** (**B**) in 2.9 M DME/toluene at -90 °C.

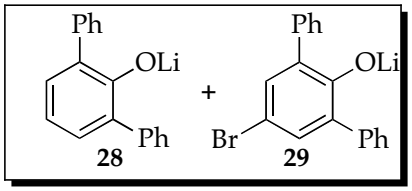


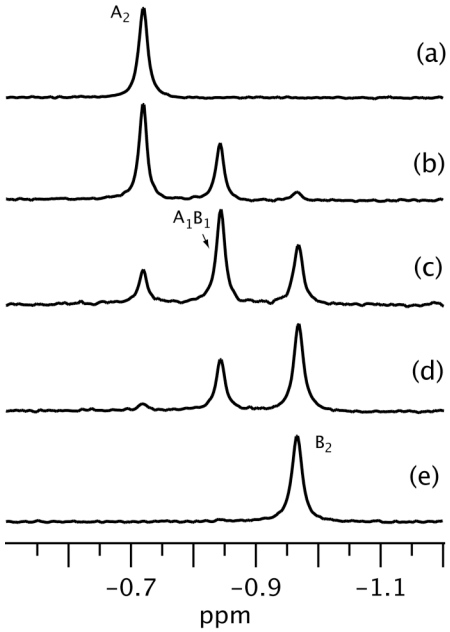


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**25** (**A**) and [^{6}Li]**26** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.53, 0.74, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

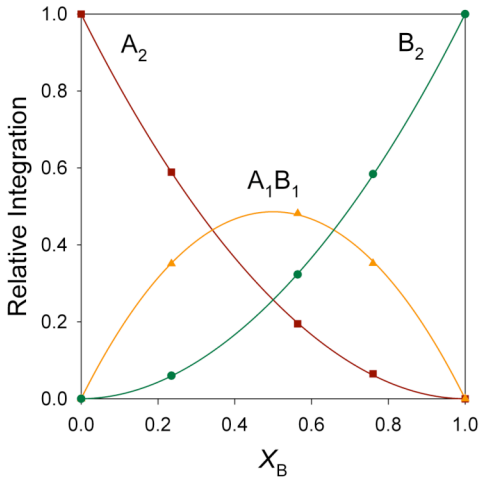


Job plot showing the relative integrations versus mole fractions of **26** for 0.10 M mixtures of phenolates [^{6}Li]**25** (**A**) and [^{6}Li]**26** (**B**) in 2.9 M DME/toluene at -90 °C.

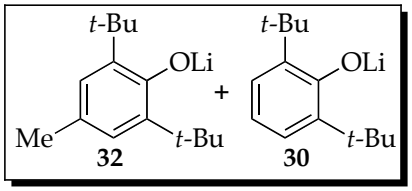


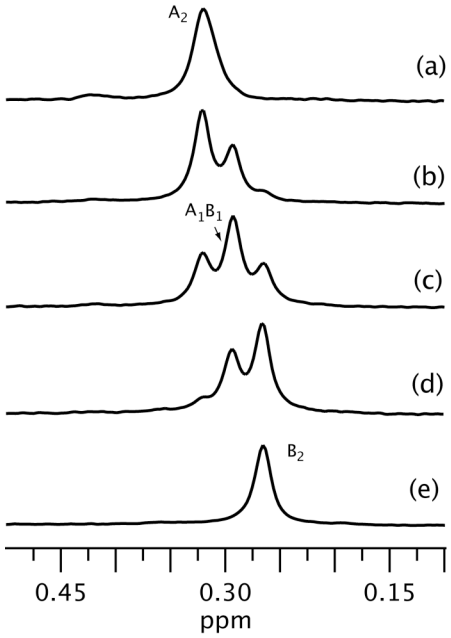


^{6}Li NMR spectra of 0.05 M solutions of [^{6}Li]**28** (**A**) and [^{6}Li]**29** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.56, 0.76, 1.00 respectively.

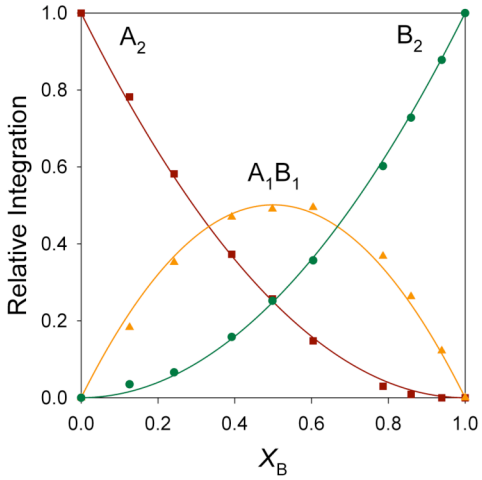


Job plot showing the relative integrations versus mole fractions of **29** for 0.05 M mixtures of phenolates [^{6}Li]**28** (**A**) and [^{6}Li]**29** (**B**) in 2.9 M DME/toluene at -90 °C.



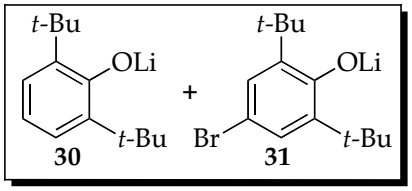


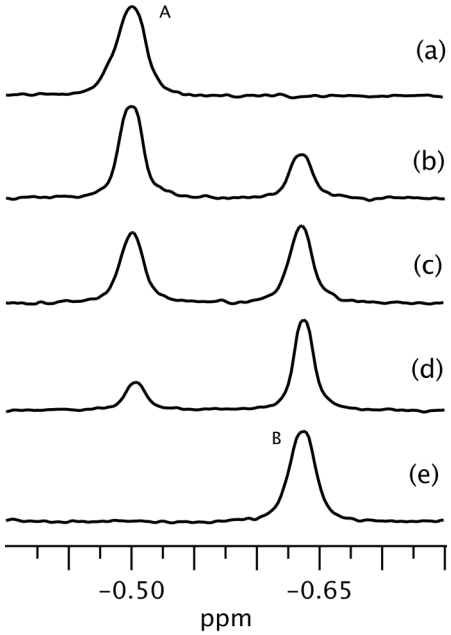
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**32** (**A**) and [^{6}Li]**30** (**B**) at 0.22 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.50, 0.79, 1.00 respectively.



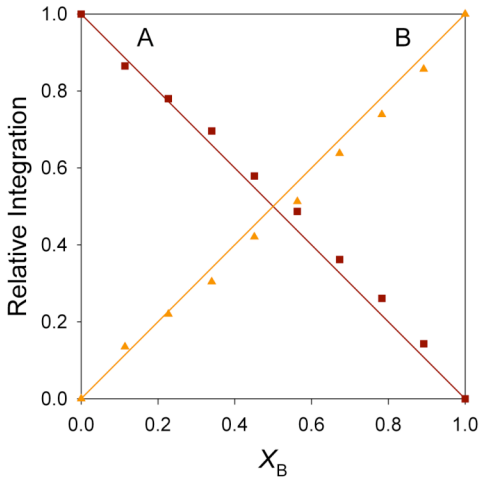
Job plot showing the relative integrations versus mole fractions of **30** for 0.10 M mixtures of phenolates [^{6}Li]**32** (**A**) and [^{6}Li]**30** (**B**) in 0.22 M DME/toluene at -90 °C.

Monomer Job plot in DME



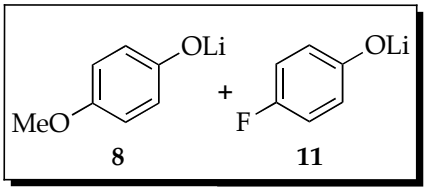


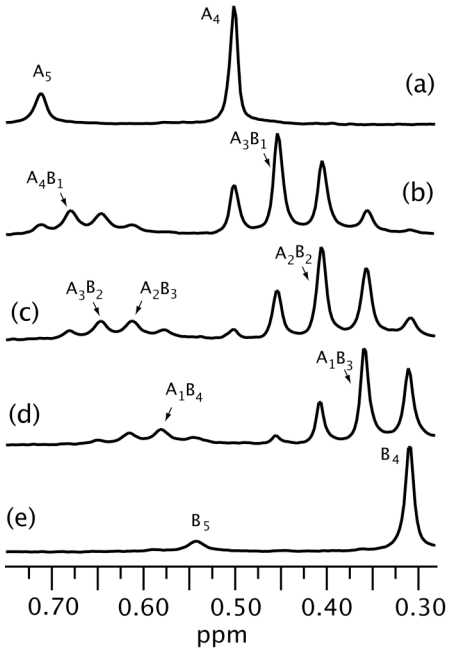
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**30** (**A**) and [^{6}Li]**31** (**B**) at 2.9 M DME/toluene at -90 °C. The intended mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.56, 0.78, 1.00 respectively.



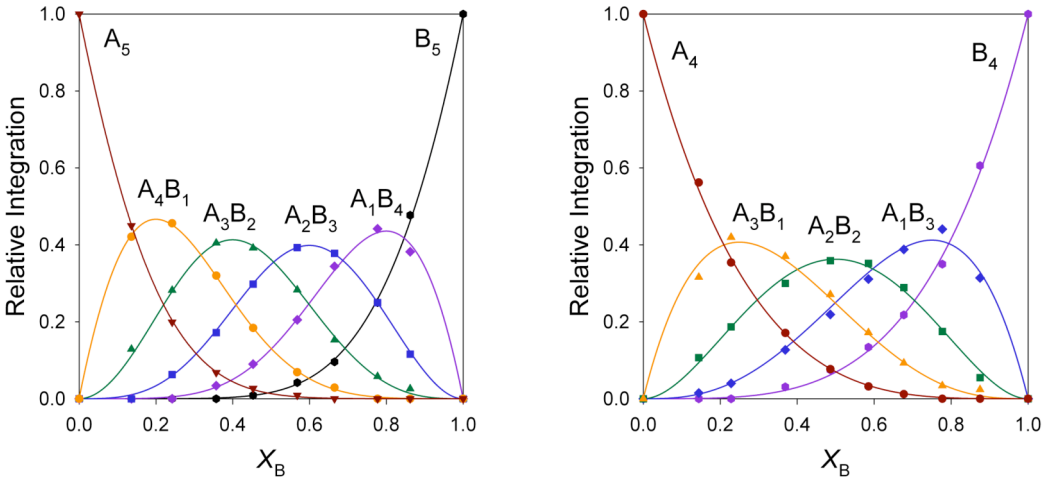
Job plot showing the relative integrations versus intended mole fractions of **31** for 0.10 M mixtures of phenolates [^{6}Li]**30** (**A**) and [^{6}Li]**31** (**B**) in 2.9 M DME/toluene at -90 °C.

Double Job plots in DME

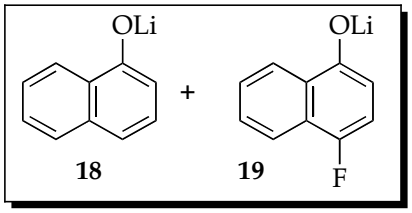


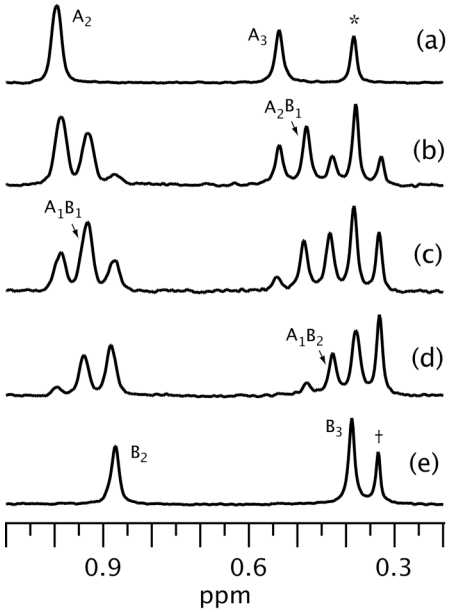


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**8** (**A**) and [^{6}Li]**11** (**B**) at 2.9 M DME/toluene at -50 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.36, 0.57, 0.77, 1.00 respectively.

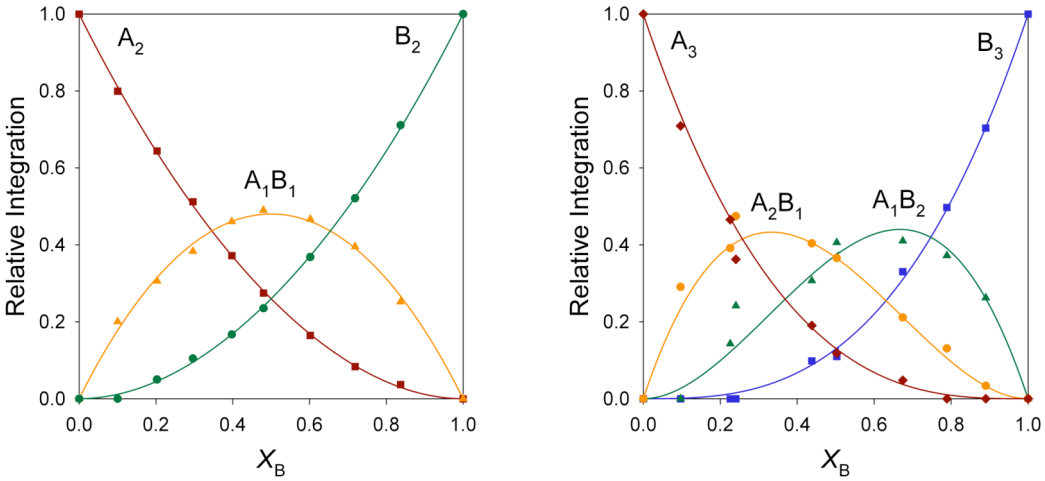


Job plots showing the relative integrations versus mole fractions of **11** (within the given ensemble) for 0.10 M mixtures of phenolates [^{6}Li]**8** (**A**) and [^{6}Li]**11** (**B**) in 2.9 M DME/toluene at -50 °C.

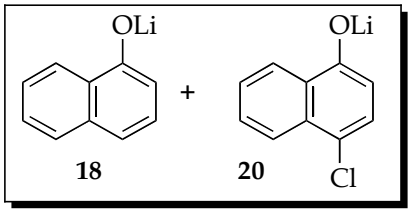


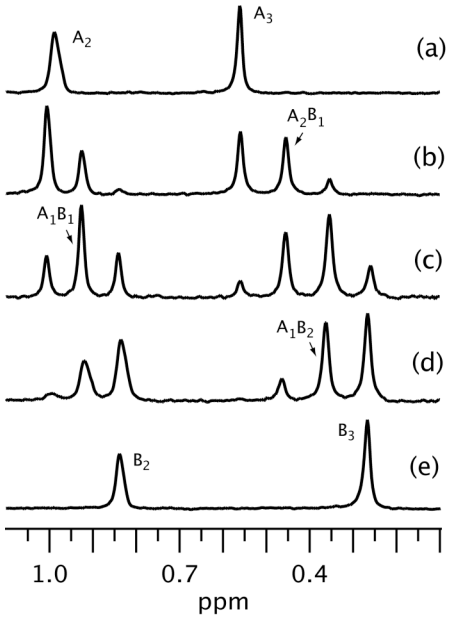


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**19** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.49, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate. Due to overlap of $\mathbf{B}_3$ homoaggregate with **A**·LiHMDS mixed aggregate, the contribution to the peak's integration from $\mathbf{B}_3$ was calculated as follows. Constant excess LiHMDS was assumed, therefore constant relative integration for **A**·LiHMDS + **B**·LiHMDS. Subtracting the measured **B**·LiHMDS integration from this for each tube gave a calculated **A**·LiHMDS integration, which was subtracted from the overlapped peak's integration to give a value for $\mathbf{B}_3$.

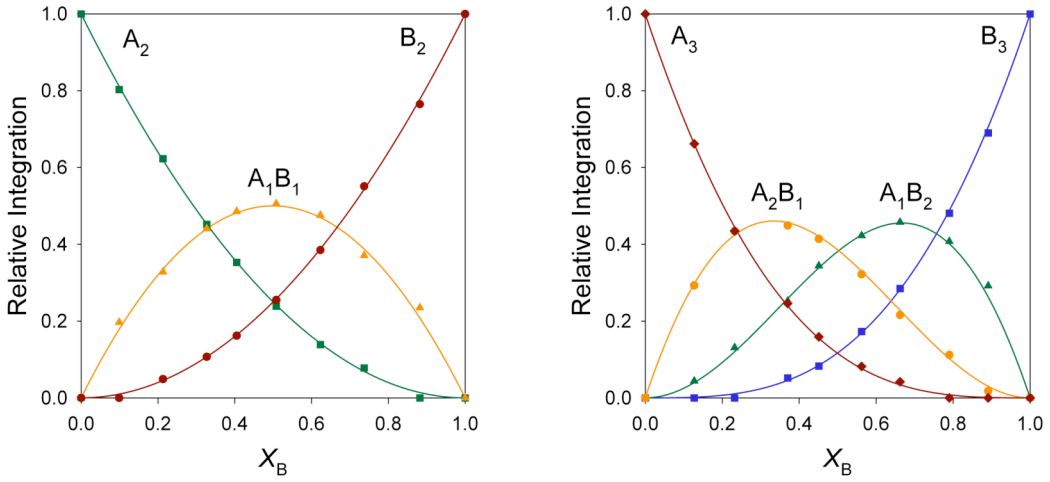


Job plots showing the relative integrations versus mole fractions of **19** (within the given ensemble) for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**19** (**B**) in 2.9 M DME/toluene at -90 °C.

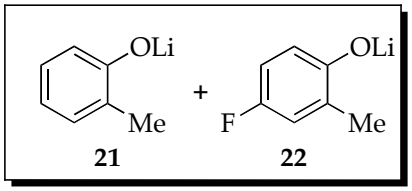


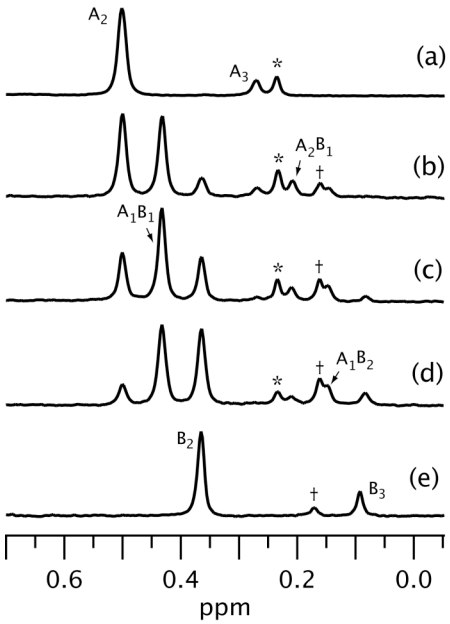


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**20** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.22, 0.54, 0.77, 1.00 respectively.

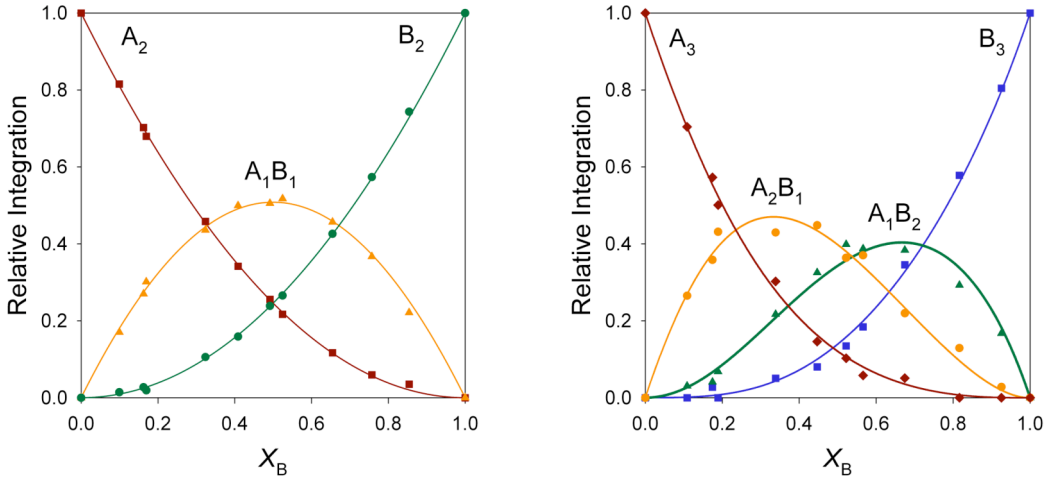


Job plots showing the relative integrations versus mole fractions of **20** (within the given ensemble) for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**20** (**B**) in 2.9 M DME/toluene at -90 °C.



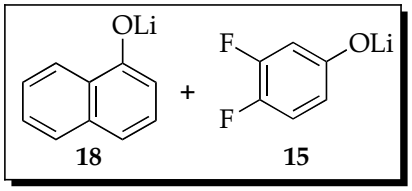


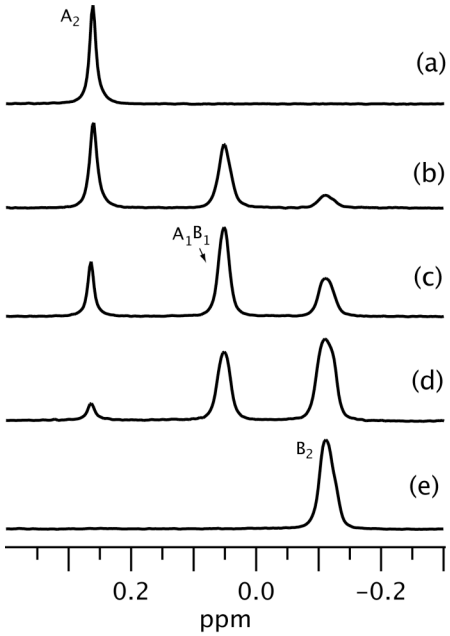
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**21** (**A**) and [^{6}Li]**22** (**B**) at 2.9 M DME/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.50, 0.66, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.



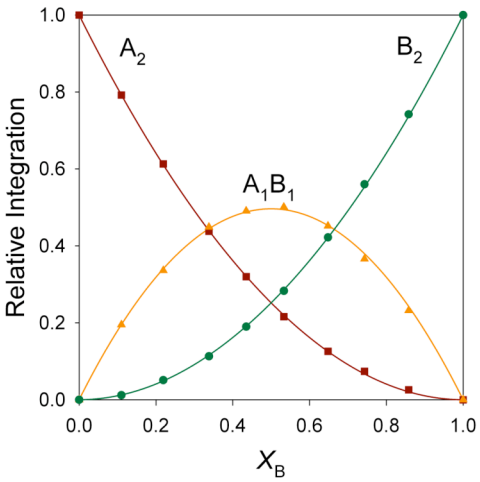
Job plots showing the relative integrations versus mole fractions of **22** (within the given ensemble) for 0.10 M mixtures of phenolates [^{6}Li]**21** (**A**) and [^{6}Li]**22** (**B**) in 2.9 M DME/toluene at -90 °C.

Job plots in TMEDA

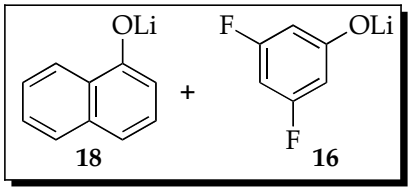


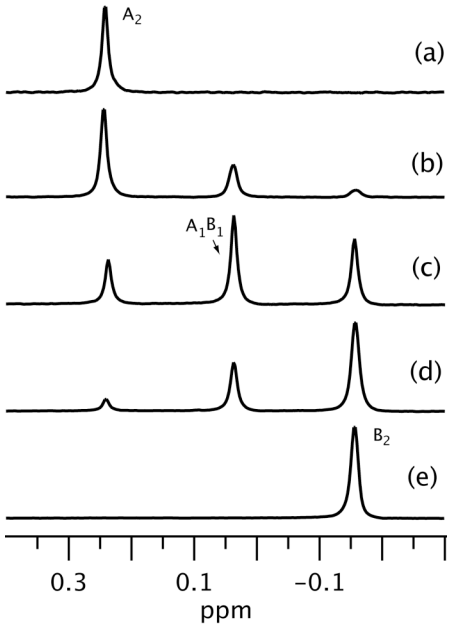


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**15** (**B**) at 0.22 M TMEDA/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.53, 0.74, 1.00 respectively.

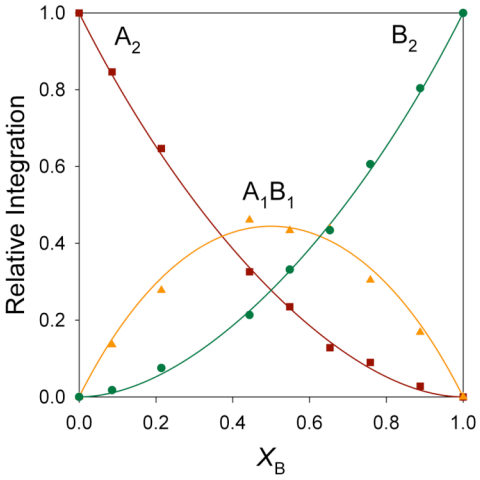


Job plot showing the relative integrations versus mole fractions of **15** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**15** (**B**) in 0.22 M TMEDA/toluene at -90 °C.



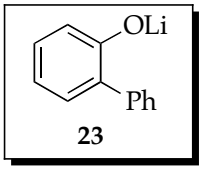


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) and [^{6}Li]**16** (**B**) at 0.22 M TMEDA/toluene at -90 °C. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.21, 0.55, 0.76, 1.00 respectively.

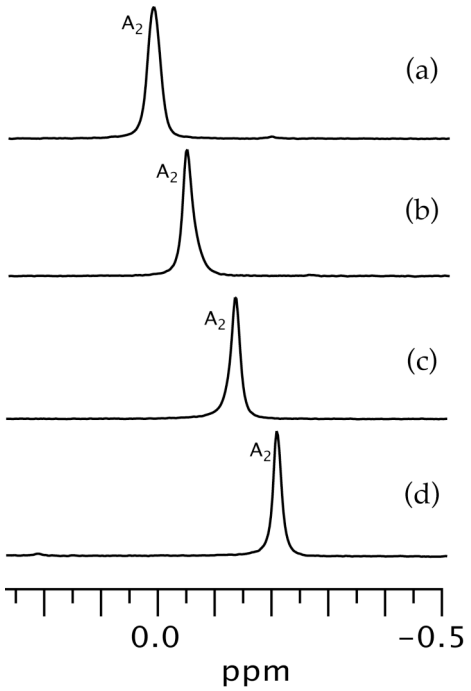


Job plot showing the relative integrations versus mole fractions of **16** for 0.10 M mixtures of phenolates [^{6}Li]**18** (**A**) and [^{6}Li]**16** (**B**) in 0.22 M TMEDA/toluene at -90 °C.

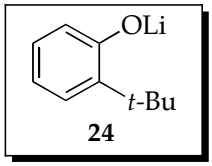
Solvent swaps



23



^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**23** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene.



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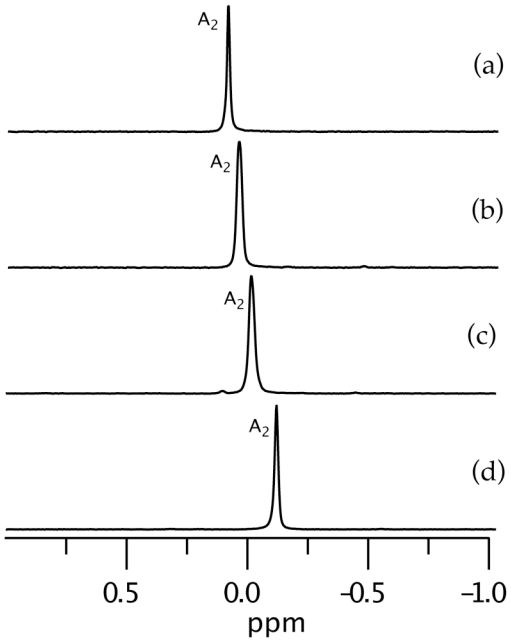
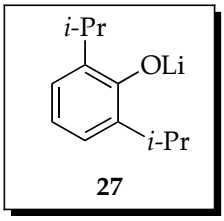


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**24** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene.



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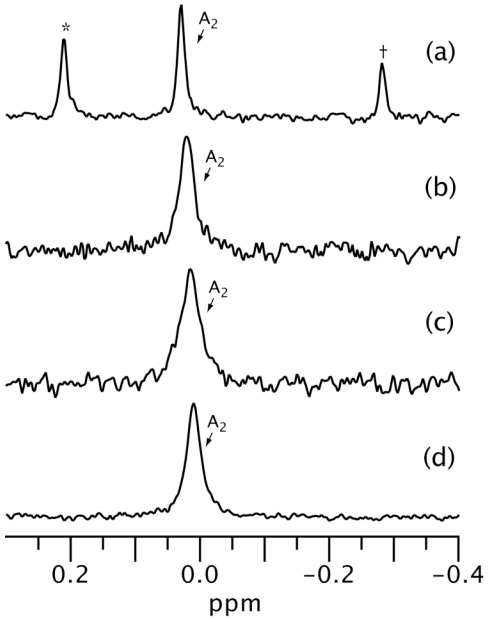
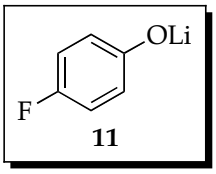


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**27** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene. † denotes excess LiHMDS dimer and * denotes **A.**LiHMDS mixed aggregate



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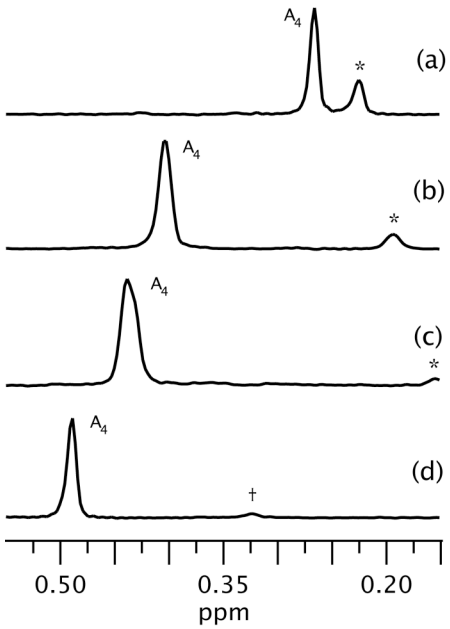
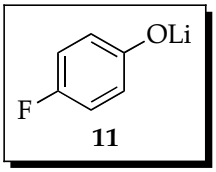


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**11** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 33%, respectively, of the DME/toluene solvent with THF/toluene. * denotes **A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.



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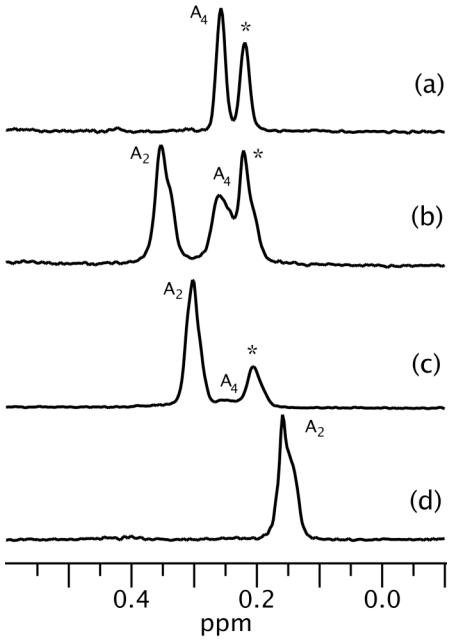
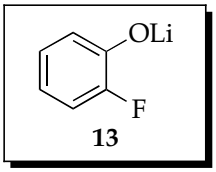


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**11** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 2.0 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 5% and 11%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes **A**·LiHMDS mixed aggregate.



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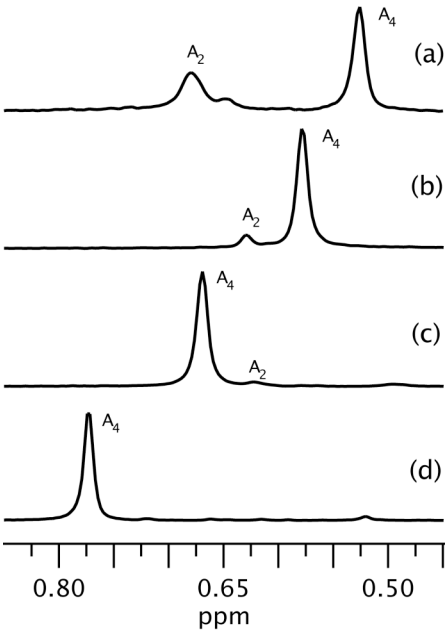
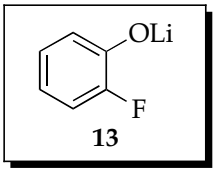


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**13** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with THF/toluene.



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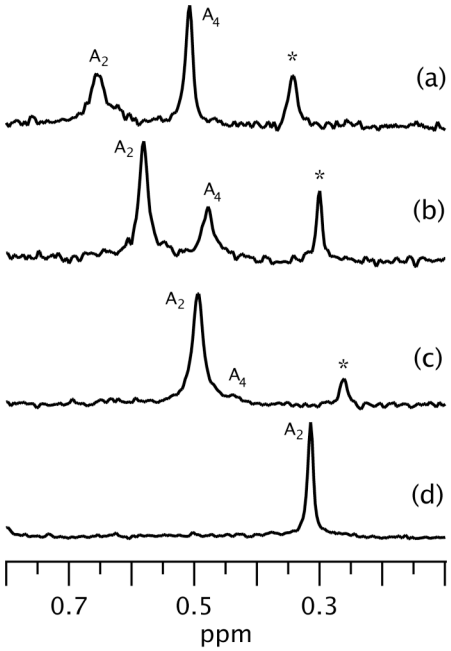
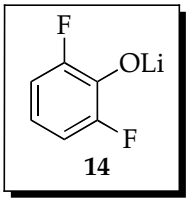


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**13** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.22 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes **A**·LiHMDS mixed aggregate.



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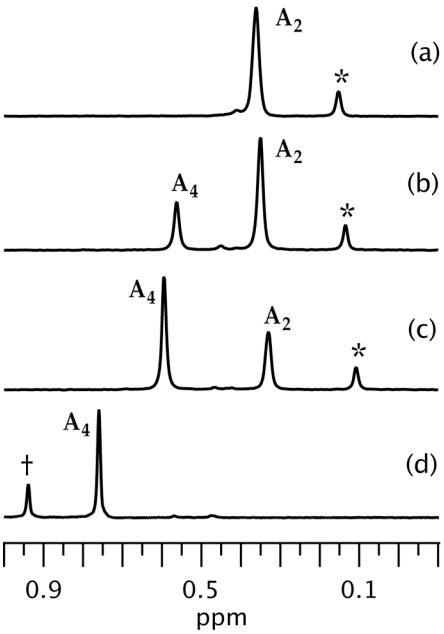
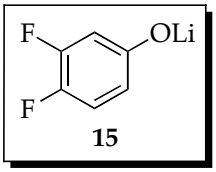


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**14** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 33%, respectively, of the DME/toluene solvent with THF/toluene. * denotes **A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.



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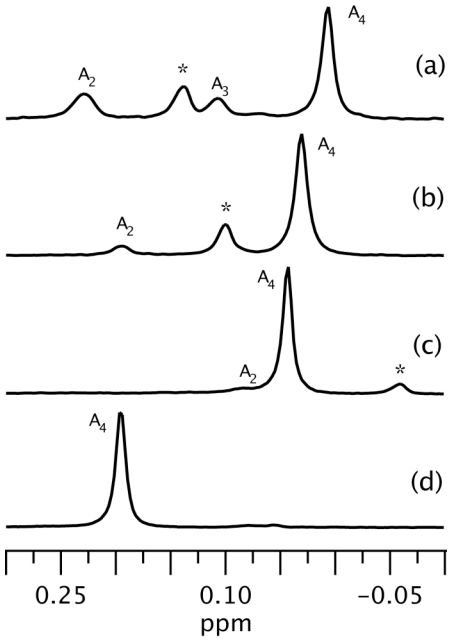
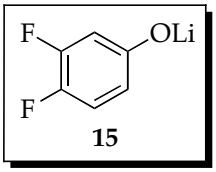


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**15** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 72%, respectively, of the DME/toluene solvent with THF/toluene. * denotes **A**·LiHMDS mixed aggregate.



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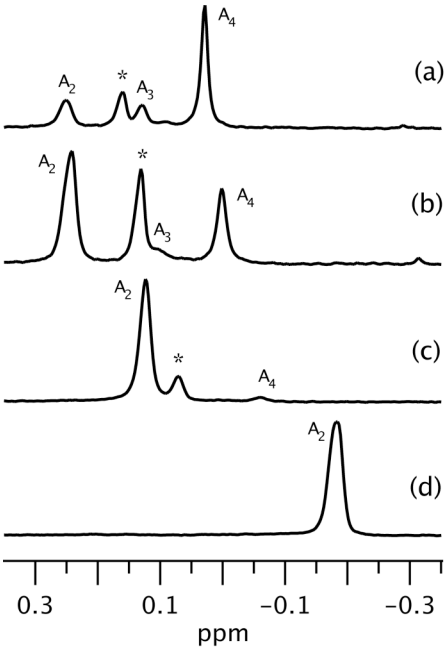
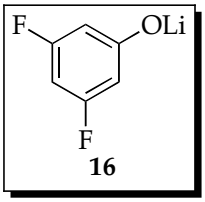


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**15** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.22 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes **A**·LiHMDS mixed aggregate.



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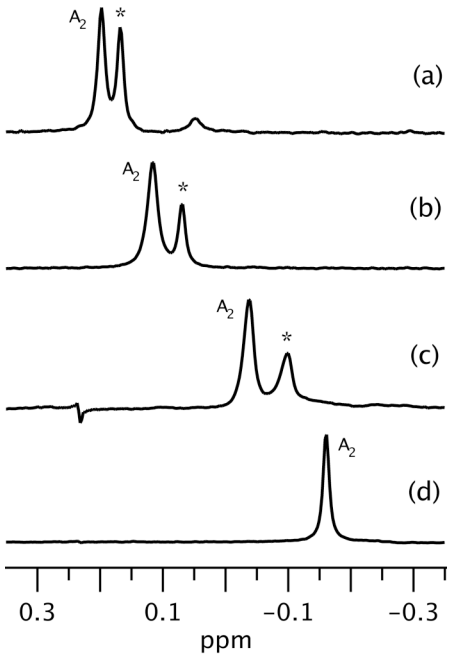
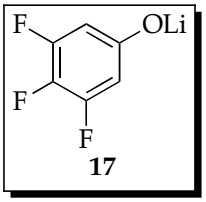


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**16** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.18 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 33% and 72%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes **A**·LiHMDS mixed aggregate.



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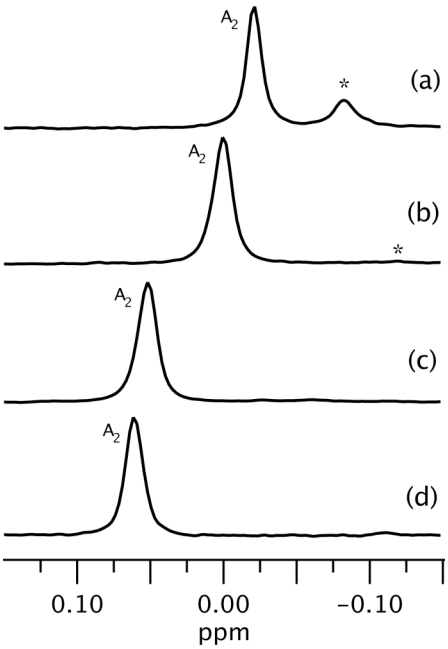
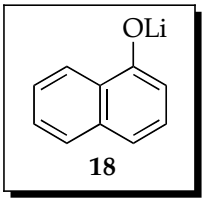


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**17** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 22% and 50%, respectively, of the DME/toluene solvent with THF/toluene. * denotes **A**·LiHMDS mixed aggregate.



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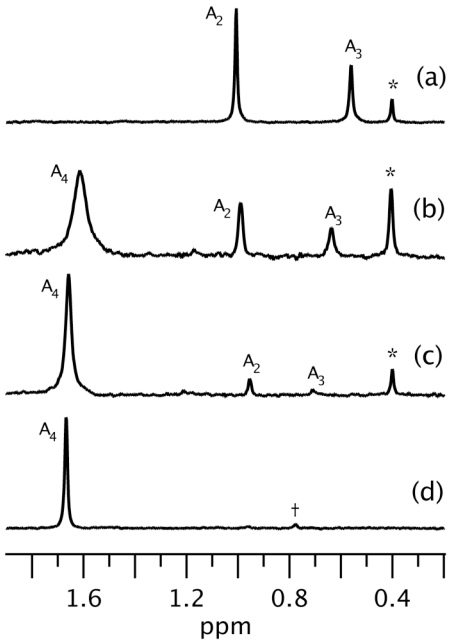
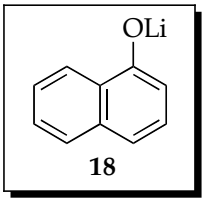


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) at -90 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 6% and 11%, respectively, of the DME/toluene solvent with THF/toluene. * denotes **A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.



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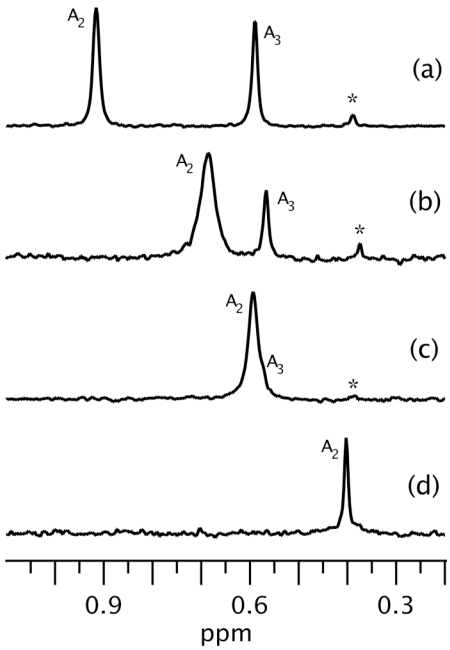
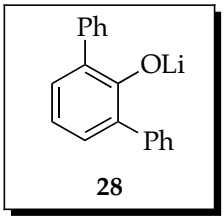
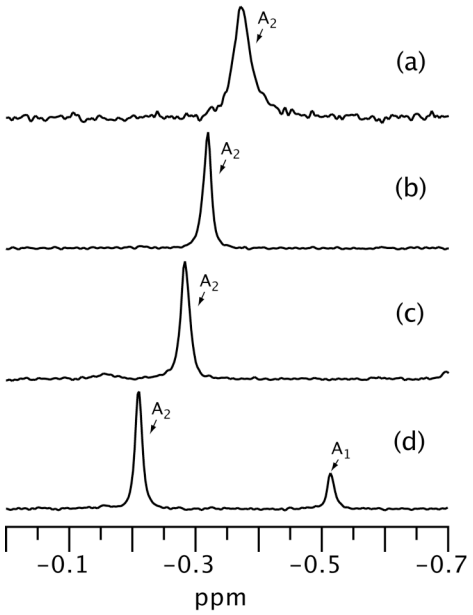


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) at -70 °C showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 2.0 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 3% and 6%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes **A**·LiHMDS mixed aggregate.

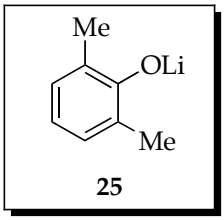
Solvent concentration scans in THF



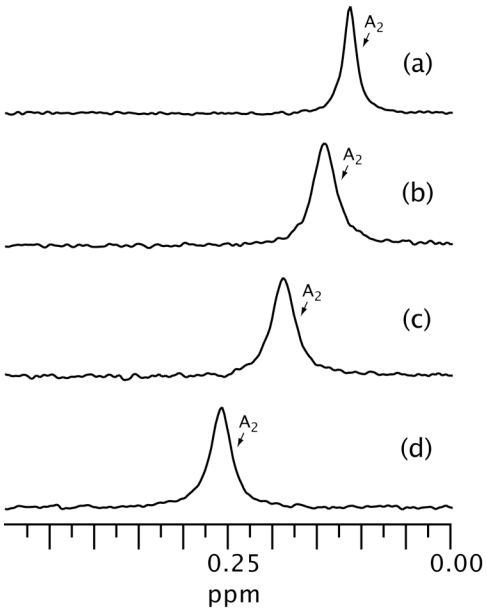
28



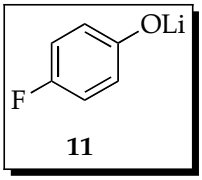
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**28** (**A**) at -90 °C. The solvent systems in tubes (a)-(c) are 1.2 M, 2.0 M, 6.1 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M). A_1 was tentatively assigned based on chemical shift similarity with other monomers.)



25



^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**25** (**A**) at -90 °C. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively.



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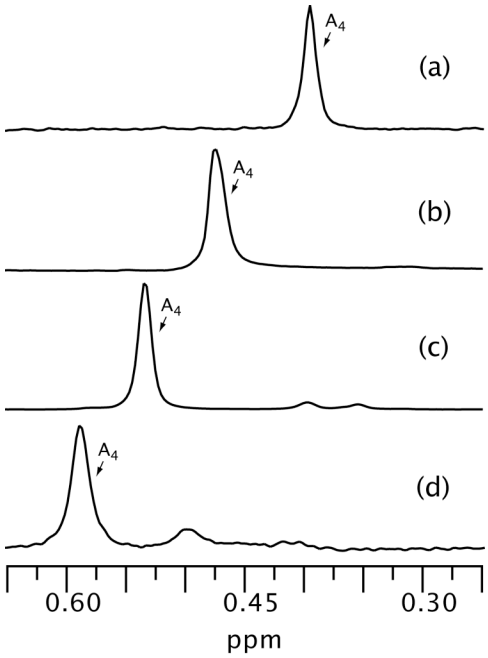
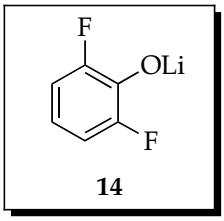


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**11** (**A**) at -90 °C. The solvent systems in tubes (a)-(c) are 0.12 M, 2.0 M, 6.1 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).



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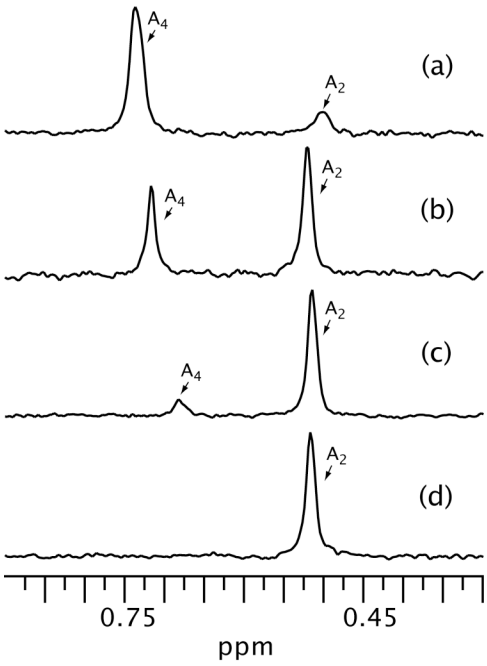
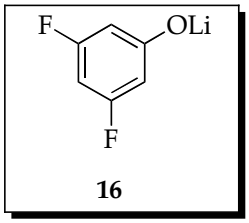
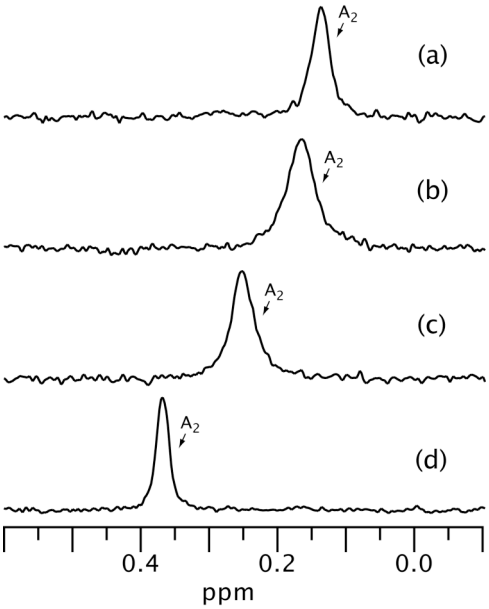


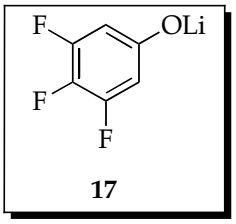
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**14** (**A**) at -90 °C. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively. (A_2 was tentatively assigned based on chemical shift similarity with other dimers.)



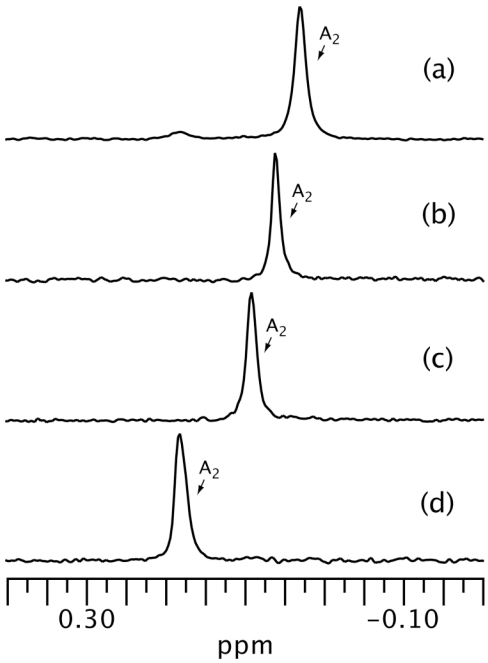
16



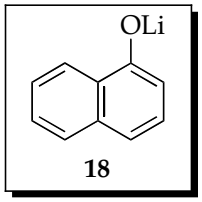
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**16** (**A**) at -90 °C. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively



17



^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**17** (**A**) at -90 °C. The solvent systems in tubes (a)-(d) are 3.0 M, 4.0 M, 6.1 M and 8.0 M THF/toluene, respectively.



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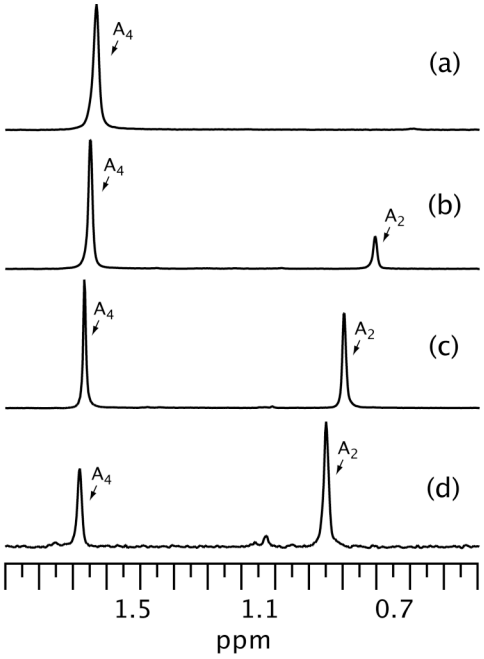
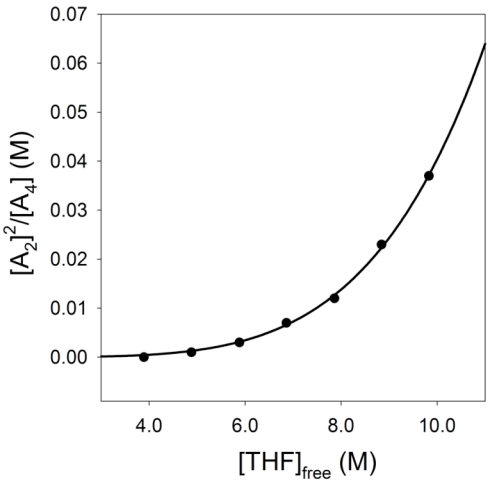


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) at -90 °C. The solvent systems in tubes (a)-(c) are 2.0 M, 6.0 M, 8.0 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).

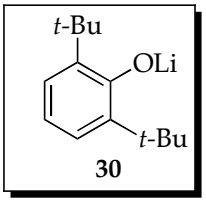


Plot of $[A_2]^2/[A_4]$ of 0.10 M [^{6}Li]**8** (**A**) in toluene at -90 ºC. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 6*10^{-7} \pm 4*10^{-7}$, $n = 2.4 \pm 0.3$) :

$$[A_2]^2/[A_4] = K_{eq} * [THF]^{2n}$$

The equation, assuming a tetrasolvated tetramer was derived from the following equilibrium:

$$A_4THF_4 + 2n\ THF \rightleftharpoons 2\ A_2THF_{(n+2)}$$



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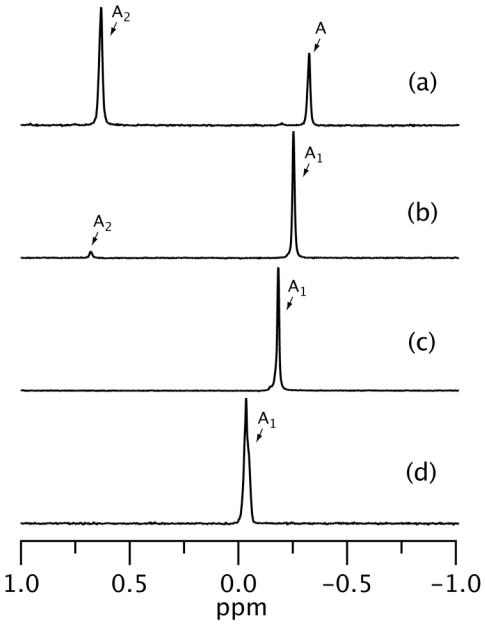
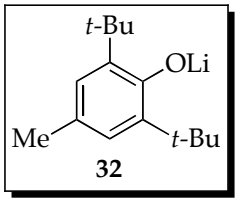


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**30** (**A**) at -90 ºC. The solvent system in tubes (a)-(d) are 2.0 M , 4.0 M, 6.0 M, 10.0 M THF/toluene respectively.



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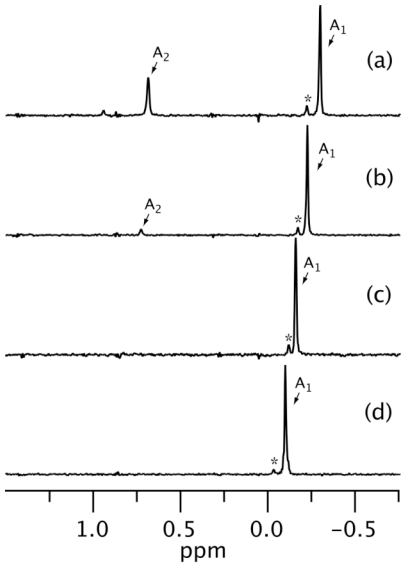
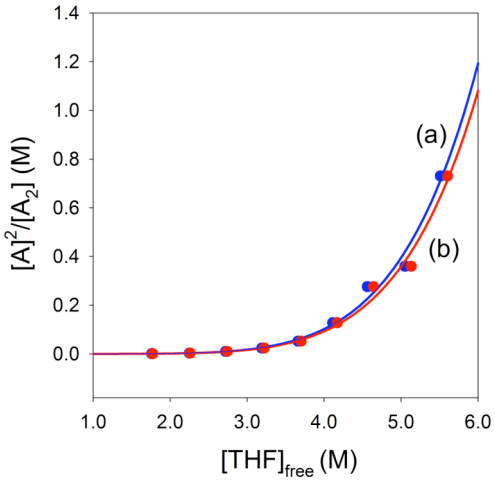


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**32** (**A**) at -90 ºC. The solvent systems in tubes (a)-(c) are 4.0 M, 6.0 M, 8.0 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).



(a) Plot of $[A]^2/[A_2]$ of 0.10 M [^{6}Li]**32** (**A**) in toluene at -90 ºC. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 2*10^{-5} \pm 3*10^{-5}$, $n = 3.0 \pm 0.8$) :

$$[A]^2/[A_2] = K_{eq} * [THF]^{2n}$$

The equation, assuming a tetrasolvated dimer was derived from the following equilibrium:

$$A_2THF_4 + 2n\ THF \rightleftharpoons 2\ A_1THF_{(n+2)}$$

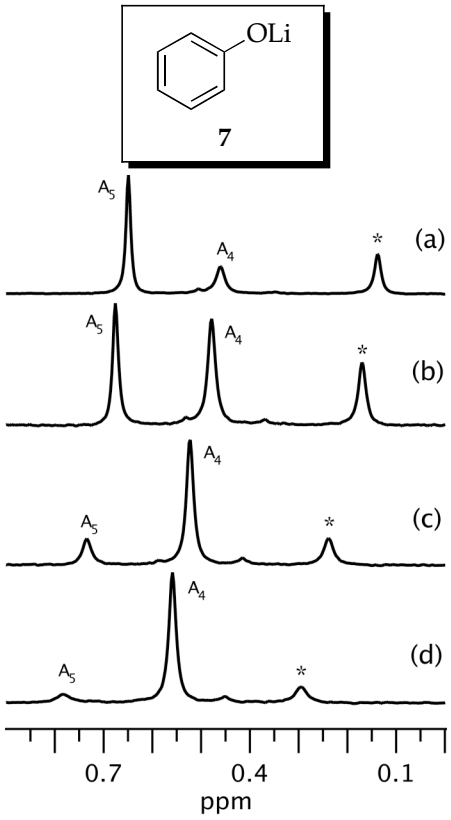
(b) Plot of $[A]^2/[A_2]$ of 0.10 M [^{6}Li]**32** (**A**) in toluene at -90 ºC. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 2*10^{-5} \pm 4*10^{-5}$, $n = 3.0 \pm 0.9$) :

$$[A]^2/[A_2] = K_{eq} * [THF]^{2n}$$

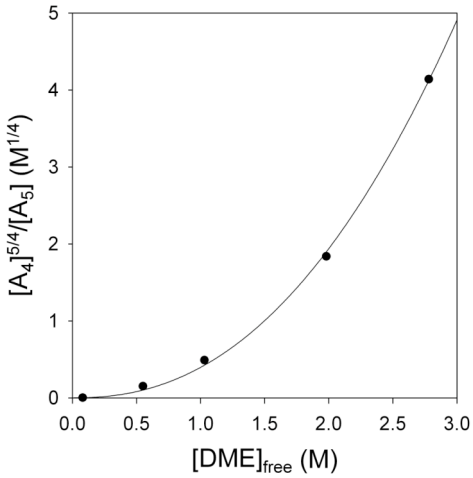
The equation, assuming a disolvated dimer was derived from the following equilibrium:

$$A_2THF_2 + 2n\ THF \rightleftharpoons 2\ A_1THF_{(n+1)}$$

Solvent concentration scans in DME



^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**7** (**A**) at -30 °C. The solvent systems in tubes (a)-(d) are 0.64 M, 1.1 M, 2.1 M and 2.9 M DME/toluene, respectively. * denotes **A**·LiHMDS mixed aggregate.

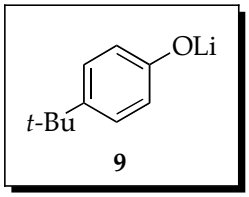


Plot of $[A_4]^{5/4}/[A_5]$ vs. [DME] for 0.10 M [^{6}Li]**7** (**A**) in toluene at -30 °C. The data are fit by non-linear least-squares methods to the following power function (K_{eq} = 0.40 ± 0.06, n = 2.7 ± 0.2):

$$[A_4]^{5/4}/[A_5] = K_{eq}*[DME]^{5-n}$$

The equation, assuming a tetrasolvated tetramer, was derived from the following equilibrium:

$$A_5DME_n + (5\text{-}n)\ DME \rightleftharpoons 5/4\ A_4DME_4$$



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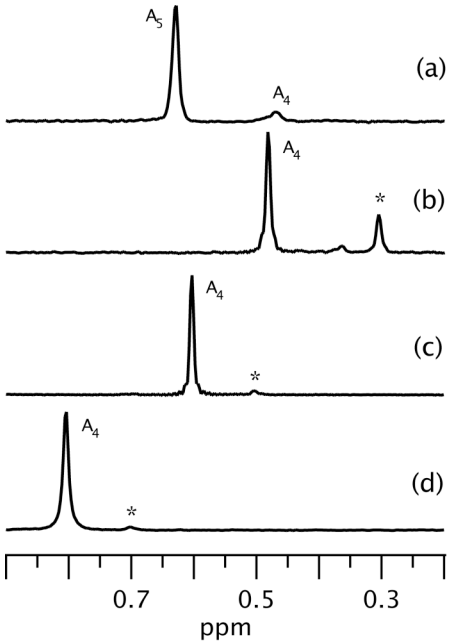
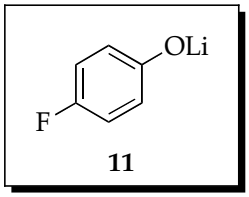


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**9** (**A**) at -90 °C (tube (a) at -30 °C, tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate.



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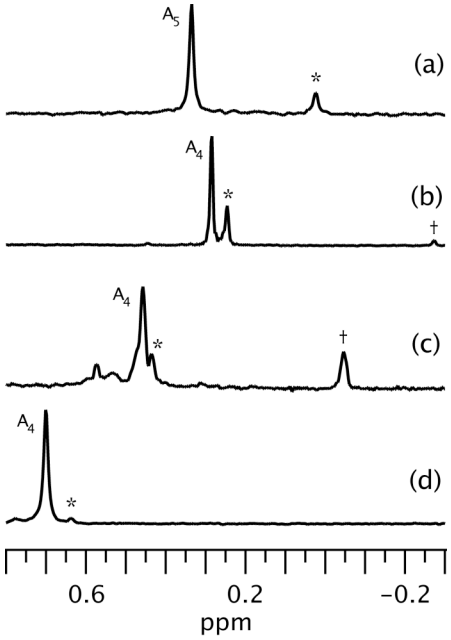
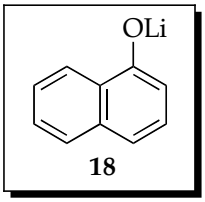


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**11** (**A**) at -90 °C (tube (a) at -30 °C, tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.22 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.



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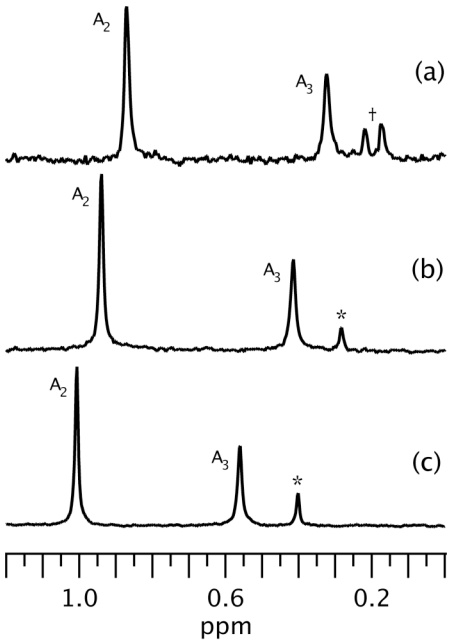
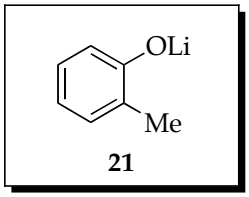


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**18** (**A**) at -90 °C. The solvent systems in tubes (a)-(c) are 0.23 M, 1.1 M and 2.9 M DME/toluene, respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes [^{6}Li,^{15}N]**A**·LiHMDS mixed aggregate.



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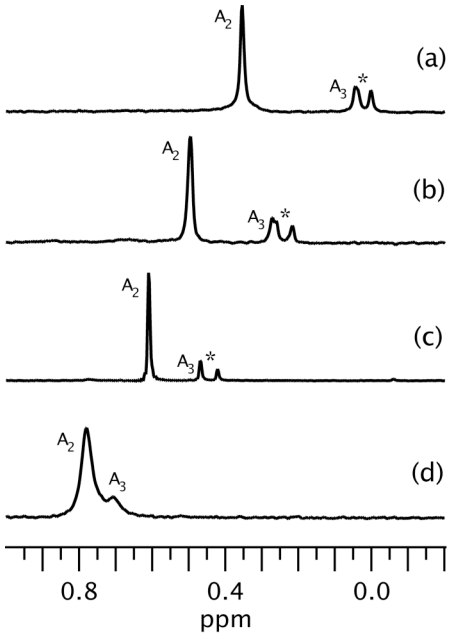
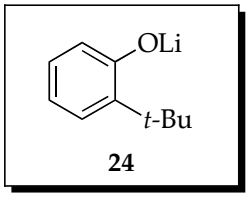
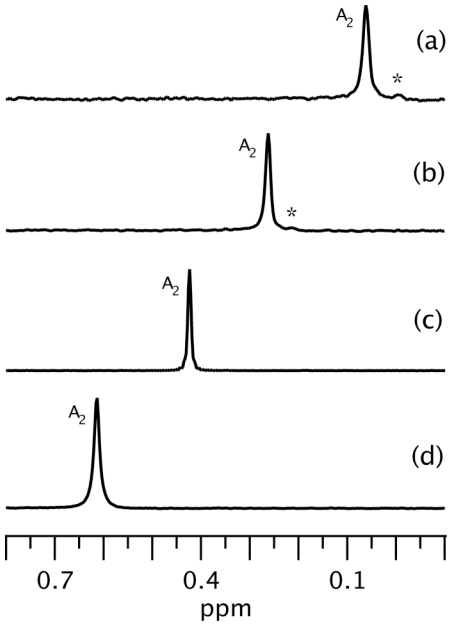


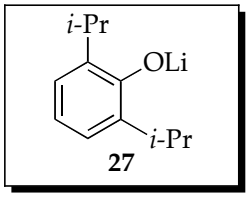
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**21** (**A**) at -90 °C (tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes [^{6}Li,^{15}N]**A**·LiHMDS mixed aggregate, half of which overlaps the $\mathbf{A}_3$ peak.



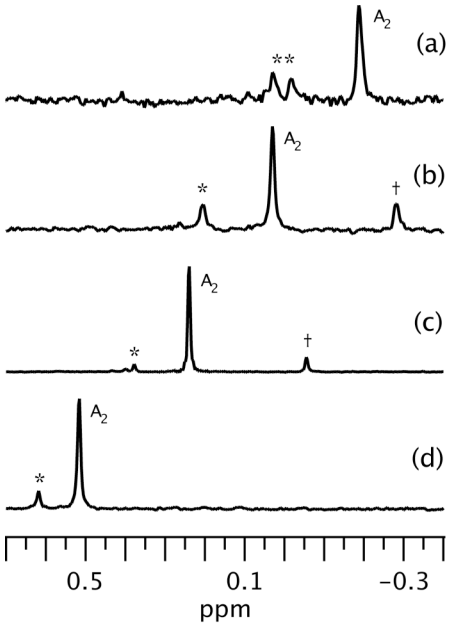
24



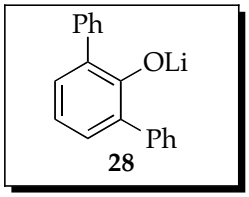
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**24** (**A**) at -90 °C (tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate.



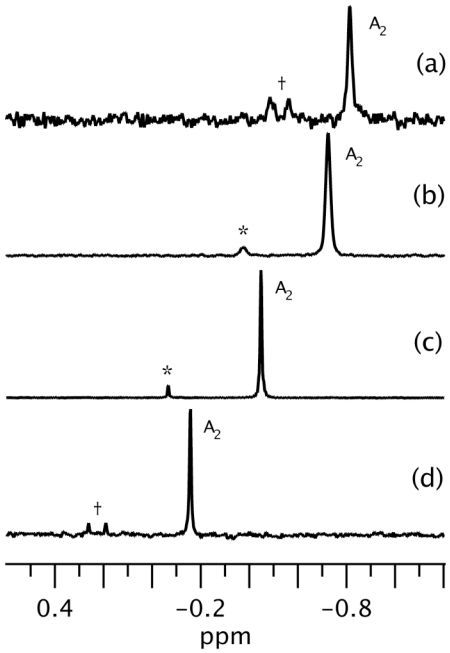
27



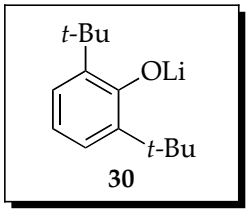
^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**27** (**A**) at -90 °C (tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate; ** denotes [^{6}Li,^{15}N]**A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.



28



^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**28** (**A**) at -90 °C (tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes excess LiHMDS; † denotes excess [^{6}Li,^{15}N]LiHMDS.



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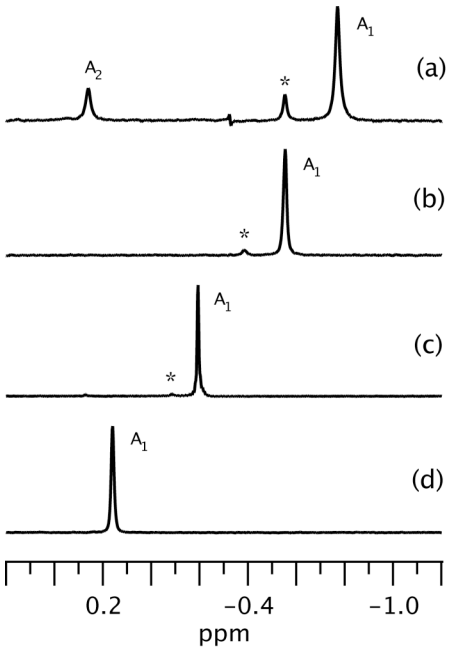
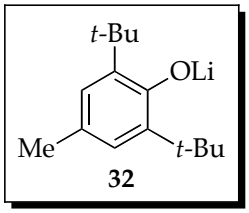


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**24** (**A**) at -90 °C (tube (d) at -70 °C). The solvent systems in tubes (a)-(c) are 0.21 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes excess LiHMDS.



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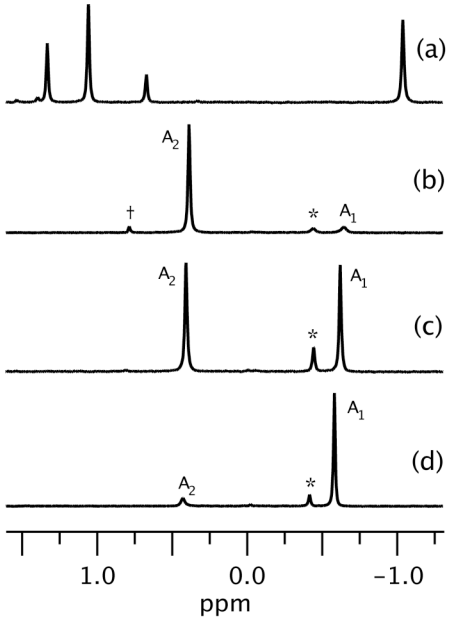
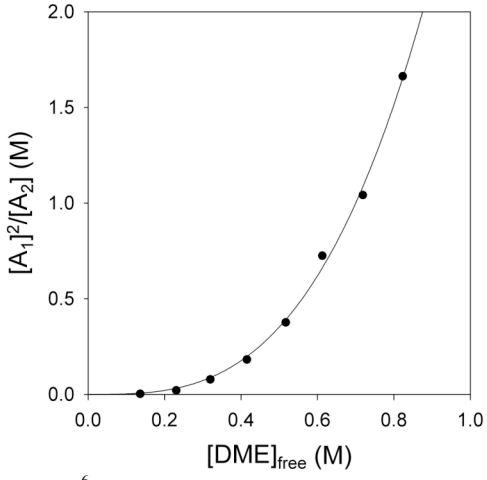


^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]**32** (**A**) at -70 °C. The solvent in tube (a) is toluene without added DME; the peaks have not been assigned. The solvent systems in tubes (b)-(d) are 0.22 M, 0.43 M and 0.87 M DME/toluene, respectively. * denotes excess LiHMDS monomer; † denotes LiHMDS dimer.



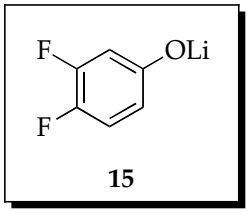
Plot of $[A_1]^2/[A_2]$ vs. [DME] for 0.10 M [^{6}Li]**32** (**A**) in toluene at -70 °C. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 3.0 \pm 0.2$, $n = 1.6 \pm 0.1$):

$$[A_1]^2/[A_2] = K_{eq}*[DME]^{2n}$$

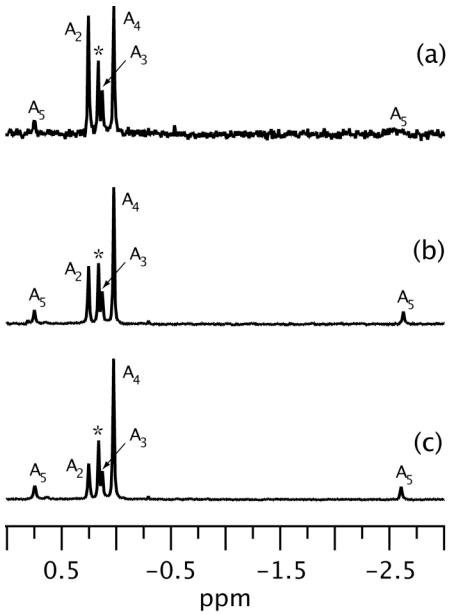
The equation, assuming a monosolvated dimer, was derived from the following equilibrium:

$$A_2DME_1 + 2n\ DME \rightleftharpoons 2\ A_1DME_{n+1/2}$$

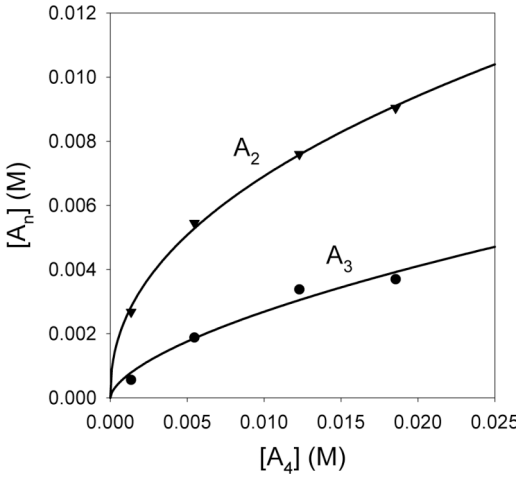
Phenolate concentration studies in DME



15



^{6}Li NMR spectra of solutions of [^{6}Li]**15** (**A**) at 2.9 M DME/toluene at -90 °C. The total lithium ion concentrations in tubes (a) – (c) are 0.018 N, 0.055 N and 0.109 N, respectively. * denotes excess LiHMDS.

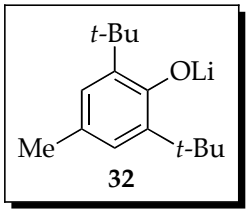


Plots of [A_2] vs. [A_4] and [A_3] vs. [A_4] for [^{6}Li]**15** (**A**) in 2.9 M DME/toluene at -90 °C. The data are fit by non-linear least-squares methods to the following power function (A_2: $K_{eq} = 19 \pm 2$, $n = 1.8 \pm 0.1$; A_3: $K_{eq} = 22 \pm 7$, $n = 2.5 \pm 0.5$):

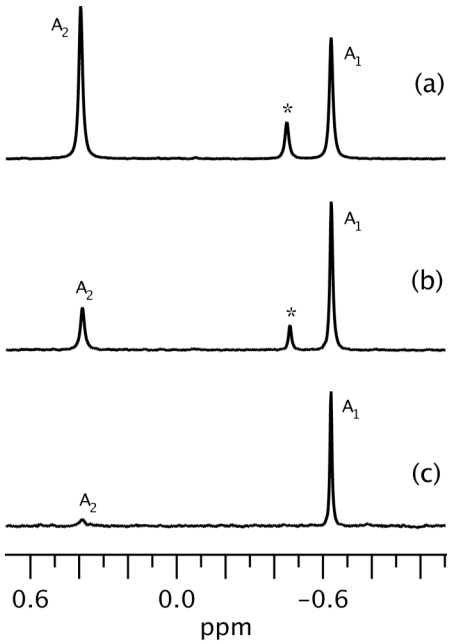
$$[A_n] = K_{eq}^{-1} * [A_4]^{n/4}$$

The equation was derived from the following equilibrium:

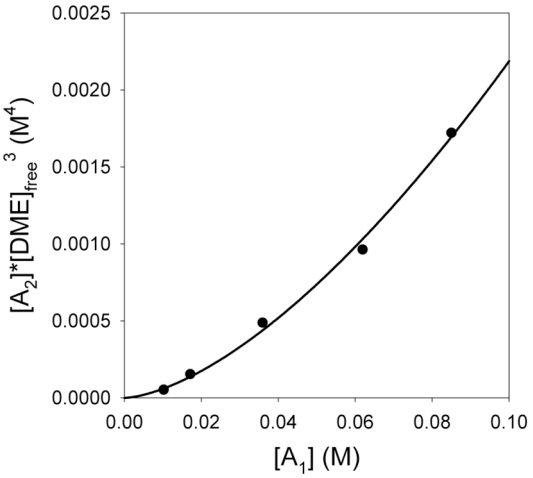
$$A_n \rightleftharpoons n/4\ A_4$$



32



^{6}Li NMR spectra of solutions of [^{6}Li]**32** (**A**) at c**A.** 0.4 M excess DME/toluene at -70 °C. The total lithium ion concentrations in tubes (a) – (c) are 0.229 N, 0.057 N and 0.011 N, respectively. * denotes excess LiHMDS.



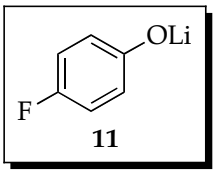
Plot of $[A_2]*[DME]_{free}^3$ vs. $[A_1]$ for [^{6}Li]**32** (**A**) in c**A.** 0.4 M excess DME/toluene at -70 °C. The data are fit by non-linear least-squares methods to the following power function ($K_{eq} = 12 \pm 3$, $n = 1.6 \pm 0.1$):

$$[A_2]*[DME]_{free}^3 = K_{eq}^{-1} * [A_1]^n$$

The equation was derived from the following equilibrium:

$$A_2DME_1 + 3\ DME \rightleftharpoons 2\ A_1DME_2$$

VI. ^{19}F NMR spectra.



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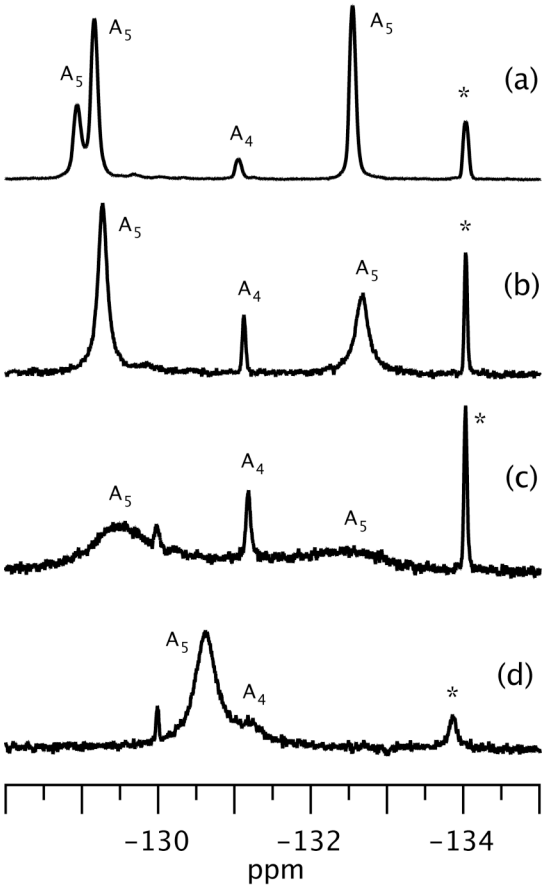
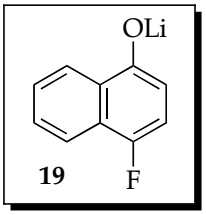
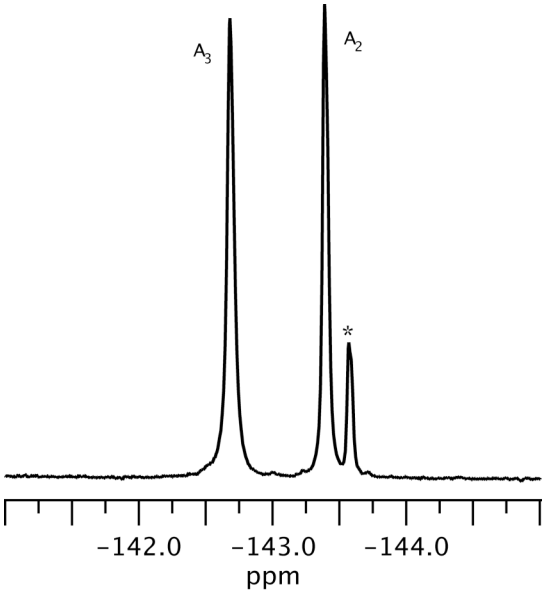
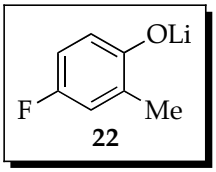


^{19}F NMR spectra of a 0.10 M solution of **11** (**A**) in 0.22 M DME/toluene at (a) -90 °C, (b) -40 °C, (c) -20 °C, and (d) 10 °C. * denotes A·LiHMDS mixed aggregate.

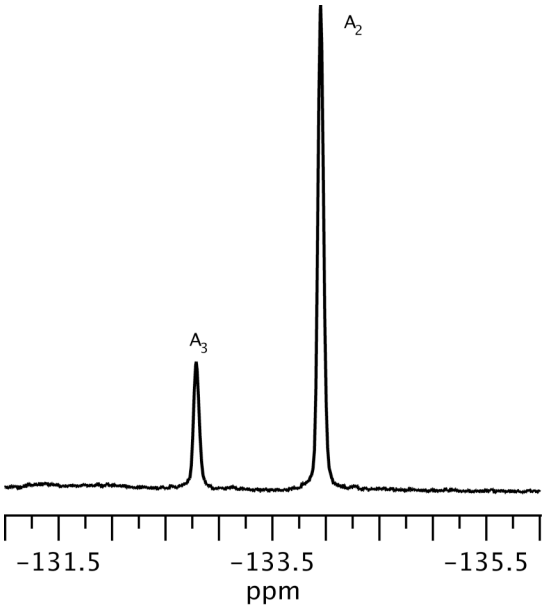




^{19}F NMR spectrum of a 0.10 M solution of **19** (**A**) in 2.9 M DME/toluene at -90 °C. * denotes A·LiHMDS mixed aggregate.



22



^{19}F NMR spectrum of a 0.10 M solution of **22** (**A**) in 2.9 M DME/toluene at -90 °C.

Effect of phenolate substitution on aggregate order equilibria
(All the energies are calculated on a per lithium basis at -90 °C)

Scheme 2

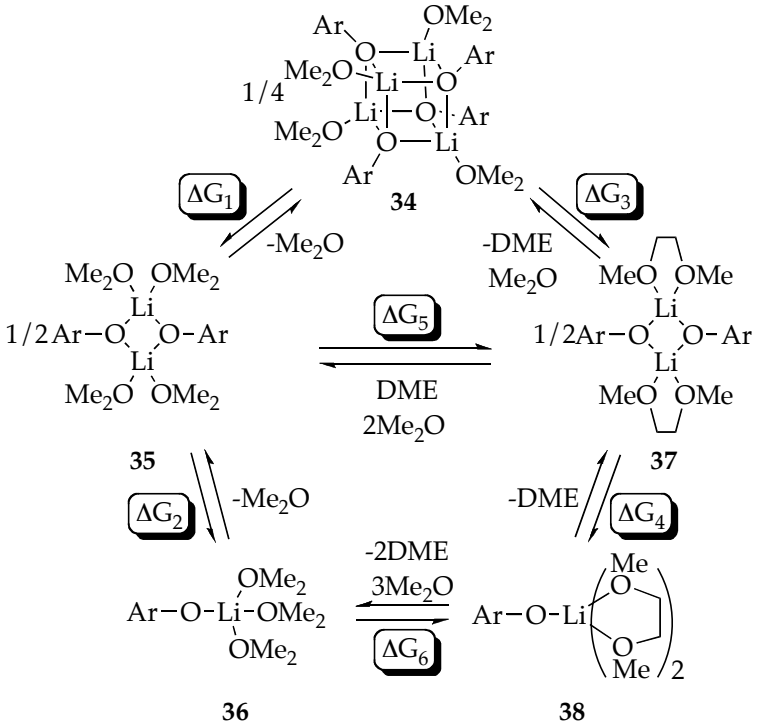
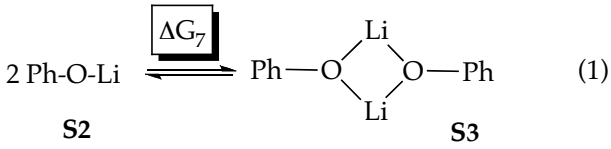


Table 3. Free energies ΔG_1-ΔG_6 reported in kcal/mol on a per lithium basis.

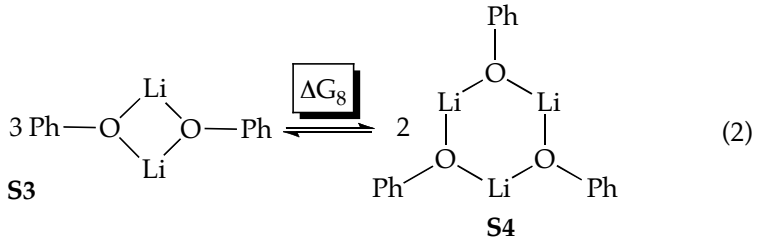
-Ar (#)	ΔG_1	ΔG_2	ΔG_3	ΔG_4	ΔG_5	ΔG_6
(**7**)	3.67	10.43	-0.11	10.05	-3.78	-4.16
(**11**)	3.79	9.86	-0.14	10.23	-3.92	-4.29
(**12**)	3.27	10.59	-0.03	8.98	-3.30	-4.91
(**13**)	3.80	9.25	-0.36	7.21	-3.47	-5.51
(**25**)	0.21	6.75	-6.22	10.06	-6.40	-3.12

Unsolvated aggregates: Phenolate as a model system



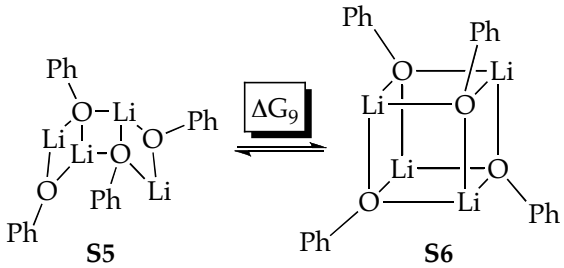
S2 **S3** (1)

ΔG_7 = -25.87 kcal/mol



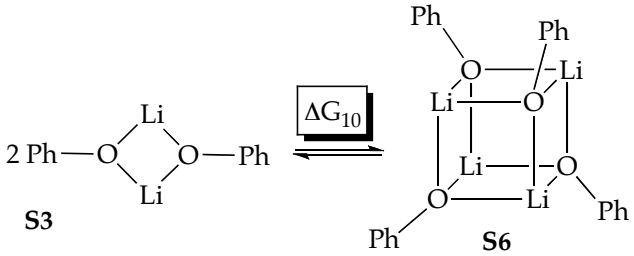
S3 **S4** (2)

ΔG_8 = -6.39 kcal/mol



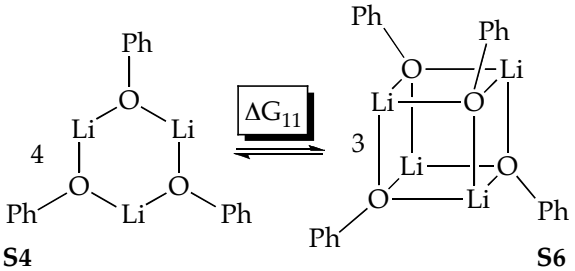
S5 **S6** (3)

ΔG_9 = -3.03 kcal/mol



S3 **S6** (4)

ΔG_{10} = -10.14 kcal/mol



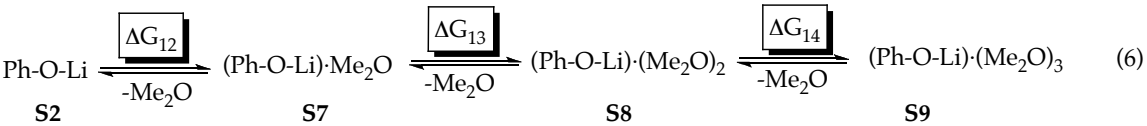
S4 **S6** (5)

ΔG_{11} = -3.75 kcal/mol

Serial solvation within same aggregates: Phenolate as a model system

Monomer solvation

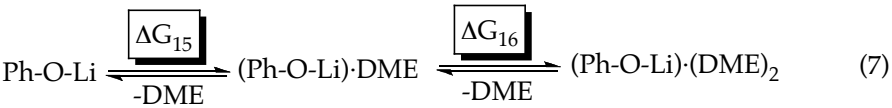
S=Me_2O



S2 **S7** **S8** **S9** (6)

ΔG_{12} = -17.53 kcal/mol ΔG_{13} = -9.86 kcal/mol ΔG_{14} = -3.16 kcal/mol

S=DME

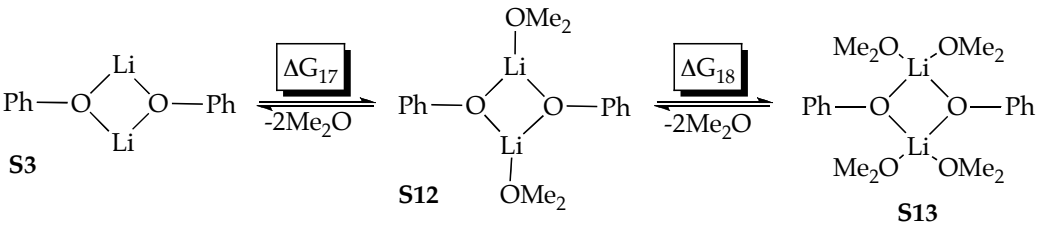


S2 **S10** **S11** (7)

ΔG_{15} = -26.35 kcal/mol ΔG_{16} = -8.36 kcal/mol

Dimer solvation

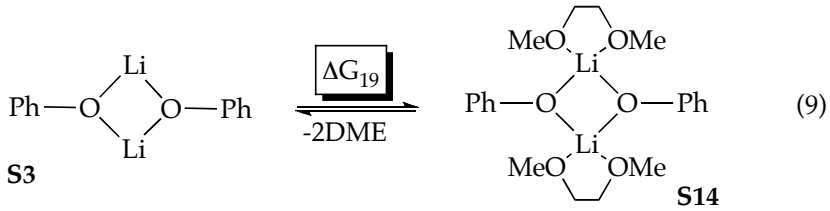
S=Me_2O



S3 **S12** **S13** (8)

ΔG_{17} = -13.37 kcal/mol ΔG_{18} = -1.64 kcal/mol

S=DME

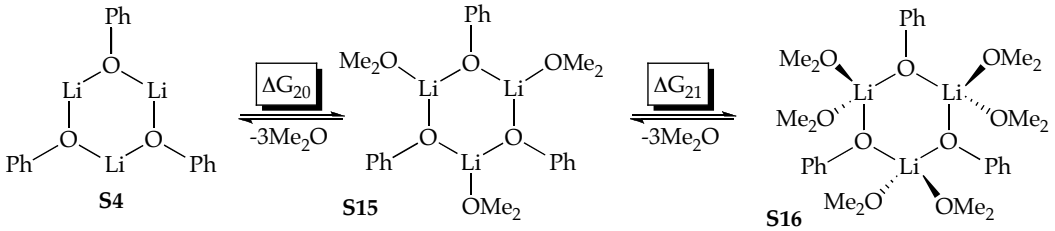


S3 **S14** (9)

ΔG_{19} = -18.79 kcal/mol

Trimer solvation

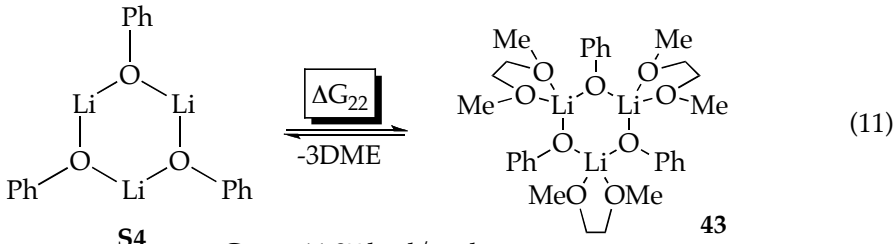
S=Me_2O



S4 **S15** **S16** (10)

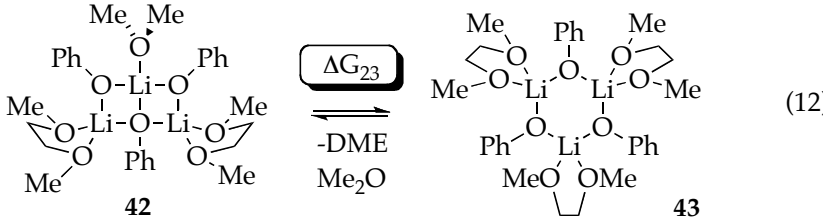
ΔG_{20} = -8.51 kcal/mol ΔG_{21} = 1.45 kcal/mol

S=DME



S4 **43** (11)

ΔG_{22} = -11.37 kcal/mol

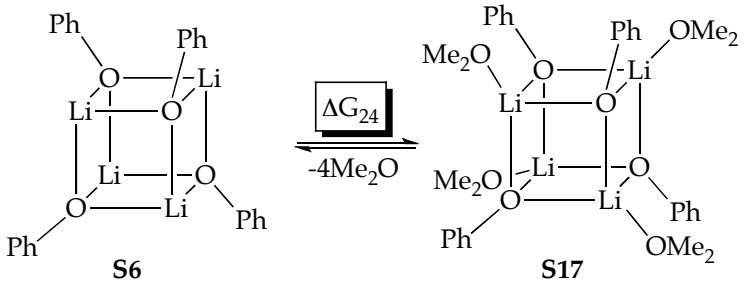


42 **43** (12)

ΔG_{23} = -0.64 kcal/mol

Tetramer solvation

S=Me_2O



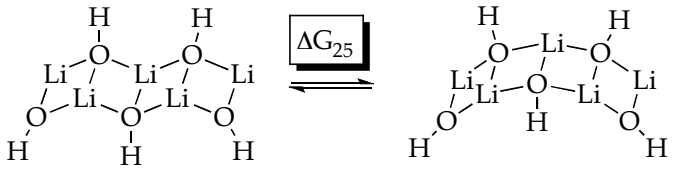
(13)

S6 **S17**

ΔG_{24} = -8.54 kcal/mol

Determination of pentamer ladder shape and solvation

LiOH pentamers as a model system

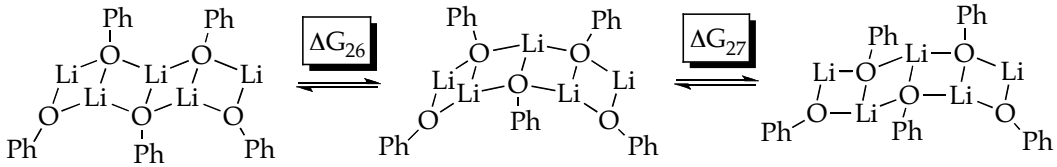


(14)

S18 **S19**

ΔG_{25} = 0.29 kcal/mol

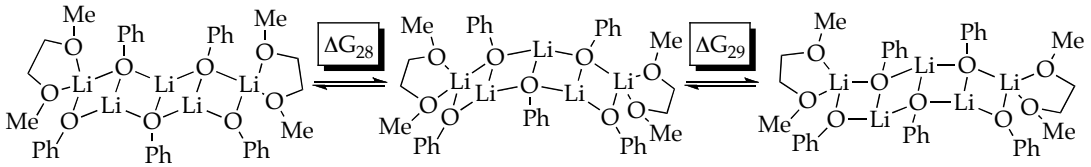
PhOLi pentamers



(15)

44 **45** **46**

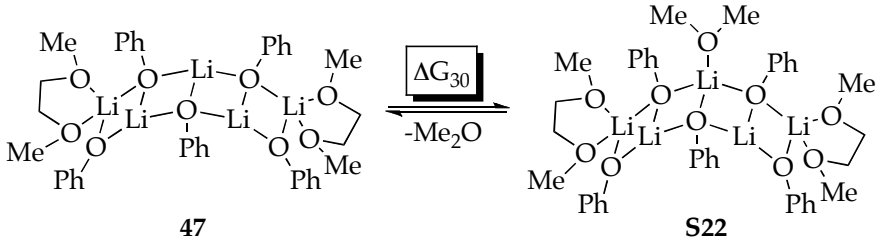
ΔG_{26} = -0.21 kcal/mol ΔG_{27} = -0.62 kcal/mol



(16)

S20 **47** **S21**

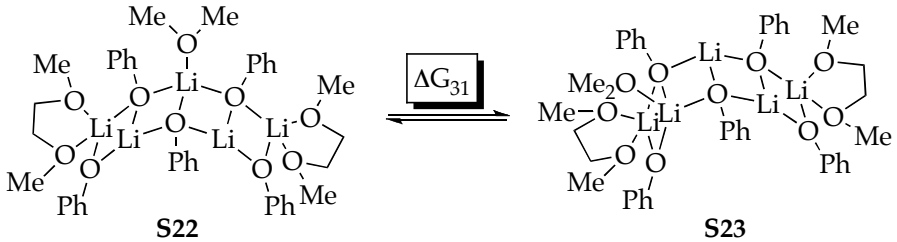
ΔG_{28} = -0.37 kcal/mol ΔG_{29} = 0.29 kcal/mol



(17)

47 **S22**

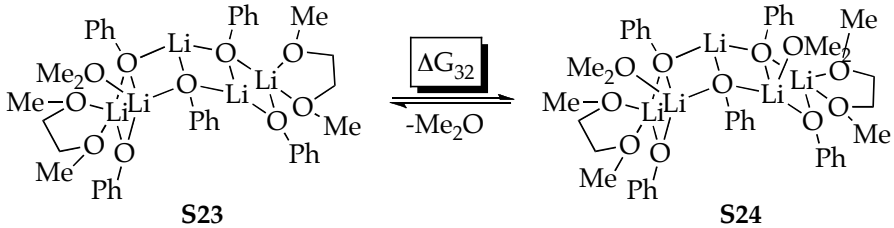
ΔG_{30} = -0.42 kcal/mol



(18)

S22 **S23**

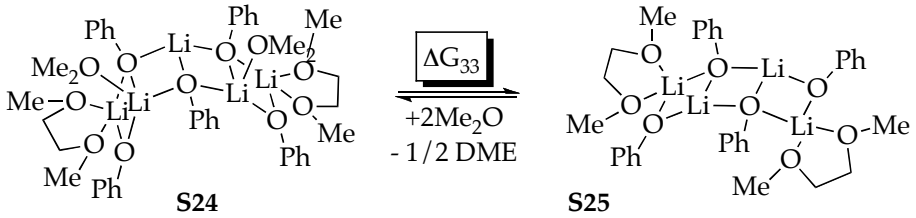
ΔG_{31} = -0.69 kcal/mol



(19)

S23 **S24**

ΔG_{32} = -0.16 kcal/mol

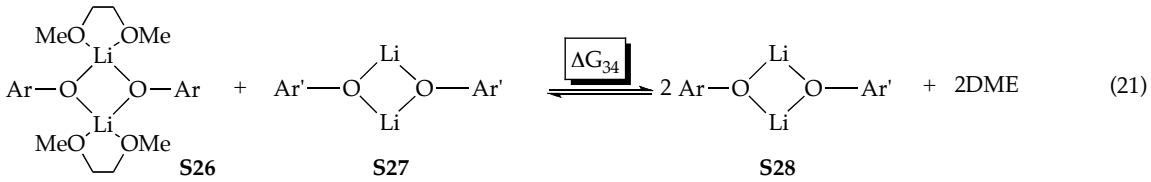


S24 **S25** (20)

ΔG_{33} = -0.34 kcal/mol

Others

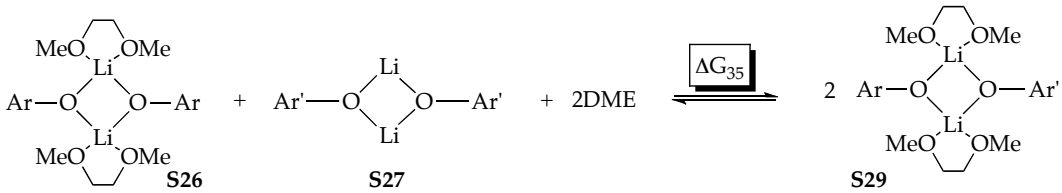
Heterodimer formation from 2,6-dimethylphenolate and 2,6-diphenylphenolate



S26 **S27** **S28** (21)

ΔG_{34} = 5.82 kcal/mol

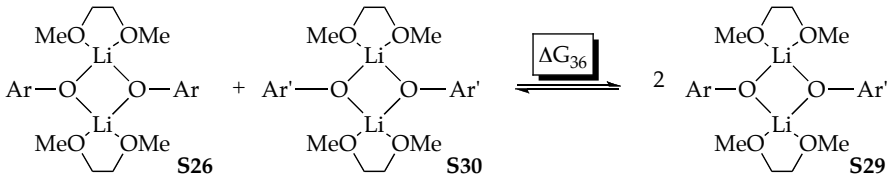
Ar'= 2,6-diphenylphenyl
Ar = 2,6-dimethylphenyl



S26 **S27** **S29** (22)

ΔG_{35} = -3.79 kcal/mol

Ar'= 2,6-diphenylphenyl
Ar = 2,6-dimethylphenyl



S26 **S30** **S29** (23)

ΔG_{36} = -0.07 kcal/mol

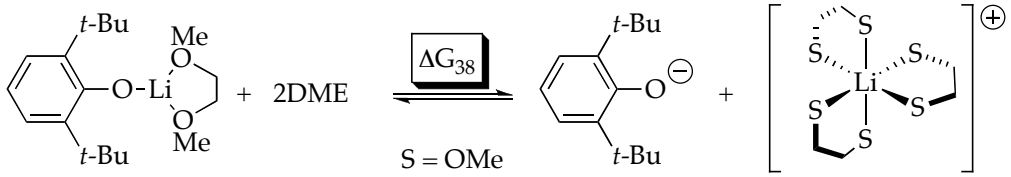
Ar'= 2,6-diphenylphenyl
Ar = 2,6-dimethylphenyl

S27 **S30** (24)

ΔG_{37} = -7.43 kcal/mol

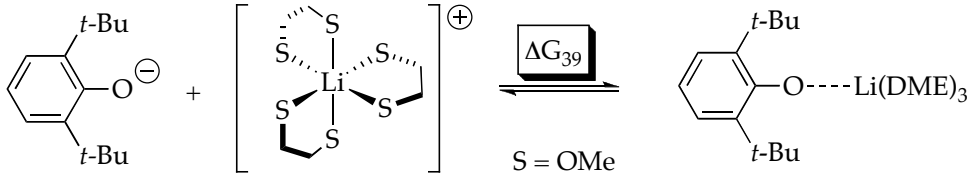
Ar'= 2,6-diphenylphenyl

2,6-di-*tert*-butylphenolate solvation



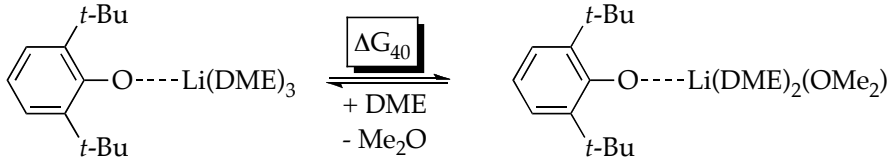
S31 **S32** **S33** (25)

ΔG_{38} = 71.79 kcal/mol



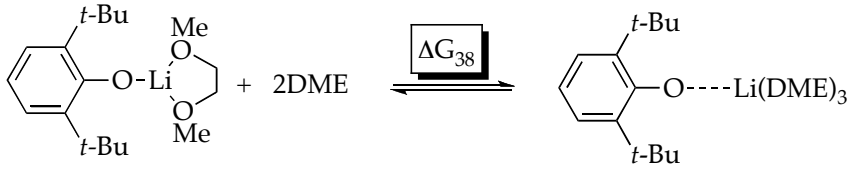
S32 **S33** **S34** (26)

ΔG_{39} = -53.85 kcal/mol



S34 **S35** (27)

ΔG_{40} = 0.45 kcal/mol



S31 **S34** (28)

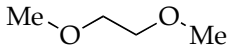
$\Delta G_{38} = 17.94$ kcal/mol

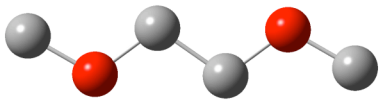
Table S1. Optimized geometry at B3LYP level of theory with 6-31G(d) basis set, free energy (G, Hartrees), and cartesian coordinates (X, Y, Z).

Me_2O
G = -154.958697
(-90 °C)

Atom	X	Y	Z
C	-1.170957	0.195262	0.000002
O	-0.000002	-0.589887	0.000011
C	1.170966	0.195268	-0.000001
H	1.232787	0.839156	0.893297
H	1.232018	0.840190	-0.892599
H	2.021804	-0.491398	-0.000758
H	-2.021793	-0.491404	-0.000504
H	-1.232665	0.839334	0.893177
H	-1.232188	0.840036	-0.892706

Table S1 (Continued).

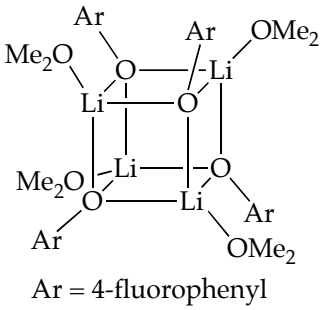




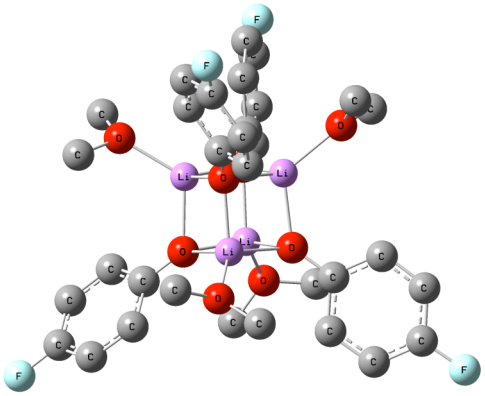
DME
G = -308.730705
(-90 °C)

Atom	X	Y	Z
C	0.646680	-0.400765	-0.000050
O	1.719768	0.518926	-0.000258
C	2.980824	-0.113586	0.000175
H	3.121588	-0.744290	-0.892664
H	3.120984	-0.744247	0.893139
H	3.737943	0.675089	0.000414
C	-0.646681	0.400794	0.000034
O	-1.719758	-0.518928	-0.000176
C	-2.980825	0.113566	0.000130
H	-3.737931	-0.675122	-0.000006
H	-3.121203	0.744001	0.893220
H	-3.121393	0.744489	-0.892585
H	-0.679907	1.052031	-0.888944
H	-0.680064	1.051766	0.889196
H	0.679807	-1.051938	-0.889082
H	0.680113	-1.051816	0.889054

Table S1 (Continued).



Ar = 4-fluorophenyl

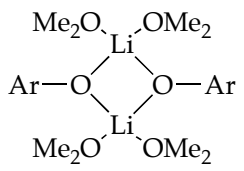


34 (Ar = 4-fluorophenyl)
G = -2274.530106
(-90 ºC)
see pg S95

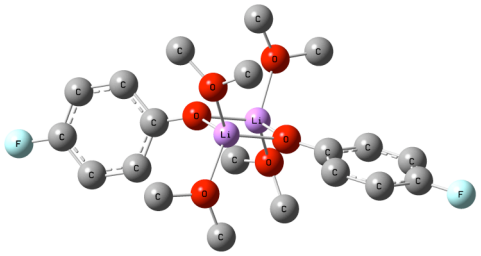
Atom	X	Y	Z	Atom	X	Y	Z
O	0.735744	0.150809	1.573617	H	5.157250	0.150038	-0.735138
Li	-0.017001	-1.448312	0.740469	C	3.849996	0.017080	-1.945639
O	-1.695349	-0.581158	0.196583	H	4.759334	1.552106	-1.776617
Li	-0.745702	-0.163833	-1.465126	H	3.887956	1.985545	0.698766
O	-0.024207	1.540155	-0.840074	H	4.692678	1.493015	1.258957
Li	-0.849327	1.053843	0.880420	C	4.271105	2.906038	0.237750
O	-1.796917	2.475885	1.877358	C	3.072861	2.224806	1.382987
C	-1.246558	3.792034	1.919375	C	-0.086855	2.720876	-1.452231
H	-1.459989	4.263700	2.887901	C	1.090128	3.423597	-1.797994
H	-0.166947	3.695068	1.792759	C	0.996948	4.653385	-2.432424
H	-1.651272	4.407918	1.107140	C	-0.215079	5.251637	-2.760649
C	-3.209780	2.463345	2.076127	H	-1.379983	4.556418	-2.424567
H	-3.535103	1.422875	2.026161	H	-1.329320	3.317515	-1.784561
H	-3.459625	2.880874	3.060853	H	-2.245264	2.790086	-1.528694
H	-3.717343	3.047192	1.296464	O	-2.346781	4.990880	-2.668129
Li	1.498159	0.474023	-0.207360	C	-0.233568	6.214964	-3.257430
O	0.846870	-1.204713	-0.996767	H	2.147226	5.299751	-2.746138
C	1.614960	-2.001632	-1.737338	H	2.061367	2.998906	-1.566874
C	2.162888	-3.189951	-1.201027	H	-1.571199	-0.448846	-3.240446
C	2.956013	-4.002237	-1.998333	C	-1.417477	0.467617	-4.322966
C	3.258522	-3.708716	-3.323933	H	-0.554558	0.194142	-4.945538
C	2.725881	-2.530169	-3.852921	H	-2.322157	0.476781	-4.945658
C	1.921701	-1.687243	-3.085250	H	-1.262383	1.457089	-3.889555
H	1.516442	-0.772134	-3.510415	C	-1.794704	-1.788371	-3.678772
H	2.944229	-2.264714	-4.884759	C	-1.962875	-2.394304	-2.786582
H	3.884163	-4.377859	-3.903772	C	-2.684255	-1.836052	-4.320844
O	3.459032	-5.137382	-1.454012	C	-0.921824	-2.169839	-4.223165
C	1.964006	-3.465274	-0.170206	C	-2.942473	-0.980349	0.438134
H	3.361561	1.111041	-0.297515	C	-3.915794	-0.990536	-0.587601
H	4.344057	0.687785	-1.240599	H	-5.205791	-1.416412	-0.307075

Atom	X	Y	Z
H	-5.612124	-1.838804	0.954341
H	-4.654677	-1.818908	1.972062
O	-3.346129	-1.399496	1.730835
C	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
H	-6.112054	-1.418770	-1.315682
C	-3.655156	-0.659195	-1.587531
H	-0.087743	-3.230405	1.587431
H	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
C	-0.739019	-4.053244	-0.156392
C	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
C	0.388471	-4.380480	3.253585
C	0.544499	-2.607314	3.419761
C	-1.079476	-3.368106	3.417819
H	1.352599	0.184225	2.754704
H	0.861372	0.987474	3.808956
H	1.526453	1.004317	5.026471
F	2.673442	0.259171	5.278606
F	3.156961	-0.539318	4.238279
F	2.517961	-0.584212	2.999185
F	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
H	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table S1 (Continued).



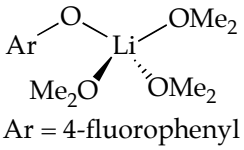
Ar = 4-fluorophenyl



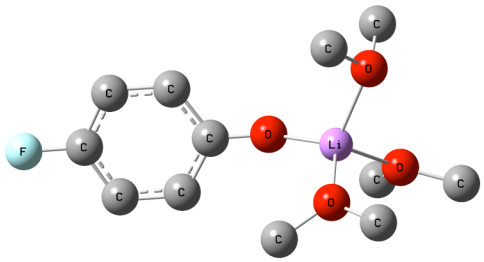
35 (Ar = 4-fluorophenyl)
G = -1447.170703
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
C	0.712005	2.348694	-2.488717	H	-2.058337	-3.016962	-1.788696
O	0.052675	2.673072	-1.268433	H	-1.393482	-3.806125	-0.327580
Li	0.080046	1.282401	0.199056	H	-0.911815	-4.389085	-1.947608
O	1.421497	-0.029965	0.050047	C	2.725180	-0.084700	-0.154282
Li	0.006549	-1.249657	0.220751	C	3.538030	1.077545	-0.107292
O	-1.353603	0.055344	0.364053	C	4.912328	1.014122	-0.329757
C	-2.626378	0.067943	0.003651	C	5.541185	-0.202736	-0.608522
C	-3.667535	0.202271	0.957272	C	4.759828	-1.360451	-0.661316
C	-5.007994	0.209199	0.573851	C	3.384528	-1.308647	-0.441680
C	-5.372992	0.084694	-0.769537	H	2.786054	-2.216461	-0.494713
C	-4.363633	-0.046098	-1.727643	H	5.227381	-2.319297	-0.878787
C	-3.019803	-0.054988	-1.355091	H	5.501093	1.928702	-0.282643
H	-2.238138	-0.154703	-2.105933	H	3.061761	2.030462	0.115601
H	-4.625560	-0.141738	-2.780087	C	-1.196404	3.330441	-1.472101
H	-6.418970	0.091086	-1.063174	H	-1.598612	3.560241	-0.483706
H	-3.393900	0.307998	2.005004	H	-1.052142	4.261788	-2.037571
O	-0.072037	-2.505366	1.810642	H	-1.900699	2.679027	-2.005217
C	1.121202	-2.981043	2.422053	H	0.926785	3.261255	-3.062503
H	0.987253	-4.008607	2.789198	H	1.646053	1.850213	-2.224534
H	1.905711	-2.958445	1.664219	H	0.093768	1.677842	-3.101827
H	1.414120	-2.334713	3.261281	O	0.066508	2.559243	1.772124
C	-1.161479	-2.412678	2.720594	C	-0.312044	1.952116	3.002671
H	-2.001669	-1.983043	2.173955	H	-1.000288	1.146099	2.744934
H	-1.429130	-3.406676	3.106869	H	-0.809377	2.681847	3.657407
H	-0.908223	-1.758090	3.566967	H	0.566005	1.541427	3.521714
O	-0.077860	-2.598371	-1.289081	C	1.022167	3.597698	1.935839
C	0.354783	-2.162190	-2.573127	H	1.234758	3.992728	0.940736
H	-0.461989	-1.663872	-3.114447	H	0.619767	4.399727	2.571109
H	0.711332	-3.014334	-3.168872	H	1.948883	3.213478	2.384846
H	1.172849	-1.459897	-2.408000	F	6.902589	-0.259595	-0.827029
C	-1.175158	-3.502813	-1.353063	F	-5.984603	0.343907	1.539504

Table S1 (Continued).



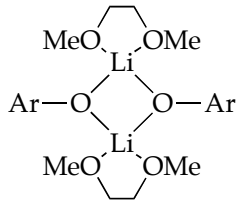
Ar = 4-fluorophenyl



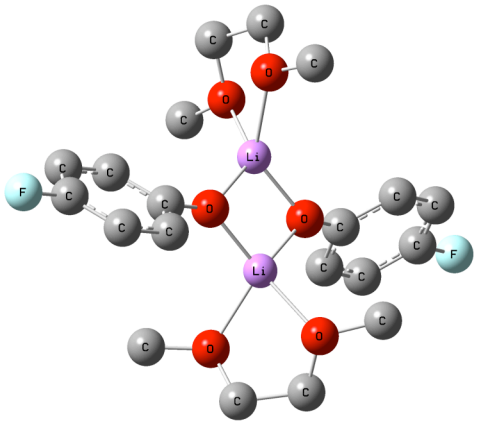
36 (Ar = 4-fluorophenyl)
G = -878.527894
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.407914	0.042926	-0.016230	O	2.302122	1.863833	0.116697
O	-0.249428	0.079559	-0.608913	C	2.267815	2.484653	-1.169042
O	2.533308	-0.935191	-1.381516	H	2.773431	3.459627	-1.137977
C	1.762198	-1.561106	-2.410325	H	2.793730	1.818771	-1.855218
H	1.811664	-2.655079	-2.315380	H	1.231661	2.610806	-1.507309
H	0.738442	-1.212769	-2.263741	C	1.638998	2.652073	1.104793
H	2.138585	-1.268780	-3.400711	H	0.583969	2.798289	0.839885
C	3.898778	-1.311292	-1.397052	H	1.702105	2.101582	2.044966
H	4.014701	-2.392298	-1.231167	H	2.132672	3.627681	1.213011
H	4.369254	-1.049548	-2.355972	C	-1.550318	0.035861	-0.440959
H	4.397890	-0.765474	-0.592624	C	-2.252288	-1.197599	-0.348051
O	1.641266	-0.701826	1.839799	C	-3.634212	-1.250215	-0.165355
C	2.841078	-0.936062	2.558412	C	-4.354370	-0.066095	-0.074789
H	2.741629	-0.614293	3.605028	C	-3.719819	1.167357	-0.166199
H	3.112716	-2.001528	2.540812	C	-2.338926	1.215124	-0.348186
H	3.627901	-0.350763	2.076575	H	-1.835501	2.175666	-0.434209
C	0.515027	-1.386797	2.390399	H	-4.311045	2.076612	-0.097031
H	0.322850	-1.042769	3.416046	F	-5.705248	-0.113668	0.105843
H	-0.338340	-1.157601	1.751708	H	-4.158242	-2.199876	-0.096926
H	0.691540	-2.471563	2.402319	H	-1.680022	-2.118875	-0.436393

Table S1 (Continued).



Ar = 4-fluorophenyl

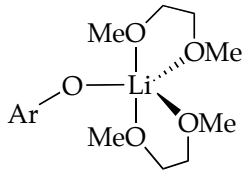


37 (Ar = 4-fluorophenyl)
G = -1444.809759
(-90 ºC)
see pg S95

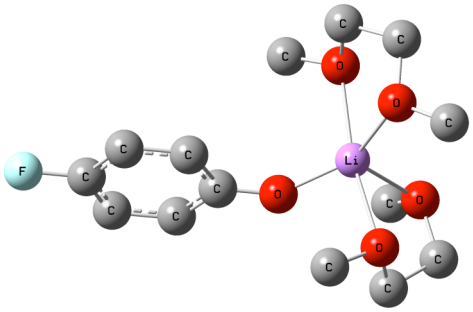
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.006243	-1.242034	0.194769	H	-2.890605	1.342308	-1.580848
O	-0.262288	-2.783350	-1.143046	Li	-0.047593	1.281600	0.159552
C	-0.129667	-4.032806	-0.476716	O	1.347151	0.055556	0.281737
C	0.958394	-3.876735	0.565856	C	2.653889	0.063483	0.074390
O	0.559213	-2.824066	1.437518	C	3.231027	-0.577159	-1.052134
C	1.527798	-2.529811	2.444334	C	4.609246	-0.577073	-1.270129
H	1.691905	-3.407399	3.084648	C	5.441203	0.065586	-0.361813
H	2.475831	-2.211072	1.994986	C	4.924282	0.706302	0.757724
H	1.121019	-1.712136	3.040748	C	3.545909	0.702397	0.972122
H	1.081136	-4.817086	1.124034	H	3.128871	1.193607	1.848233
H	1.916455	-3.623484	0.087685	H	5.601239	1.198997	1.450035
H	-1.081155	-4.303172	0.005572	F	6.786120	0.067497	-0.571768
H	0.139627	-4.827141	-1.189106	H	5.043215	-1.067569	-2.137039
C	-1.369904	-2.730126	-2.040891	H	2.567029	-1.069735	-1.759373
H	-2.310890	-2.922542	-1.510224	O	0.427216	2.817139	-1.127871
H	-1.243334	-3.460461	-2.851697	C	-0.286189	3.988018	-0.754605
H	-1.394061	-1.719623	-2.449207	C	-0.175008	4.111929	0.753115
O	-1.386718	-0.017096	0.095462	O	-0.637810	2.888982	1.309303
C	-2.707322	-0.069493	0.039121	C	-0.636040	2.860444	2.731002
C	-3.442153	0.698609	-0.898713	H	-1.298141	3.637954	3.135663
C	-4.833711	0.636182	-0.970658	H	-1.009969	1.877803	3.022934
C	-5.522171	-0.201612	-0.102014	H	0.378739	3.004807	3.127919
C	-4.848128	-0.974539	0.835511	H	-0.786997	4.955372	1.106268
C	-3.456459	-0.906630	0.904173	H	0.870984	4.288337	1.046632
H	-2.918577	-1.496391	1.643382	H	-1.340758	3.901200	-1.057672
H	-5.414625	-1.617105	1.503745	H	0.146567	4.877840	-1.235666
F	-6.880171	-0.266530	-0.171263	C	0.501494	2.598224	-2.531819
H	-5.388604	1.226842	-1.694250	H	-0.500551	2.474648	-2.966333

Atom	X	Y	Z
H	1.081158	1.684394	-2.671067
H	1.011951	3.434960	-3.027632

Table S1 (Continued).



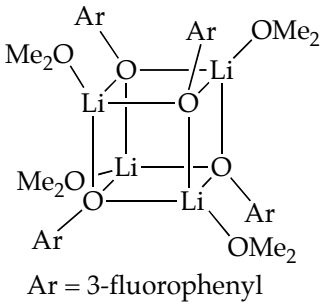
Ar = 4-fluorophenyl



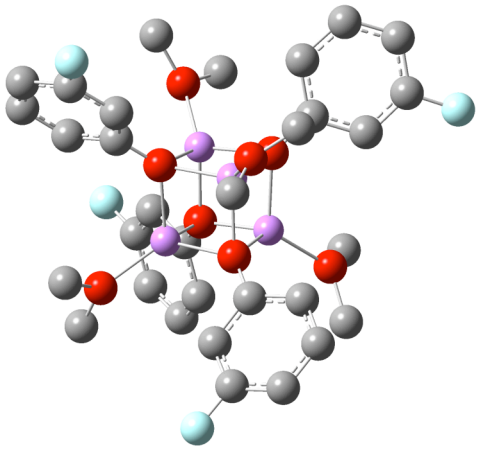
38 (Ar = 4-fluorophenyl)
G = -1031.12015
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.198501	0.067794	0.084324	H	-1.209352	3.997120	0.635242
O	0.455603	-0.624172	0.319410	H	-0.308935	3.010566	-0.548526
C	1.734756	-0.431380	0.112938	C	0.291949	2.165627	1.852071
C	2.219249	0.428490	-0.914044	H	0.386488	1.321312	2.534043
C	3.582796	0.633137	-1.129084	H	0.274701	3.107162	2.419558
C	4.504565	-0.018723	-0.320497	H	1.144035	2.156226	1.163043
C	4.088302	-0.870821	0.696547	O	-2.483202	-0.985956	1.408452
C	2.726207	-1.072183	0.908242	C	-2.878444	-2.209535	0.780161
H	2.391228	-1.739056	1.699588	C	-1.866414	-2.678970	-0.250782
H	4.833580	-1.367372	1.312340	O	-1.822085	-1.688474	-1.273523
F	5.838314	0.179306	-0.526793	C	-0.817722	-1.960586	-2.250832
H	3.936693	1.290548	-1.918997	H	0.174007	-1.945848	-1.788561
H	1.490412	0.928533	-1.550077	H	-1.003803	-2.930143	-2.735336
O	-0.937575	1.994899	1.144292	H	-0.883118	-1.167830	-2.999909
C	-1.144848	3.001510	0.167939	H	-0.869000	-2.785690	0.194723
C	-2.443275	2.690607	-0.543981	H	-2.184054	-3.648527	-0.668839
O	-2.332832	1.389281	-1.109546	H	-3.041543	-2.989055	1.536933
C	-3.504012	0.992597	-1.815895	H	-3.833816	-2.004628	0.285425
H	-3.341317	-0.035420	-2.137581	C	-1.721512	-1.165612	2.608943
H	-4.387219	1.037549	-1.162515	H	-0.725050	-1.560459	2.385897
H	-3.669365	1.643080	-2.686142	H	-2.259539	-1.824094	3.304157
H	-3.284311	2.717252	0.165306	H	-1.621889	-0.175062	3.056879
H	-2.627003	3.437142	-1.331547				

Table S1 (Continued).



Ar = 3-fluorophenyl

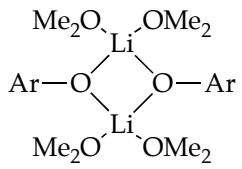


34 (Ar = 3-fluorophenyl)
G = -2274.544259
(-90 ºC)
see pg S95

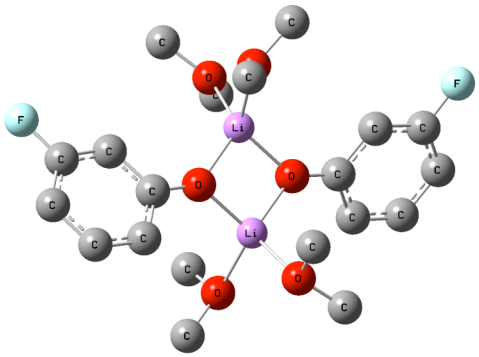
Atom	X	Y	Z
O	0.735744	0.150809	1.573617
Li	-0.017001	-1.448312	0.740469
O	-1.695349	-0.581158	0.196583
Li	-0.745702	-0.163833	-1.465126
O	-0.024207	1.540155	-0.840074
Li	-0.849327	1.053843	0.880420
O	-1.796917	2.475885	1.877358
C	-1.246558	3.792034	1.919375
H	-1.459989	4.263700	2.887901
H	-0.166947	3.695068	1.792759
H	-1.651272	4.407918	1.107140
C	-3.209780	2.463345	2.076127
H	-3.535103	1.422875	2.026161
H	-3.459625	2.880874	3.060853
H	-3.717343	3.047192	1.296464
Li	1.498159	0.474023	-0.207360
O	0.846870	-1.204713	-0.996767
C	1.614960	-2.001632	-1.737338
C	2.162888	-3.189951	-1.201027
C	2.956013	-4.002237	-1.998333
C	3.258522	-3.708716	-3.323933
C	2.725881	-2.530169	-3.852921
C	1.921701	-1.687243	-3.085250
H	1.516442	-0.772134	-3.510415
H	2.944229	-2.264714	-4.884759
H	3.884163	-4.377859	-3.903772
F	3.459032	-5.137382	-1.454012
H	1.964006	-3.465274	-0.170206
O	3.361561	1.111041	-0.297515
C	4.344057	0.687785	-1.240599
H	5.157250	0.150038	-0.735138
H	3.849996	0.017080	-1.945639
H	4.759334	1.552106	-1.776617
C	3.887956	1.985545	0.698766
H	4.692678	1.493015	1.258957
H	4.271105	2.906038	0.237750
H	3.072861	2.224806	1.382987
C	-0.086855	2.720876	-1.452231
C	1.090128	3.423597	-1.797994
C	0.996948	4.653385	-2.432424
C	-0.215079	5.251637	-2.760649
C	-1.379983	4.556418	-2.424567
C	-1.329320	3.317515	-1.784561
H	-2.245264	2.790086	-1.528694
H	-2.346781	4.990880	-2.668129
H	-0.233568	6.214964	-3.257430
F	2.147226	5.299751	-2.746138
H	2.061367	2.998906	-1.566874
O	-1.571199	-0.448846	-3.240446
C	-1.417477	0.467617	-4.322966
H	-0.554558	0.194142	-4.945538
H	-2.322157	0.476781	-4.945658
H	-1.262383	1.457089	-3.889555
C	-1.794704	-1.788371	-3.678772
H	-1.962875	-2.394304	-2.786582
H	-2.684255	-1.836052	-4.320844

Atom	X	Y	Z
H	-0.921824	-2.169839	-4.223165
C	-2.942473	-0.980349	0.438134
C	-3.915794	-0.990536	-0.587601
C	-5.205791	-1.416412	-0.307075
C	-5.612124	-1.838804	0.954341
C	-4.654677	-1.818908	1.972062
C	-3.346129	-1.399496	1.730835
H	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
F	-6.112054	-1.418770	-1.315682
H	-3.655156	-0.659195	-1.587531
O	-0.087743	-3.230405	1.587431
C	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
H	-0.739019	-4.053244	-0.156392
H	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
H	0.388471	-4.380480	3.253585
H	0.544499	-2.607314	3.419761
H	-1.079476	-3.368106	3.417819
C	1.352599	0.184225	2.754704
C	0.861372	0.987474	3.808956
C	1.526453	1.004317	5.026471
C	2.673442	0.259171	5.278606
C	3.156961	-0.539318	4.238279
C	2.517961	-0.584212	2.999185
H	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
F	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table S1 (Continued).



Ar = 3-fluorophenyl

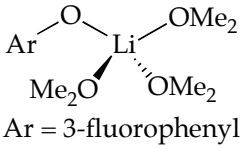


35 (Ar = 3-fluorophenyl)
G = -1447.179435
(-90 ºC)
see pg S95

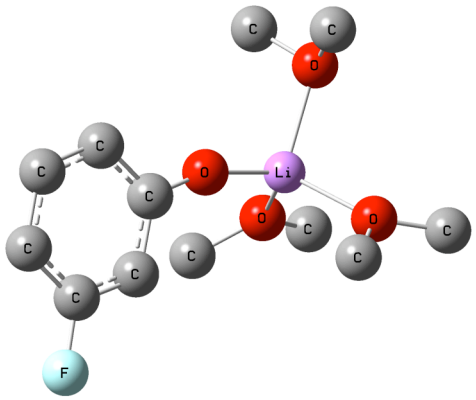
Atom	X	Y	Z	Atom	X	Y	Z
C	1.458824	3.479209	-1.593307	H	-1.317371	-3.659031	0.943165
O	0.275448	2.683630	-1.585101	C	0.983440	-2.076774	2.680157
Li	0.018402	1.432308	-0.015548	H	1.512603	-2.945249	3.096248
O	1.378282	0.139699	0.128705	H	1.702993	-1.336906	2.329574
Li	-0.007119	-1.140366	0.018519	H	0.346662	-1.637732	3.461692
O	-1.369584	0.164424	-0.137338	C	2.694339	0.188485	0.199758
C	-2.685451	0.225129	-0.184624	C	3.505283	-0.802802	-0.409044
C	-3.363993	1.359074	-0.708871	C	4.886199	-0.728823	-0.309270
C	-4.754724	1.410387	-0.758984	C	5.549033	0.288046	0.369170
C	-5.543171	0.350814	-0.299028	C	4.755553	1.269960	0.970856
C	-4.873838	-0.756345	0.210536	C	3.365588	1.230634	0.895105
C	-3.491920	-0.845797	0.278417	H	2.764850	2.000893	1.372907
H	-3.030350	-1.734966	0.695851	H	5.236804	2.081209	1.512874
F	-5.606304	-1.805211	0.667494	H	6.632100	0.299797	0.418405
H	-6.626735	0.371065	-0.330508	F	5.624598	-1.699406	-0.908037
H	-5.240694	2.293320	-1.168611	H	3.047968	-1.617542	-0.961267
H	-2.769176	2.191134	-1.078144	O	-0.222471	2.740206	1.515323
O	-0.239844	-2.538759	-1.440260	C	-1.255588	3.715881	1.401007
C	0.775119	-3.489968	-1.734282	H	-1.154856	4.476748	2.187488
H	1.463518	-3.108196	-2.501513	H	-2.246055	3.247033	1.466041
H	0.333879	-4.432799	-2.087380	H	-1.141793	4.185120	0.421909
H	1.323745	-3.667904	-0.807686	C	-0.255950	2.056757	2.765832
C	-1.045568	-2.220671	-2.571334	H	-0.104396	2.762739	3.594213
H	-0.433532	-1.787871	-3.375609	H	-1.213265	1.535253	2.898902
H	-1.786391	-1.494049	-2.237766	H	0.557498	1.329697	2.747408
H	-1.549670	-3.120696	-2.949802	C	0.064862	2.006984	-2.822387
O	0.203644	-2.461201	1.551629	H	0.920812	1.361825	-3.062986
C	-0.792796	-3.423563	1.870880	H	-0.086335	2.730503	-3.635526
H	-0.335482	-4.337537	2.275692	H	-0.830192	1.395632	-2.697504
H	-1.506113	-3.024243	2.605583	H	2.349751	2.856143	-1.743525

Atom	X	Y	Z
H	1.403661	4.241711	-2.382722
H	1.521829	3.966928	-0.618629

Table S1 (Continued).



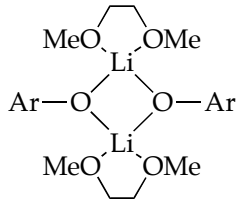
Ar = 3-fluorophenyl



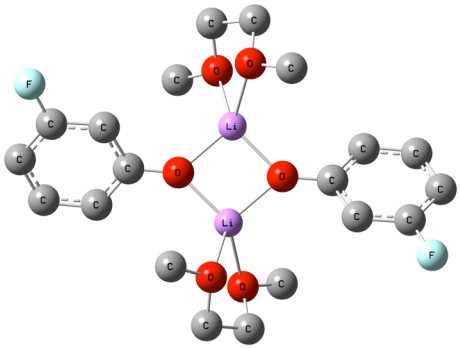
36 (Ar = 3-fluorophenyl)
G = -878.531702
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.378461	0.048354	0.000246	C	2.337501	2.415802	-1.180218
O	1.857924	-0.968527	-1.669990	H	2.973556	3.311018	-1.212283
C	0.747467	-1.326298	-2.495390	H	2.572237	1.768830	-2.027394
H	0.595219	-2.414478	-2.486363	H	1.279688	2.703153	-1.222708
H	-0.122490	-0.822346	-2.074063	C	2.328488	2.417987	1.183919
H	0.917641	-0.995186	-3.529305	H	1.270285	2.705057	1.217996
C	3.074961	-1.567570	-2.081782	H	2.557170	1.772771	2.034087
H	3.014166	-2.664308	-2.031321	H	2.963958	3.313503	1.218950
H	3.329379	-1.274928	-3.110710	O	-0.300665	0.582950	-0.009208
H	3.857884	-1.215467	-1.405699	C	-1.607031	0.553549	-0.006606
O	1.843502	-0.964730	1.676854	C	-2.326991	-0.674171	-0.005614
C	3.056991	-1.564801	2.097604	C	-3.713256	-0.670558	-0.002791
H	3.303569	-1.273100	3.128702	C	-4.474469	0.492256	-0.000819
H	2.995960	-2.661461	2.045787	C	-3.774351	1.705412	-0.001864
H	3.845291	-1.212580	1.427867	C	-2.384769	1.746460	-0.004676
C	0.726474	-1.322962	2.493098	H	-1.857533	2.697345	-0.005611
H	0.888176	-0.992172	3.528469	H	-4.335095	2.638129	-0.000450
H	-0.140407	-0.819343	2.065142	H	-5.557594	0.440893	0.001356
H	0.574498	-2.411165	2.482505	F	-4.358074	-1.869871	-0.001921
O	2.600043	1.660066	0.003572	H	-1.790781	-1.619100	-0.007394

Table S1 (Continued).



Ar = 3-fluorophenyl

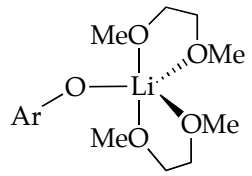


37 (Ar = 3-fluorophenyl)
G = -1444.816497
(-90 ºC)
see pg S95

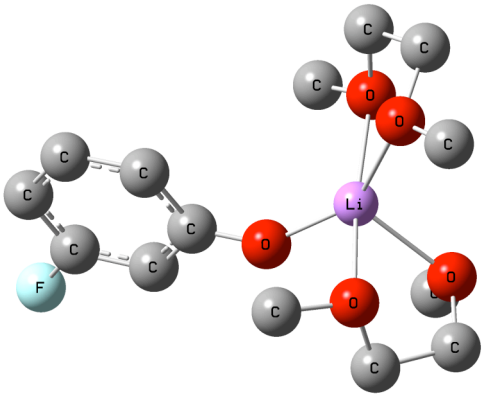
Atom	X	Y	Z
Li	-0.280725	-1.237855	0.125577
O	1.335896	-0.307888	0.120693
Li	0.280725	1.237855	0.125577
O	-1.335896	0.307888	0.120692
C	-2.629805	0.551570	0.100412
C	-3.199188	1.628821	0.830739
C	-4.570191	1.872301	0.803867
C	-5.442157	1.068000	0.062507
C	-4.877685	0.015208	-0.649450
C	-3.518065	-0.259116	-0.652461
H	-3.130953	-1.080647	-1.248395
F	-5.695127	-0.786819	-1.380451
H	-6.512311	1.239610	0.031501
H	-4.975304	2.703114	1.377601
H	-2.536892	2.250450	1.428987
O	0.233727	2.844114	-1.156595
C	0.434764	4.034436	-0.403269
C	1.514084	3.746513	0.620650
O	1.066961	2.649322	1.409553
C	2.023857	2.223033	2.380193
H	2.223687	3.028711	3.099661
H	1.586081	1.368208	2.896995
H	2.958085	1.912896	1.896689
H	2.459564	3.487806	0.121133
H	1.681161	4.634082	1.249276
H	0.747428	4.860793	-1.059113
H	-0.500780	4.321941	0.099943
C	-0.855622	2.930289	-2.075947
H	-1.796623	3.125223	-1.546658

Atom	X	Y	Z
H	-0.671041	3.720187	-2.816497
H	-0.921005	1.963608	-2.576444
C	2.629805	-0.551570	0.100413
C	3.199188	-1.628822	0.830740
C	4.570191	-1.872302	0.803867
C	5.442157	-1.068001	0.062507
C	4.877685	-0.015208	-0.649450
C	3.518065	0.259116	-0.652460
H	3.130954	1.080647	-1.248395
F	5.695127	0.786818	-1.380452
H	6.512311	-1.239611	0.031501
H	4.975303	-2.703115	1.377601
H	2.536891	-2.250450	1.428987
O	-0.233726	-2.844113	-1.156595
C	0.855622	-2.930288	-2.075947
H	0.921005	-1.963608	-2.576444
H	1.796623	-3.125223	-1.546658
H	0.671040	-3.720187	-2.816497
C	-0.434764	-4.034436	-0.403269
C	-1.514084	-3.746512	0.620650
O	-1.066961	-2.649322	1.409553
C	-2.023857	-2.223033	2.380193
H	-2.223687	-3.028711	3.099662
H	-1.586081	-1.368208	2.896996
H	-2.958085	-1.912896	1.896690
H	-1.681161	-4.634082	1.249276
H	-2.459564	-3.487805	0.121133
H	0.500780	-4.321940	0.099943
H	-0.747428	-4.860792	-1.059113

Table S1 (Continued).



Ar = 3-fluorophenyl

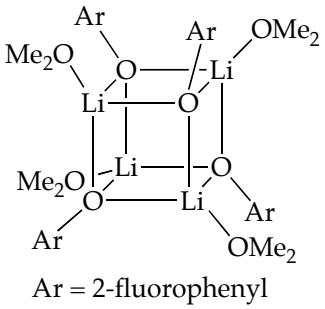


38 (Ar = 3-fluorophenyl)
G = -1031.124934
(-90 ºC)
see pg S95

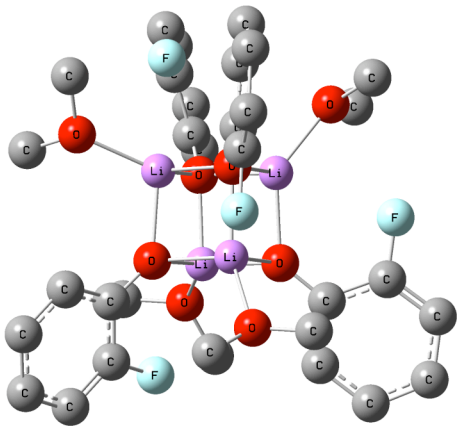
Atom	X	Y	Z
Li	-1.153085	0.036651	0.091490
O	0.576143	-0.506063	0.121610
C	1.797434	-0.175294	-0.198233
C	2.088636	0.716139	-1.274338
C	3.397157	1.060896	-1.601562
C	4.488412	0.551196	-0.890186
C	4.202295	-0.318283	0.158577
C	2.916758	-0.686821	0.517204
H	2.761070	-1.372676	1.344532
F	5.241217	-0.831698	0.872375
H	5.515031	0.805652	-1.129026
H	3.577586	1.741600	-2.431598
H	1.253452	1.115551	-1.847194
O	-0.950202	1.937894	1.176197
C	-1.412323	2.952455	0.300395
C	-2.749649	2.509681	-0.252277
O	-2.564833	1.254810	-0.897824
C	-3.765252	0.746267	-1.470942
H	-3.530339	-0.244312	-1.858434
H	-4.555962	0.664902	-0.711273
H	-4.114139	1.401050	-2.281672
H	-3.484150	2.403984	0.560415
H	-3.125241	3.257750	-0.966958

Atom	X	Y	Z
H	-1.532697	3.908961	0.833618
H	-0.690690	3.102813	-0.517410
C	0.334076	2.234747	1.728724
H	0.626375	1.376777	2.332914
H	0.277104	3.136213	2.355378
H	1.078094	2.373688	0.936017
O	-2.163441	-1.174346	1.512829
C	-2.512020	-2.415802	0.892150
C	-1.586545	-2.759839	-0.262202
O	-1.750861	-1.742649	-1.245759
C	-0.848785	-1.892604	-2.341684
H	0.185869	-1.801576	-1.997142
H	-1.005485	-2.860045	-2.840560
H	-1.070685	-1.086629	-3.045284
H	-0.539055	-2.784599	0.064612
H	-1.860949	-3.743563	-0.677743
H	-2.511270	-3.224949	1.635055
H	-3.533312	-2.294062	0.515687
C	-1.262969	-1.307223	2.619587
H	-0.266716	-1.610496	2.281981
H	-1.664446	-2.021599	3.350863
H	-1.198943	-0.319366	3.079664

Table S1 (Continued).



Ar = 2-fluorophenyl

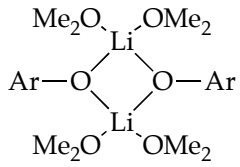


34 (Ar = 2-fluorophenyl)
G = -2274.550937
(-90 ºC)
see pg S95

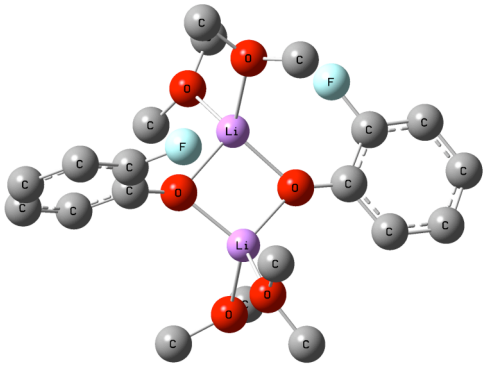
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.131471	0.810447	0.787185	C	2.282027	-1.529222	-1.513018
O	-0.987765	0.833110	-1.198929	C	3.538563	-0.885000	-1.550878
Li	-0.725424	-1.124095	-1.052409	C	4.684275	-1.448624	-2.082098
O	-0.926484	-1.170829	0.890505	C	4.620465	-2.740446	-2.617861
Li	1.010576	-0.820464	1.017547	C	3.402842	-3.422345	-2.598105
O	1.223863	-0.930785	-0.984264	C	2.257087	-2.833211	-2.056103
Li	0.956615	1.010868	-0.918915	H	1.309697	-3.364560	-2.038656
O	0.813719	1.132889	1.034904	H	3.339672	-4.427754	-3.007907
C	1.417690	2.084002	1.735792	H	5.510010	-3.199182	-3.038880
C	0.672928	3.082333	2.398648	H	5.609930	-0.880145	-2.066860
C	1.233991	4.101477	3.146257	F	3.604932	0.380233	-1.023305
C	2.627115	4.171161	3.261739	O	2.581824	-1.660187	1.941533
C	3.409890	3.213859	2.614606	C	2.809167	-3.053870	1.745920
C	2.821375	2.190986	1.864231	H	3.864140	-3.297882	1.930920
H	3.433669	1.455932	1.348344	H	2.171161	-3.645718	2.414771
H	4.493738	3.259446	2.690132	H	2.570098	-3.276537	0.704781
H	3.085314	4.963845	3.845357	C	2.944336	-1.231093	3.252057
H	0.582587	4.827351	3.624579	H	2.741623	-0.160389	3.308627
F	-0.690835	3.019669	2.275358	H	2.358634	-1.761916	4.012842
O	1.660988	2.425912	-2.146927	H	4.014938	-1.407095	3.425697
C	2.780292	3.252204	-1.837037	C	-1.715988	-1.962580	1.604312
H	2.656915	4.244434	-2.292757	C	-1.261080	-2.570579	2.793856
H	2.819152	3.348178	-0.750903	C	-2.034357	-3.404275	3.583047
H	3.711977	2.797240	-2.196057	C	-3.352818	-3.672684	3.199880
C	1.518987	2.195795	-3.544143	C	-3.852911	-3.086969	2.034921
H	1.414353	3.147508	-4.083135	C	-3.055183	-2.247754	1.253238
H	2.385189	1.648084	-3.940764	H	-3.453744	-1.773859	0.360098
H	0.610647	1.606726	-3.681242	H	-4.878844	-3.279196	1.729928

Atom	X	Y	Z
H	-3.973609	-4.324620	3.806974
H	-1.601349	-3.830612	4.483524
F	0.028276	-2.305193	3.174766
O	-1.162336	-2.610286	-2.352056
C	-0.984793	-2.273901	-3.723639
H	-1.883392	-1.786892	-4.125140
H	-0.136009	-1.589422	-3.777004
H	-0.760234	-3.171867	-4.315607
C	-2.208444	-3.555757	-2.150400
H	-2.292096	-3.720111	-1.074910
H	-3.162027	-3.171932	-2.535361
H	-1.968145	-4.503569	-2.652167
C	-1.927715	1.454663	-1.895619
C	-3.102589	0.779862	-2.295739
C	-4.130987	1.366539	-3.010816
C	-4.024454	2.715236	-3.369568
C	-2.883897	3.428341	-2.994917
C	-1.856837	2.814913	-2.272661
H	-0.972657	3.373214	-1.976902
H	-2.789819	4.477681	-3.264119
H	-4.822104	3.193837	-3.929485
H	-5.001268	0.771279	-3.272507
F	-3.210183	-0.543219	-1.942512
O	-2.906600	1.329076	1.600902
C	-3.093923	1.041150	2.984191
H	-4.158949	0.881842	3.200318
H	-2.546743	0.123059	3.202207
H	-2.711271	1.861682	3.605119
C	-3.615507	2.497115	1.195789
H	-3.270015	3.375232	1.756973
H	-3.422822	2.641827	0.132230
H	-4.693909	2.362030	1.357312

Table S1 (Continued).



Ar = 2-fluorophenyl

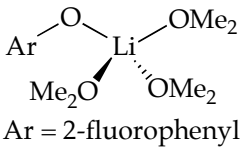


35 (Ar = 2-fluorophenyl)
G =-1447.181069
(-90 ºC)
see pg S95

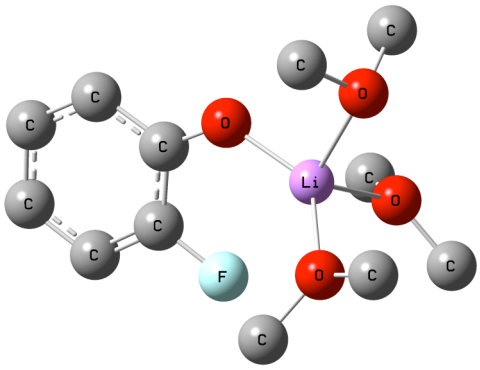
Atom	X	Y	Z	Atom	X	Y	Z
C	0.695895	-3.523938	2.026441	H	-1.299534	1.337689	-2.507705
O	-0.077670	-2.349590	1.820078	C	0.465869	3.949277	-1.580878
Li	0.074958	-1.145543	0.184386	H	-0.101780	4.747284	-2.080482
O	1.385338	0.219345	-0.085941	H	0.736903	4.266131	-0.572587
Li	-0.011512	1.456825	0.055137	H	1.377048	3.742271	-2.160359
O	-1.331795	0.167368	0.411193	C	2.693648	0.188236	-0.189335
C	-2.638971	0.094949	0.272894	C	3.499767	1.332138	-0.407776
C	-3.551142	0.374739	1.319505	C	4.890646	1.249660	-0.507082
C	-4.933493	0.286396	1.145120	C	5.547200	0.023358	-0.394893
C	-5.478216	-0.086137	-0.084950	C	4.786545	-1.133379	-0.182024
C	-4.612950	-0.371506	-1.146878	C	3.412047	-1.028380	-0.085519
C	-3.246567	-0.279210	-0.950524	F	2.673356	-2.166715	0.117183
F	-2.417025	-0.566016	-2.008591	H	5.248179	-2.112726	-0.090295
H	-4.984543	-0.664066	-2.125207	H	6.628290	-0.041346	-0.472790
H	-6.553102	-0.154344	-0.223099	H	5.465683	2.157392	-0.676393
H	-5.590754	0.510765	1.982275	H	2.997465	2.292012	-0.507858
H	-3.135701	0.663486	2.282501	O	-0.094352	-2.605348	-1.208777
O	0.275999	2.819982	1.554148	C	-1.244325	-3.436415	-1.309073
C	1.253832	2.484989	2.535266	H	-0.969090	-4.431438	-1.688085
H	0.858646	1.742024	3.242084	H	-1.993947	-2.985435	-1.969230
H	1.562131	3.381687	3.091426	H	-1.656122	-3.530320	-0.302264
H	2.109044	2.063764	2.005376	C	0.527329	-2.370199	-2.466385
C	-0.909319	3.364216	2.123139	H	0.884418	-3.313894	-2.903004
H	-1.376877	2.650007	2.814061	H	-0.174546	-1.890772	-3.161836
H	-1.596874	3.568846	1.300185	H	1.374464	-1.708729	-2.282732
H	-0.687898	4.297244	2.660683	C	-0.443715	-1.706216	3.033829
O	-0.326995	2.777198	-1.447538	H	0.448994	-1.432830	3.615991
C	-0.731777	2.245910	-2.707620	H	-1.080904	-2.361797	3.644761
H	-1.361722	2.969887	-3.243308	H	-0.994153	-0.808632	2.749695
H	0.145633	2.006172	-3.324861	H	1.642522	-3.287524	2.530501

Atom	X	Y	Z
H	0.135382	-4.252760	2.629712
H	0.907412	-3.941872	1.042099

Table S1 (Continued).



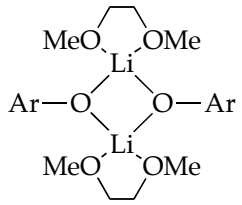
Ar = 2-fluorophenyl



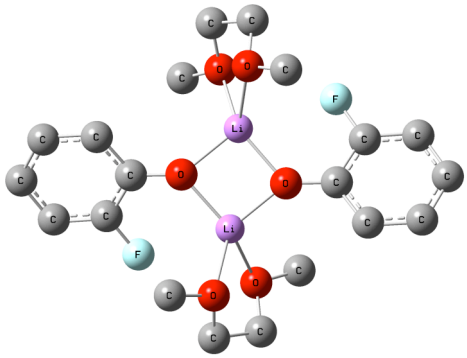
36 (Ar = 2-fluorophenyl)
G = -878.534652
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.962569	0.114765	0.022497	C	-2.238953	2.379044	1.232300
O	-1.364745	-0.798189	1.788717	H	-2.926702	3.236303	1.257435
C	-0.277365	-0.736816	2.713578	H	-2.522689	1.656720	1.999632
H	0.365084	-1.620114	2.613350	H	-1.211299	2.719561	1.408920
H	0.295083	0.155130	2.457610	C	-1.943707	2.561352	-1.101926
H	-0.656426	-0.671756	3.743098	H	-0.888088	2.836120	-1.003656
C	-2.141613	-1.976860	1.931839	H	-2.086001	1.995136	-2.025406
H	-1.529062	-2.874713	1.768337	H	-2.580615	3.456942	-1.124547
H	-2.592072	-2.029369	2.933498	O	0.556223	1.110044	0.052662
H	-2.933174	-1.938060	1.180707	C	1.792566	0.713014	-0.066947
O	-1.833120	-0.992263	-1.448195	C	2.140447	-0.662330	-0.105217
C	-3.181695	-0.825945	-1.865357	C	3.423736	-1.157133	-0.226947
H	-3.228330	-0.417098	-2.885054	C	4.489294	-0.253081	-0.318468
H	-3.717016	-1.786345	-1.846564	C	4.212020	1.116850	-0.284869
H	-3.646405	-0.124032	-1.171310	C	2.905794	1.589418	-0.162309
C	-1.086518	-1.837938	-2.320723	H	2.700451	2.657056	-0.136995
H	-1.037687	-1.405527	-3.329797	H	5.029424	1.831773	-0.355114
H	-0.085619	-1.920048	-1.899872	H	5.508063	-0.616663	-0.414315
H	-1.548916	-2.833558	-2.380141	H	3.580479	-2.232669	-0.246602
O	-2.328133	1.704994	-0.023001	F	1.088155	-1.563692	-0.013544

Table S1 (Continued).



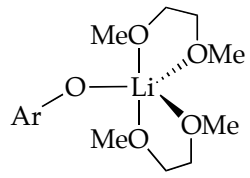
Ar = 2-fluorophenyl



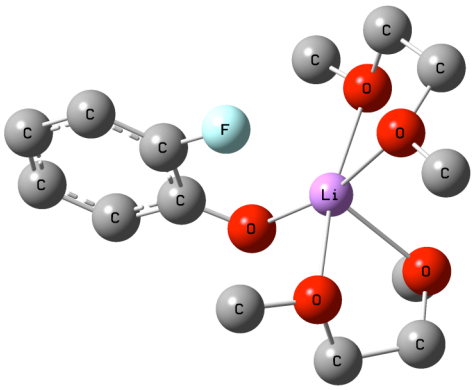
37 (Ar = 2-fluorophenyl)
G = -1444.81867
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.306657	-1.263473	0.130257	H	-1.021266	3.448276	-2.962537
O	1.318826	-0.317157	0.291133	H	-1.035633	1.689633	-2.632222
Li	0.306608	1.263506	0.130246	C	2.616839	-0.490645	0.219713
O	-1.318886	0.317192	0.290934	C	3.296521	-1.620160	0.736658
C	-2.616908	0.490651	0.219602	C	4.682418	-1.758783	0.630310
C	-3.296567	1.620213	0.736473	C	5.458858	-0.778841	0.008689
C	-4.682474	1.758805	0.630216	C	4.825897	0.358504	-0.508592
C	-5.458948	0.778782	0.008766	C	3.453629	0.475172	-0.391692
C	-4.826010	-0.358614	-0.508432	F	2.835727	1.594778	-0.895718
C	-3.453732	-0.475250	-0.391622	H	5.384161	1.149973	-1.001297
F	-2.835856	-1.594911	-0.895557	H	6.536064	-0.888170	-0.073393
H	-5.384301	-1.150149	-1.001001	H	5.160799	-2.643508	1.044801
H	-6.536161	0.888087	-0.073247	H	2.700459	-2.377866	1.240722
H	-5.160835	2.643570	1.044644	O	0.033585	-2.788942	-1.252892
H	-2.700478	2.377986	1.240405	C	1.109325	-2.679988	-2.181498
O	-0.033531	2.789099	-1.252788	H	1.035523	-1.689311	-2.632315
C	-0.013543	4.026703	-0.555106	H	2.077257	-2.772832	-1.673746
C	1.126095	3.972450	0.442282	H	1.021358	-3.447944	-2.962686
O	0.892732	2.858197	1.298734	C	0.013766	-4.026574	-0.555253
C	1.935968	2.649047	2.247815	C	-1.125881	-3.972512	0.442135
H	2.014345	3.507617	2.929012	O	-0.892667	-2.858268	1.298640
H	1.671463	1.754356	2.813256	C	-1.935949	-2.649287	2.247708
H	2.896692	2.489000	1.743273	H	-2.014259	-3.507910	2.928845
H	2.084030	3.842982	-0.078542	H	-1.671548	-1.754610	2.813220
H	1.157389	4.905934	1.024474	H	-2.896674	-2.489303	1.743149
H	0.142813	4.863611	-1.253204	H	-1.157056	-4.906026	1.024286
H	-0.971542	4.181241	-0.035492	H	-2.083831	-3.843147	-0.078687
C	-1.109305	2.680305	-2.181372	H	0.971787	-4.180999	-0.035646
H	-2.077215	2.773244	-1.673594	H	-0.142478	-4.863478	-1.253380

Table S1 (Continued).



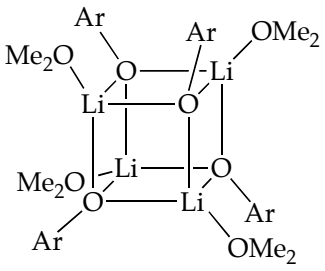
Ar = 2-fluorophenyl



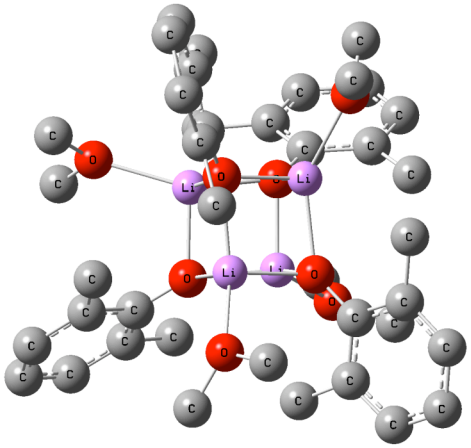
38 (Ar = 2-fluorophenyl)
G = -1031.128842
(-90 ºC)
see pg S95

Atom	X	Y	Z
Li	-0.693387	0.024169	0.079772
O	0.805444	-0.706814	0.969456
C	1.987865	-0.429742	0.500144
C	2.151864	0.358625	-0.670001
C	3.358616	0.709012	-1.239813
C	4.540061	0.263607	-0.631848
C	4.448182	-0.518407	0.523978
C	3.213712	-0.857684	1.077892
H	3.155720	-1.466148	1.977451
H	5.358309	-0.871152	1.005132
H	5.504825	0.523692	-1.056855
H	3.370195	1.317169	-2.140736
F	0.972355	0.792054	-1.267154
O	-0.777244	1.954916	1.070387
C	-1.193468	2.938976	0.137790
C	-2.411806	2.402172	-0.583280
O	-2.049429	1.177502	-1.203639
C	-3.120192	0.581247	-1.920963
H	-2.750628	-0.372764	-2.296217
H	-3.984526	0.406111	-1.263523
H	-3.432866	1.221697	-2.758554
H	-3.233639	2.233378	0.129598
H	-2.749142	3.132062	-1.336158
H	-1.452256	3.880155	0.648681
H	-0.384567	3.141532	-0.579576
C	0.378105	2.339241	1.813576
H	0.669656	1.469274	2.400527
H	0.146398	3.191608	2.468304
H	1.204293	2.606447	1.142342
O	-2.266748	-0.966267	1.266376
C	-2.520654	-2.239439	0.673652
C	-1.323490	-2.765709	-0.099896
O	-1.059135	-1.839054	-1.150276
C	0.054031	-2.227010	-1.951677
H	0.958775	-2.324527	-1.341312
H	-0.152934	-3.178620	-2.463066
H	0.203087	-1.438831	-2.691345
H	-0.438600	-2.844371	0.544766
H	-1.561115	-3.758320	-0.517098
H	-2.822113	-2.966629	1.440933
H	-3.362027	-2.097986	-0.013535
C	-1.764454	-1.035577	2.606028
H	-0.754030	-1.454676	2.627888
H	-2.448517	-1.621219	3.236238
H	-1.728684	-0.007011	2.969255

Table S1 (Continued).



Ar = 2,6-dimethylphenol

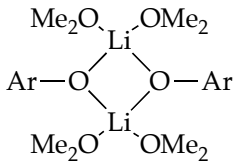


34 (Ar = 2,6-dimethylphenyl)
G = -1877.563983
(-90 ºC)
see pg S95

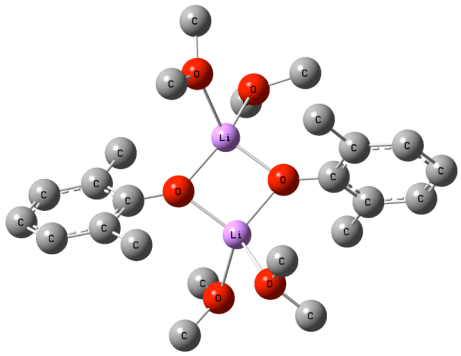
Atom	X	Y	Z	Atom	X	Y	Z
O	1.477324	-0.265196	1.017951	H	0.212759	6.018435	-3.690344
Li	1.309959	-0.313251	-0.949540	H	1.442634	4.041298	-4.573922
O	-0.266862	-1.475763	-1.015106	C	1.644386	1.570131	-3.514058
Li	-1.306956	0.317607	-0.955298	H	2.105634	1.819850	-4.475736
O	-1.481266	0.266035	1.011929	H	2.433966	1.190107	-2.855913
Li	-0.315671	-1.308187	0.953249	H	0.949583	0.737057	-3.688209
O	-1.383369	-2.841583	2.083747	O	1.378645	2.840123	2.091960
C	-1.880849	-2.610263	3.401667	C	2.062710	3.929887	1.474851
H	-1.783415	-3.521065	4.009527	H	3.140989	3.731121	1.428268
H	-1.281575	-1.816200	3.845578	H	1.666792	4.042184	0.464915
H	-2.929532	-2.293666	3.370613	H	1.892776	4.857095	2.040528
C	-2.066796	-3.928369	1.460536	C	1.870636	2.606199	3.411390
H	-1.665699	-4.039380	0.452520	H	2.921231	2.295685	3.384362
H	-1.901994	-4.857147	2.025132	H	1.765023	3.513833	4.022654
H	-3.144298	-3.726910	1.408767	H	1.273935	1.806736	3.848957
Li	0.311773	1.308761	0.956694	C	-2.643570	0.245167	1.687755
O	0.270616	1.479524	-1.010274	C	-2.766774	0.922266	2.931855
C	0.250462	2.640284	-1.688718	C	-3.979997	0.899518	3.625384
C	0.931284	2.761537	-2.931104	C	-5.088358	0.211997	3.133612
C	0.910400	3.973667	-3.626658	C	-4.966649	-0.469860	1.924480
C	0.220973	5.082486	-3.138633	C	-3.771959	-0.470993	1.193770
C	-0.464975	4.962276	-1.931617	C	-3.703557	-1.235120	-0.108205
C	-0.467748	3.768922	-1.198828	H	-3.766167	-0.575560	-0.982474
C	-1.237200	3.700927	0.099988	H	-2.772777	-1.799434	-0.210819
H	-1.944179	4.534688	0.174989	H	-4.538064	-1.940844	-0.186671
H	-1.801117	2.769494	0.199956	H	-5.817245	-1.023348	1.529655
H	-0.580648	3.764649	0.976663	H	-6.025035	0.202399	3.684051
H	-1.020415	5.813166	-1.540146	H	-4.048924	1.428477	4.574383

Atom	X	Y	Z
C	-1.575628	1.630620	3.520631
H	-1.828343	2.092336	4.481285
H	-0.746857	0.931513	3.698796
H	-1.188241	2.418811	2.865224
O	-2.821646	1.403505	-2.078705
C	-3.930825	2.069185	-1.476730
H	-3.758446	3.152663	-1.445608
H	-4.851583	1.868127	-2.042839
H	-4.038055	1.686425	-0.461146
C	-2.596749	1.874786	-3.406820
H	-1.747106	1.326715	-3.811773
H	-3.482226	1.690024	-4.031686
H	-2.361890	2.945420	-3.403622
C	-0.246622	-2.637110	-1.692625
C	-0.926450	-2.759056	-2.935450
C	-0.905302	-3.971705	-3.630096
C	-0.216870	-5.080472	-3.140581
C	0.468020	-4.959632	-1.933026
C	0.470785	-3.765661	-1.201240
C	1.240272	-3.696740	0.097502
H	1.807517	-2.767115	0.194624
H	0.584736	-3.755635	0.975284
H	1.944475	-4.532681	0.174405
H	1.022753	-5.810434	-1.540392
H	-0.208542	-6.016834	-3.691585
H	-1.436636	-4.039866	-4.577836
C	-1.638889	-1.568042	-3.520042
H	-0.943552	-0.736351	-3.698291
H	-2.102664	-1.819946	-4.479929
H	-2.426704	-1.185809	-2.861093
O	2.832786	-1.394728	-2.081059
C	2.607561	-1.874833	-3.406045
H	2.345486	-2.938941	-3.393512
H	1.776004	-1.309456	-3.824662
H	3.502781	-1.718657	-4.024721
C	3.937250	-2.062430	-1.473074
H	4.859869	-1.870458	-2.039325
H	4.044738	-1.672853	-0.460143
H	3.758598	-3.144721	-1.435082
C	2.638895	-0.247740	1.695141
C	2.759926	-0.927172	2.938133
C	3.973224	-0.908802	3.631738
C	5.083428	-0.223344	3.141265
C	4.963538	0.461582	1.933652
C	3.768717	0.467515	1.203253
C	3.700544	1.235037	-0.096732
H	4.541139	1.933084	-0.178616
H	3.751614	0.576262	-0.972309
H	2.774344	1.807822	-0.193031
H	5.815544	1.013729	1.540019
H	6.020204	-0.217598	3.691587
H	4.040710	-1.439608	4.579804
C	1.566747	-1.633303	3.525536
H	0.739169	-0.932602	3.702947
H	1.178243	-2.420499	2.869620
H	1.817597	-2.095776	4.486323

Table S1 (Continued).



Ar = 2,6-dimethylphenyl

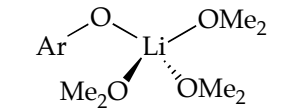


35 (Ar = 2,6-dimethylphenyl)
G = -1405.835621
(-90 ºC)
see pg S95

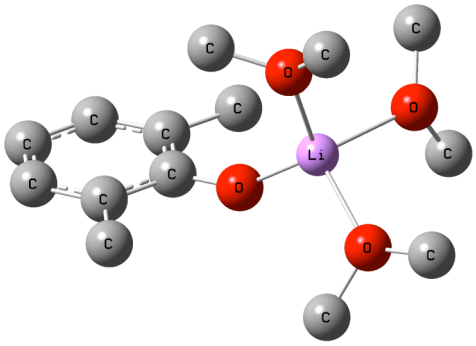
Atom	X	Y	Z	Atom	X	Y	Z
C	1.789011	-3.408701	1.270354	H	-2.340257	3.010479	0.048577
O	0.801830	-2.446600	1.639699	H	-2.528769	4.031659	1.506489
Li	0.071547	-1.232035	0.070917	O	0.516945	2.799151	-1.382577
O	1.430031	0.069257	-0.159048	C	0.390579	4.212812	-1.345969
Li	0.039086	1.362430	0.013282	H	1.376864	4.693478	-1.416675
O	-1.313776	0.046559	0.066252	H	-0.239239	4.573223	-2.172497
C	-2.627662	-0.085473	-0.049038	H	-0.068773	4.464937	-0.389948
C	-3.400925	-0.611176	1.025803	C	1.173935	2.335950	-2.558878
C	-4.785161	-0.748796	0.883948	H	2.171631	2.786906	-2.646760
C	-5.438470	-0.378577	-0.292063	H	1.274649	1.256288	-2.453225
C	-4.685346	0.149613	-1.341370	H	0.584888	2.580688	-3.454209
C	-3.299734	0.307690	-1.242598	C	2.755423	-0.001132	-0.176118
C	-2.507130	0.898469	-2.383442	C	3.542016	0.788628	0.710763
H	-1.954075	1.797029	-2.079716	C	4.935081	0.681797	0.694277
H	-1.751235	0.200096	-2.765173	C	5.590264	-0.179832	-0.185216
H	-3.164571	1.171588	-3.216460	C	4.826190	-0.938884	-1.071858
H	-5.182387	0.452004	-2.262266	C	3.430364	-0.864101	-1.087757
H	-6.514961	-0.492784	-0.386516	C	2.632773	-1.673197	-2.080994
H	-5.360188	-1.150641	1.717246	H	3.294464	-2.254806	-2.732465
C	-2.711850	-0.992107	2.313005	H	1.944958	-2.376381	-1.594084
H	-2.142970	-0.149057	2.728811	H	2.013465	-1.031043	-2.722556
H	-3.437469	-1.316677	3.067126	H	5.321863	-1.604972	-1.776933
H	-1.987792	-1.805405	2.172515	H	6.674494	-0.251691	-0.186235
O	-0.804339	2.871967	1.383188	H	5.515453	1.291225	1.385773
C	-0.519129	2.912572	2.774617	C	2.853967	1.742715	1.653603
H	-1.027580	2.094719	3.305220	H	3.578924	2.259856	2.292145
H	-0.839835	3.870501	3.209302	H	2.283823	2.507685	1.108090
H	0.560038	2.807388	2.890109	H	2.138429	1.223010	2.304758
C	-2.197539	3.053313	1.128907	O	-0.659246	-2.908888	-0.965107
H	-2.791193	2.257589	1.593193	C	-1.584698	-3.722772	-0.244192

Atom	X	Y	Z
H	-1.683881	-4.706313	-0.725073
H	-2.568417	-3.239265	-0.191291
H	-1.182148	-3.844810	0.762089
C	-1.090414	-2.686464	-2.305306
H	-1.157011	-3.639204	-2.849756
H	-2.066756	-2.186582	-2.320192
H	-0.343138	-2.050276	-2.782469
C	1.189773	-1.713929	2.798277
H	2.139127	-1.191099	2.627952
H	1.291962	-2.387667	3.661200
H	0.399600	-0.987920	2.997696
H	2.737913	-2.916579	1.021855
H	1.949738	-4.126666	2.087208
H	1.408990	-3.933753	0.392766

Table S1 (Continued).



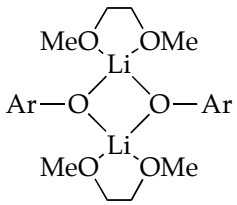
Ar = 2,6-dimethylphenyl



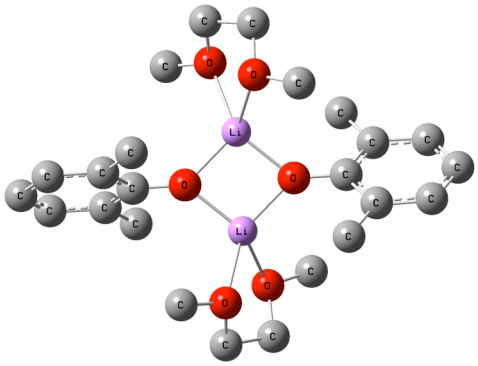
36 (Ar = 2,6-dimethylphenyl)
G = -857.865913
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.161651	-0.021204	-0.014584	H	1.522711	2.830959	-1.586953
O	2.311890	-1.160157	-1.233425	C	2.239428	2.634280	0.955519
C	1.577719	-1.932630	-2.186074	H	1.367693	3.283346	0.798248
H	1.665527	-3.005088	-1.962413	H	2.124613	2.096887	1.898070
H	0.540616	-1.607204	-2.092156	H	3.148479	3.251575	0.986593
H	1.956034	-1.744638	-3.200966	O	-0.494445	-0.097924	-0.632936
C	3.694531	-1.465132	-1.207887	C	-1.787409	-0.002875	-0.406185
H	3.866205	-2.509763	-0.909398	C	-2.584837	-1.170244	-0.207262
H	4.152864	-1.301992	-2.194351	C	-3.953708	-1.046691	0.041877
H	4.161563	-0.795901	-0.481425	C	-4.577943	0.200495	0.096449
O	1.320985	-0.491468	1.961537	C	-3.805879	1.345701	-0.107828
C	2.454014	-1.010829	2.638125	C	-2.434223	1.268134	-0.355794
H	2.532456	-0.593491	3.652485	C	-1.614846	2.510012	-0.594357
H	2.404643	-2.106896	2.709678	H	-0.799451	2.605307	0.136860
H	3.337894	-0.724297	2.063323	H	-2.233118	3.412810	-0.530575
C	0.094168	-0.777119	2.637928	H	-1.137223	2.491903	-1.583941
H	0.080184	-0.287942	3.621890	H	-4.278382	2.327241	-0.075716
H	-0.712903	-0.396399	2.012378	H	-5.644645	0.278563	0.290086
H	-0.028682	-1.860268	2.772341	H	-4.542752	-1.951228	0.192028
O	2.334417	1.652597	-0.070787	C	-1.931062	-2.526262	-0.293489
C	2.415717	2.230681	-1.371659	H	-1.546066	-2.727601	-1.303154
H	3.312103	2.860898	-1.458466	H	-2.639950	-3.324078	-0.043717
H	2.476260	1.402885	-2.079592	H	-1.068409	-2.611488	0.381303

Table S1 (Continued).



Ar = 2,6-dimethylphenyl

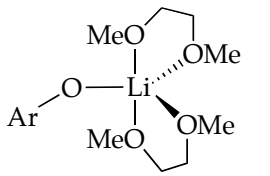


37 (Ar = 2,6-dimethylphenyl)
G = -1403.482645
(-90 ºC)
see pg S95

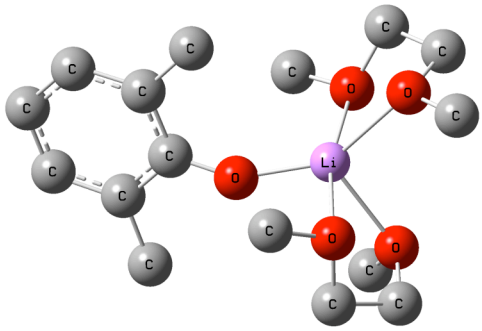
Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000105	1.264150	0.000152	H	0.585857	-4.958286	-1.103507
O	1.380002	0.000087	0.000124	H	-0.585656	-4.958054	1.104527
Li	-0.000012	-1.264069	-0.000007	H	-1.531473	-4.087807	-0.135380
O	-1.380125	-0.000008	-0.000020	C	-1.669153	-2.724919	2.104970
C	-2.707710	-0.000058	-0.000133	H	-2.600839	-2.642593	1.532151
C	-3.433432	-0.607438	-1.063893	H	-1.731662	-3.570973	2.803108
C	-4.831069	-0.595210	-1.043836	H	-1.509194	-1.801109	2.660853
C	-5.541174	-0.000224	-0.000351	C	2.707587	0.000036	-0.000074
C	-4.831299	0.594863	1.043234	C	3.433291	0.607108	-1.064023
C	-3.433667	0.607265	1.063500	C	4.830928	0.594766	-1.044056
C	-2.680868	1.243742	2.205910	C	5.541052	-0.000033	-0.000477
H	-2.019941	0.524937	2.709297	C	4.831195	-0.594808	1.043298
H	-2.028199	2.061086	1.872414	C	3.433563	-0.607089	1.063661
H	-3.371293	1.648546	2.954287	C	2.680790	-1.243208	2.206287
H	-5.371425	1.061041	1.866384	H	3.371237	-1.647896	2.954707
H	-6.627947	-0.000290	-0.000434	H	2.019979	-0.524210	2.709550
H	-5.371013	-1.061435	-1.867079	H	2.028003	-2.060560	1.873046
C	-2.680380	-1.243787	-2.206207	H	5.371336	-1.060828	1.866528
H	-2.019189	-0.524971	-2.709229	H	6.627825	-0.000059	-0.000632
H	-2.027933	-2.061303	-1.872690	H	5.370858	1.060750	-1.867446
H	-3.370635	-1.648336	-2.954879	C	2.680220	1.243254	-2.206438
O	-0.548089	-2.880475	1.235577	H	3.370463	1.647552	-2.955256
C	-0.604027	-4.068237	0.456937	H	2.018920	0.524384	-2.709237
C	0.604222	-4.068331	-0.456109	H	2.027876	2.060912	-1.873071
O	0.548275	-2.880738	-1.235009	O	0.548212	2.880767	1.235483
C	1.669317	-2.725395	-2.104471	C	1.669245	2.725160	2.104908
H	1.731796	-3.571612	-2.802414	H	1.509013	1.801591	2.661114
H	1.509357	-1.801714	-2.660570	H	2.600895	2.642354	1.532098
H	2.601018	-2.642949	-1.531694	H	1.732027	3.571431	2.802759
H	1.531669	-4.087760	0.136210	C	0.604488	4.068281	0.456488

Atom	X	Y	Z
C	-0.603803	4.068488	-0.456502
O	-0.548273	2.880640	-1.235035
C	-1.669433	2.725329	-2.104348
H	-1.731692	3.571296	-2.802612
H	-1.509826	1.801373	-2.660088
H	-2.601116	2.643411	-1.531464
H	-0.585184	4.958241	-1.104173
H	-1.531216	4.088401	0.135856
H	1.531913	4.087380	-0.135876
H	0.586428	4.958296	1.103815

Table S1 (Continued).



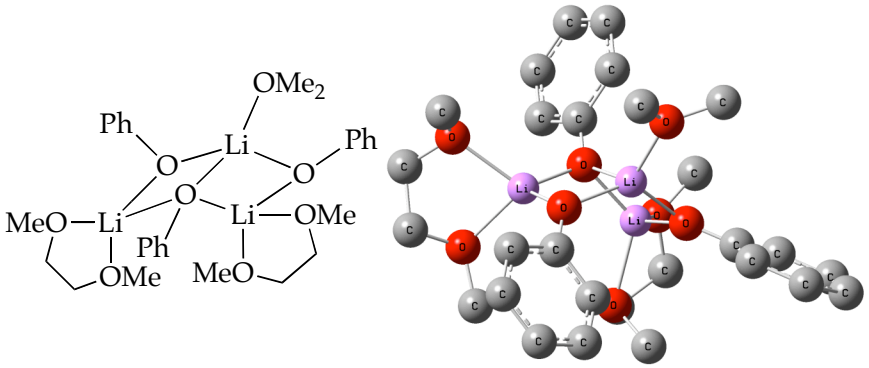
Ar = 2,6-dimethylphenyl



38 (Ar = 2,6-dimethylphenyl)
G = -1010.456279
(-90 ºC)
see pg S95

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.007765	0.065022	-0.008274	H	4.034853	1.802107	2.060908
O	-0.708989	-0.430986	0.065006	H	3.481048	1.991821	-0.986644
C	-1.991086	-0.167000	0.162496	H	3.280923	3.276985	0.238082
C	-2.474892	0.859049	1.032199	H	1.720957	3.606229	-1.671819
C	-3.844252	1.122635	1.110826	H	0.837338	3.316532	-0.149063
C	-4.773344	0.402959	0.357916	C	-0.402230	1.983005	-2.009867
C	-4.309537	-0.606375	-0.488172	H	-0.806622	1.031393	-2.351778
C	-2.949838	-0.901464	-0.599966	H	-0.312588	2.685222	-2.850974
C	-2.466776	-1.997825	-1.514734	H	-1.078285	2.394168	-1.251260
H	-3.306348	-2.510740	-1.997775	O	2.219863	-1.221806	-1.205231
H	-1.810090	-1.611607	-2.307636	C	2.608343	-2.377579	-0.456435
H	-1.878478	-2.748924	-0.969444	C	1.615441	-2.687318	0.649451
H	-5.021014	-1.182258	-1.079795	O	1.633608	-1.588392	1.551857
H	-5.835752	0.619639	0.433023	C	0.668770	-1.730311	2.594180
H	-4.188676	1.909741	1.781490	H	-0.342290	-1.734329	2.175651
C	-1.489615	1.637400	1.867236	H	0.856129	-2.649634	3.168500
H	-1.999302	2.378308	2.493827	H	0.785157	-0.866618	3.252816
H	-0.905547	0.981750	2.527181	H	0.602374	-2.813554	0.243597
H	-0.753870	2.172187	1.249118	H	1.911895	-3.615350	1.166514
O	0.885664	1.709509	-1.455369	H	2.721905	-3.243584	-1.122063
C	1.502591	2.855920	-0.895161	H	3.585484	-2.151765	-0.016001
C	2.792666	2.413235	-0.238505	C	1.508150	-1.522673	-2.407933
O	2.476260	1.423306	0.733884	H	0.562846	-2.034572	-2.197185
C	3.618011	0.981801	1.459944	H	2.129756	-2.136702	-3.074004
H	3.286193	0.170089	2.106240	H	1.298531	-0.564931	-2.885935
H	4.394524	0.607517	0.777218				

Table S1 (Continued).

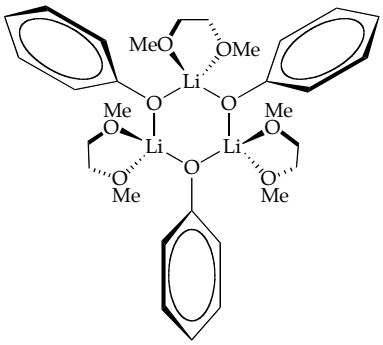


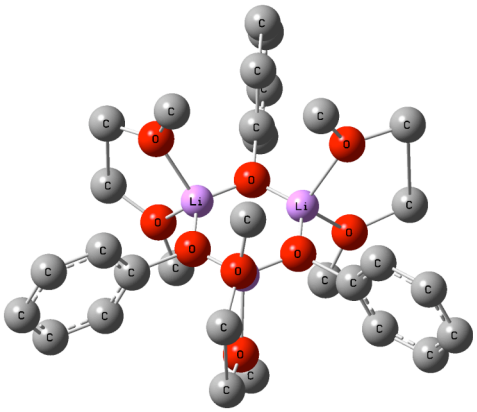
42
G = -1715.709887
(-90 ºC)
see pg S98

Atom	X	Y	Z	Atom	X	Y	Z
O	-0.362622	1.356205	0.261324	H	-2.731934	-6.041634	-1.101597
Li	1.192905	0.898882	-0.747318	H	-4.456857	-4.631303	0.018359
O	1.838030	-0.482937	0.292522	H	-3.879349	-2.374198	0.857100
Li	0.147311	-0.440884	1.155202	O	0.322252	-0.688748	3.123277
O	-1.525389	-1.215285	0.621335	C	-0.702566	-1.352063	3.852374
Li	-1.976241	0.440570	-0.089876	H	-0.370939	-2.351357	4.168260
O	-2.870056	0.400431	-1.954577	H	-1.549590	-1.446689	3.171506
C	-4.276735	0.405075	-1.734291	H	-0.986762	-0.770926	4.741830
C	-4.546372	1.493978	-0.708021	C	1.541342	-0.563655	3.843520
O	-3.797201	1.247357	0.484449	H	1.399026	0.050591	4.744650
C	-4.530176	0.607226	1.526673	H	2.257861	-0.084762	3.174852
H	-3.816760	0.392200	2.323149	H	1.925769	-1.550206	4.135650
H	-5.315955	1.274490	1.904792	C	2.933254	-1.217776	0.389319
H	-4.980400	-0.334459	1.187675	C	4.204600	-0.708717	0.018875
H	-4.203969	2.458493	-1.096325	C	5.358400	-1.485544	0.116738
H	-5.619254	1.565470	-0.487468	C	5.299100	-2.799708	0.587176
H	-4.813069	0.624460	-2.670819	C	4.055990	-3.319971	0.961143
H	-4.602200	-0.580214	-1.368165	C	2.896619	-2.552848	0.866961
C	-2.436852	-0.591962	-2.888382	H	1.934422	-2.972437	1.151538
H	-1.359144	-0.460613	-2.999195	H	3.986620	-4.342050	1.329254
H	-2.651474	-1.599787	-2.514055	H	6.199288	-3.403347	0.663124
H	-2.928265	-0.439514	-3.859312	H	6.316183	-1.056540	-0.173475
C	-1.825385	-2.435573	0.199589	H	4.261376	0.320921	-0.329661
C	-3.128695	-2.974835	0.347590	O	2.313047	2.434489	-1.474729
C	-3.445548	-4.251381	-0.117280	C	2.874594	2.076544	-2.731355
C	-2.482433	-5.046781	-0.743075	C	1.770297	1.380019	-3.514533
C	-1.187127	-4.539297	-0.886633	O	1.217275	0.285750	-2.783424
C	-0.859912	-3.264359	-0.428983	C	1.902956	-0.961115	-2.967652
H	0.152051	-2.880738	-0.535768	H	2.928893	-0.923600	-2.585534
H	-0.417936	-5.146114	-1.361129	H	1.346019	-1.704379	-2.397688

Atom	X	Y	Z
H	1.905895	-1.230961	-4.032234
H	2.143776	1.045548	-4.492354
H	0.945634	2.081747	-3.674050
H	3.204952	2.974237	-3.275977
H	3.746327	1.421331	-2.583606
C	3.153117	3.248564	-0.659535
H	3.391643	4.188090	-1.175270
H	2.589105	3.464611	0.248934
H	4.083609	2.723256	-0.405749
C	-0.366885	2.624934	0.693490
C	0.089385	2.960634	1.988343
C	0.097658	4.285866	2.425772
C	-0.346089	5.318309	1.595105
C	-0.802238	5.000915	0.312644
C	-0.813201	3.680095	-0.135412
H	-1.160937	3.437537	-1.137502
H	-1.152490	5.790956	-0.348943
H	-0.338531	6.348439	1.940529
H	0.453066	4.512345	3.429146
H	0.427086	2.157863	2.639112

Table S1 (Continued).



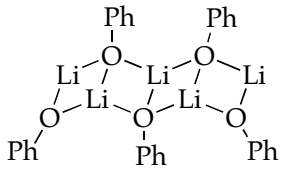


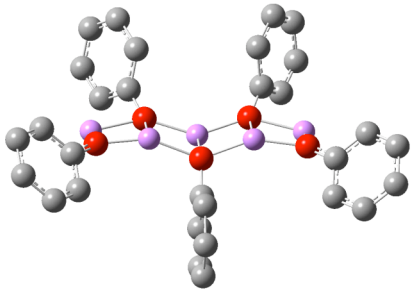
43
G = -1869.485079
(-90 ºC)
see pg S98

Atom	X	Y	Z	Atom	X	Y	Z
Li	-3.018404	1.912134	-0.001678	H	-5.404546	0.701421	2.159293
Li	-0.925925	0.703703	0.000000	C	-7.348199	0.706405	-1.209858
Li	-3.018623	-0.504047	0.000000	H	-5.402949	0.707226	-2.161619
C	-0.853911	-1.837983	0.001841	C	-8.046085	0.705576	-0.001816
C	-0.505715	-2.440833	1.210375	H	-7.898973	0.702410	2.158508
C	-0.504575	-2.443442	-1.205883	H	-7.898096	0.707707	-2.162268
C	0.190762	-3.649711	1.211942	H	-9.145689	0.706214	-0.002259
H	-0.781192	-1.964126	2.162270	O	-1.623579	1.912212	-0.001199
C	0.192150	-3.651792	-1.204238	O	-3.716005	0.703928	-0.000682
H	-0.779172	-1.967900	-2.158643	O	-1.623463	-0.504047	0.000000
C	0.539514	-4.255192	0.004750	C	1.768816	0.704332	1.479852
H	0.464800	-4.125067	2.164876	C	1.771354	0.702866	-1.475220
H	0.467619	-4.129211	-2.155901	C	-0.397071	0.701984	-3.028516
H	1.088603	-5.207888	0.005802	C	-0.402275	0.704990	3.029420
C	-0.853075	3.245600	-0.001281	H	0.374056	0.670780	-3.769656
C	-0.501975	3.848365	-1.209016	H	-1.027799	-0.155928	-3.133717
C	-0.505783	3.850647	1.207239	H	-0.979238	1.590547	-3.156721
C	0.195364	5.056748	-1.208992	H	-0.590764	1.712935	3.335065
H	-0.775840	3.371984	-2.161540	H	-1.324064	0.162365	3.001794
C	0.191804	5.058500	1.207187	H	0.264560	0.240084	3.725187
H	-0.782669	3.375171	2.159370	H	2.209075	-0.184833	1.880421
C	0.542074	5.661817	-0.001005	H	2.209063	1.593901	1.879539
H	0.471692	5.532037	-2.161297	H	2.212301	-0.186696	-1.874149
H	0.465663	5.535594	2.159477	H	2.212288	1.592038	-1.875031
H	1.091842	6.614121	-0.000802	O	0.238743	0.702780	-1.625897
C	-5.256005	0.704184	-0.000934	O	0.235948	0.704395	1.627896
C	-5.953829	0.702361	1.206650	O	-3.568283	-1.456924	-1.536879
C	-5.953374	0.705847	-1.209607	O	-3.568283	-1.455188	1.537954
C	-7.348989	0.703398	1.206322	C	-4.430106	-2.530484	-1.150056

Atom	X	Y	Z
C	-4.450174	-2.513651	1.154777
H	-4.044679	-3.461690	-1.509500
H	-5.417156	-2.367091	-1.529444
H	-4.093605	-3.448198	1.534752
H	-5.439006	-2.320013	1.514799
C	-3.181949	-1.151456	-2.879390
C	-3.164563	-1.161660	2.878010
H	-2.394700	-0.426882	-2.867887
H	-4.022271	-0.756702	-3.411299
H	-2.839800	-2.042216	-3.363518
H	-2.152904	-1.478453	3.023223
H	-3.802259	-1.678960	3.564046
H	-3.236443	-0.107935	3.049462
O	-3.568595	2.865717	1.534573
O	-3.567539	2.862573	-1.540254
C	-4.249413	4.056093	-1.145975
C	-4.247663	4.059876	1.137395
H	-3.726209	4.919339	1.503876
H	-5.251965	4.052572	1.506481
H	-3.730983	4.915825	-1.516099
H	-5.254253	4.044699	-1.513489
C	-3.340934	2.456232	2.885644
C	-3.336755	2.451579	-2.890337
H	-2.323420	2.664759	-3.159793
H	-3.998451	2.982094	-3.542727
H	-3.515710	1.400356	-2.978692
H	-2.753115	1.562189	2.893129
H	-4.279342	2.270118	3.364865
H	-2.819998	3.229991	3.409880

Table S1 (Continued).



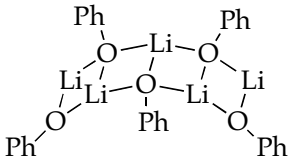


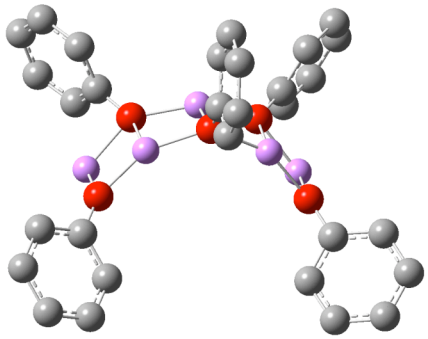
44
G = -1572.075642
(-90 °C)
see pg S99

Atom	X	Y	Z	Atom	X	Y	Z
O	-1.734417	1.530442	0.507754	C	2.312203	2.682878	0.403991
Li	0.016209	1.029169	0.896421	C	3.154090	3.248638	1.389137
O	-0.019135	-0.791315	0.249190	C	3.757589	4.495777	1.186961
Li	-1.780508	-0.347128	-0.274300	C	3.534151	5.203269	0.008054
O	-3.591463	-0.527469	-0.180613	C	2.697806	4.652970	-0.971047
Li	-3.575408	1.037540	0.629129	C	2.098056	3.410325	-0.786176
C	-4.496453	-1.458987	-0.525589	H	1.460575	2.978983	-1.553154
C	-5.527452	-1.161285	-1.439666	H	2.516290	5.197935	-1.894050
C	-6.469533	-2.127991	-1.791953	H	3.998679	6.171992	-0.148940
C	-6.409970	-3.412776	-1.247363	H	4.391120	4.914254	1.964910
C	-5.389174	-3.717916	-0.343407	H	3.276151	2.724430	2.337991
C	-4.443182	-2.758778	0.017112	C	-0.038968	-1.993261	0.890751
H	-3.651197	-2.997012	0.723131	C	-0.055765	-3.195606	0.159972
H	-5.327271	-4.714215	0.088974	C	-0.076722	-4.425528	0.819375
H	-7.144646	-4.163772	-1.524116	C	-0.081093	-4.485680	2.214707
H	-7.254644	-1.873649	-2.500732	C	-0.064317	-3.296683	2.947160
H	-5.565745	-0.164026	-1.873744	C	-0.043411	-2.062487	2.296585
Li	1.761747	-0.408743	-0.257028	H	-0.030205	-1.137845	2.871314
O	1.806375	1.445104	0.588126	H	-0.067492	-3.326492	4.034029
Li	3.631995	0.863249	0.650745	H	-0.097558	-5.444757	2.723983
O	3.564382	-0.667794	-0.219382	H	-0.090230	-5.341723	0.234607
C	4.409227	-1.627459	-0.631461	H	-0.052401	-3.149667	-0.926788
C	5.493678	-1.321340	-1.478466	C	-2.175138	2.774435	0.219844
C	6.372435	-2.318702	-1.901648	C	-2.911462	3.499165	1.184221
C	6.194973	-3.643595	-1.496820	C	-3.448521	4.755391	0.879744
C	5.120549	-3.957147	-0.660432	C	-3.264410	5.313955	-0.383464
C	4.237405	-2.967621	-0.229594	C	-2.534561	4.604222	-1.344371
H	3.404733	-3.213541	0.425212	C	-1.999826	3.351226	-1.056165
H	4.967092	-4.984113	-0.336093	H	-1.445096	2.795615	-1.807884
H	6.880490	-4.418342	-1.828733	H	-2.385663	5.030603	-2.333293
H	7.200651	-2.056493	-2.556468	H	-3.678947	6.289265	-0.619676
H	5.623158	-0.291765	-1.806892	H	-4.001469	5.297957	1.642349

Atom	X	Y	Z
H	-3.007650	3.085916	2.188611

Table S1 (Continued).



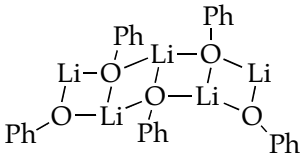


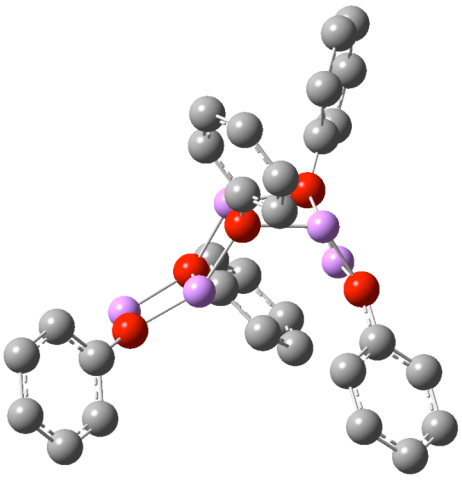
45
G = -1572.077311
(-90 °C)
see pg S99

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000653	1.556974	0.129381	C	0.002425	-1.736321	2.896866
O	-1.771208	1.557245	-0.460087	C	0.003539	-2.041607	4.258947
Li	-1.728224	-0.304600	0.410940	C	0.004042	-1.025535	5.217429
O	0.000738	-0.098846	1.138327	C	0.003402	0.306412	4.797375
Li	1.728544	-0.303623	0.407961	C	0.002302	0.623261	3.438161
O	1.769005	1.557665	-0.463503	H	0.001801	1.662796	3.114883
Li	2.965986	0.557787	-1.528135	H	0.003766	1.108665	5.531332
O	2.943323	-1.021245	-0.749065	H	0.004916	-1.267970	6.276043
C	3.514425	-2.228982	-0.898966	H	0.004030	-3.083329	4.569600
C	4.812491	-2.481059	-0.411404	H	0.002083	-2.527527	2.150388
C	5.400995	-3.735807	-0.569680	O	-2.943657	-1.022711	-0.745062
C	4.717070	-4.768704	-1.215212	Li	-2.968935	0.556873	-1.523176
C	3.430062	-4.528035	-1.702007	C	-3.515032	-2.230153	-0.896316
C	2.832624	-3.276875	-1.549479	C	-4.813142	-2.482483	-0.408996
H	1.830767	-3.088151	-1.928879	C	-5.401949	-3.736902	-0.568788
H	2.882882	-5.321514	-2.206264	C	-4.718305	-4.769164	-1.215621
H	5.178521	-5.744825	-1.335543	C	-3.431242	-4.528247	-1.702158
H	6.403433	-3.906475	-0.183261	C	-2.833493	-3.277425	-1.548118
H	5.342462	-1.677018	0.094643	H	-1.831589	-3.088445	-1.927257
C	2.589404	2.625748	-0.553808	H	-2.884265	-5.321257	-2.207366
C	3.198647	3.195060	0.585104	H	-5.180031	-5.745011	-1.337112
C	4.093315	4.253866	0.451334	H	-6.404423	-3.907824	-0.182573
C	4.416547	4.769193	-0.809704	H	-5.342850	-1.678927	0.098090
C	3.823048	4.216426	-1.942682	C	-2.591285	2.625540	-0.551446
C	2.915341	3.158084	-1.821790	C	-2.915027	3.158410	-1.819757
H	2.400990	2.769737	-2.701882	C	-3.822312	4.216991	-1.941678
H	4.050692	4.614166	-2.928459	C	-4.417597	4.769402	-0.809450
H	5.117935	5.592817	-0.902363	C	-4.096568	4.253497	0.451900
H	4.550595	4.678151	1.341737	C	-3.202303	3.194464	0.586696
H	2.964786	2.782894	1.563711	H	-2.970034	2.781881	1.565500
C	0.001793	-0.395068	2.464451	H	-4.555220	4.677515	1.341724

Atom	X	Y	Z
H	-5.118685	5.593190	-0.902931
H	-4.048273	4.615178	-2.927662
H	-2.399361	2.770271	-2.699120

Table S1 (Continued).



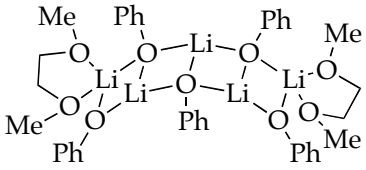


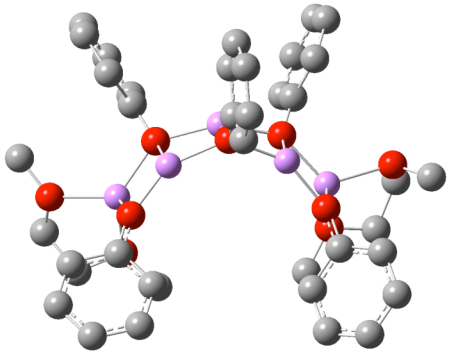
46
G = -1572.082244
(-90 °C)
see pg S99

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000653	1.556974	0.129381	H	4.050692	4.614166	-2.928459
O	-1.771208	1.557245	-0.460087	H	5.117935	5.592817	-0.902363
Li	-1.728224	-0.304600	0.410940	H	4.550595	4.678151	1.341737
O	0.000738	-0.098846	1.138327	H	2.964786	2.782894	1.563711
Li	1.728544	-0.303623	0.407961	C	0.001793	-0.395068	2.464451
O	1.769005	1.557665	-0.463503	C	0.002425	-1.736321	2.896866
Li	2.965986	0.557787	-1.528135	C	0.003539	-2.041607	4.258947
O	2.943323	-1.021245	-0.749065	C	0.004042	-1.025535	5.217429
C	3.514425	-2.228982	-0.898966	C	0.003402	0.306412	4.797375
C	4.812491	-2.481059	-0.411404	C	0.002302	0.623261	3.438161
C	5.400995	-3.735807	-0.569680	H	0.001801	1.662796	3.114883
C	4.717070	-4.768704	-1.215212	H	0.003766	1.108665	5.531332
C	3.430062	-4.528035	-1.702007	H	0.004916	-1.267970	6.276043
C	2.832624	-3.276875	-1.549479	H	0.004030	-3.083329	4.569600
H	1.830767	-3.088151	-1.928879	H	0.002083	-2.527527	2.150388
H	2.882882	-5.321514	-2.206264	O	-2.943657	-1.022711	-0.745062
H	5.178521	-5.744825	-1.335543	Li	-2.968935	0.556873	-1.523176
H	6.403433	-3.906475	-0.183261	C	-3.515032	-2.230153	-0.896316
H	5.342462	-1.677018	0.094643	C	-4.813142	-2.482483	-0.408996
C	2.589404	2.625748	-0.553808	C	-5.401949	-3.736902	-0.568788
C	3.198647	3.195060	0.585104	C	-4.718305	-4.769164	-1.215621
C	4.093315	4.253866	0.451334	C	-3.431242	-4.528247	-1.702158
C	4.416547	4.769193	-0.809704	C	-2.833493	-3.277425	-1.548118
C	3.823048	4.216426	-1.942682	H	-1.831589	-3.088445	-1.927257
C	2.915341	3.158084	-1.821790	H	-2.884265	-5.321257	-2.207366
H	2.400990	2.769737	-2.701882	H	-5.180031	-5.745011	-1.337112

Atom	X	Y	Z
H	-6.404423	-3.907824	-0.182573
H	-5.342850	-1.678927	0.098090
C	-2.591285	2.625540	-0.551446
C	-2.915027	3.158410	-1.819757
C	-3.822312	4.216991	-1.941678
C	-4.417597	4.769402	-0.809450
C	-4.096568	4.253497	0.451900
C	-3.202303	3.194464	0.586696
H	-2.970034	2.781881	1.565500
H	-4.555220	4.677515	1.341724
H	-5.118685	5.593190	-0.902931
H	-4.048273	4.615178	-2.927662
H	-2.399361	2.770271	-2.699120

Table S1 (Continued).



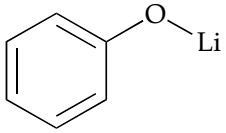


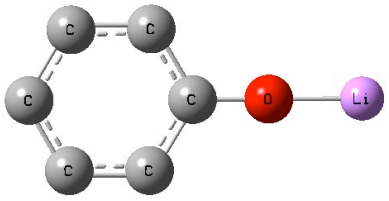
47
G = -2189.595499
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.717624	0.156932	1.276664	H	-1.504990	1.220137	-3.250580
O	-0.006416	-0.215072	1.959710	H	-2.640183	1.229288	-4.628917
Li	-0.014581	-1.494956	0.502300	H	-2.920826	2.307929	-3.218212
O	-1.828911	-1.313270	-0.042993	C	-3.025814	2.643027	0.267815
Li	-1.694479	0.199333	1.219706	C	-2.205739	3.524944	-0.475334
O	-2.771302	1.336953	0.316456	C	-2.483004	4.890512	-0.536020
Li	-3.063249	-0.072391	-0.855424	C	-3.582915	5.427869	0.137527
C	-2.298674	-2.576954	-0.132137	C	-4.397550	4.572174	0.883674
C	-2.190790	-3.300275	-1.339565	C	-4.128731	3.205342	0.951500
C	-2.671065	-4.607639	-1.434296	H	-4.758274	2.546334	1.544830
C	-3.268613	-5.229313	-0.335354	H	-5.251821	4.973520	1.425345
C	-3.378518	-4.523054	0.865343	H	-3.794714	6.492378	0.090600
C	-2.902562	-3.215825	0.971236	H	-1.827662	5.542190	-1.110696
H	-2.997417	-2.666869	1.905566	H	-1.337693	3.112708	-0.985687
H	-3.840560	-4.992048	1.731036	C	-0.043818	-0.253727	3.313033
H	-3.638806	-6.247695	-0.411622	C	-0.110846	0.938857	4.062754
H	-2.572626	-5.144729	-2.375224	C	-0.151463	0.899755	5.457383
H	-1.719201	-2.816917	-2.192355	C	-0.125921	-0.319978	6.137946
O	-5.033959	-0.660654	-1.002790	C	-0.058153	-1.506089	5.403127
C	-5.998950	0.162524	-0.344269	C	-0.017230	-1.479711	4.008529
H	-5.700032	0.209105	0.702993	H	0.036505	-2.405955	3.440036
H	-6.016052	1.180944	-0.750831	H	-0.036315	-2.464159	5.917385
H	-6.996678	-0.288077	-0.425471	H	-0.156930	-0.345857	7.223448
C	-5.273979	-0.871585	-2.393570	H	-0.201910	1.832765	6.013561
H	-4.800207	-1.827735	-2.635676	H	-0.126222	1.888610	3.532779
H	-6.350602	-0.948136	-2.597327	O	1.804077	-1.348756	-0.022453
O	-3.264965	0.276159	-2.885914	Li	2.978046	-0.072520	-0.902399
C	-4.650038	0.239117	-3.224121	O	2.848561	1.248245	0.405153
H	-5.112702	1.213463	-3.006193	C	3.341021	2.483872	0.427873
H	-4.776871	0.029252	-4.296978	C	2.493475	3.615068	0.495719
C	-2.552417	1.325266	-3.538392	C	3.018804	4.907222	0.499484

Atom	X	Y	Z
C	4.398208	5.121998	0.433045
C	5.248568	4.014699	0.369532
C	4.735472	2.717702	0.366527
H	5.399339	1.856476	0.336592
H	6.326395	4.160826	0.328441
H	4.802063	6.130655	0.438660
H	2.340022	5.755805	0.557393
H	1.418387	3.455105	0.549297
C	2.335859	-2.588378	-0.003895
C	3.065412	-3.058241	1.110130
C	3.612461	-4.342564	1.115886
C	3.451650	-5.192868	0.018830
C	2.729125	-4.740031	-1.088414
C	2.178414	-3.457873	-1.105199
H	1.615254	-3.104926	-1.966094
H	2.587848	-5.391323	-1.948104
H	3.875617	-6.192875	0.029553
H	4.167614	-4.679792	1.988271
H	3.194241	-2.400996	1.967721
O	2.726881	0.771765	-2.770275
C	4.053679	1.062306	-3.207675
H	4.050187	1.381516	-4.260665
H	4.479359	1.867922	-2.592516
C	1.854693	1.899929	-2.854003
H	1.745625	2.220290	-3.899333
H	0.886875	1.574742	-2.467286
H	2.225858	2.731229	-2.243370
O	4.783906	-0.620255	-1.700998
C	4.867424	-0.206810	-3.060132
H	5.913489	-0.010120	-3.338440
H	4.473643	-0.997933	-3.716181
C	5.548276	-1.792077	-1.419559
H	6.615084	-1.602542	-1.599300
H	5.385438	-2.034580	-0.369411
H	5.212887	-2.635187	-2.036492

Table S1 (Continued).

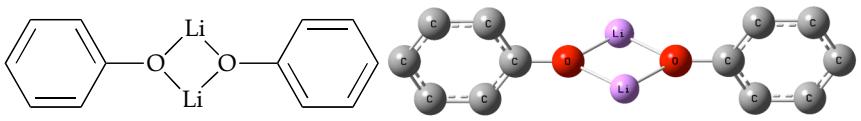




S2
G = -314.360982
(-90 ºC)
see pg S96

Atom	X	Y	Z	Atom	X	Y	Z
C	0.000137	-2.038685	0.000000	H	2.145002	0.619400	0.000000
C	-1.202935	-1.327374	0.000000	O	-0.000245	2.121447	0.000000
C	-1.208485	0.065889	0.000000	Li	-0.000416	3.743306	0.000000
C	0.000000	0.796987	0.000000	H	-2.145198	0.618957	0.000000
C	1.208602	0.065971	0.000000	H	-2.149816	-1.864023	0.000000
C	1.203173	-1.327236	0.000000	H	0.000151	-3.125338	0.000000
H	2.150113	-1.863799	0.000000				

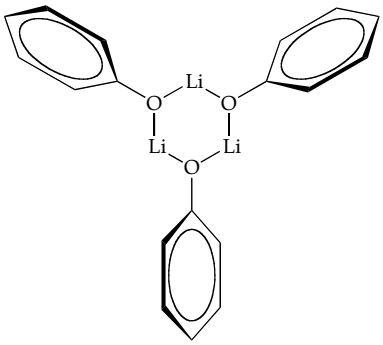
Table S1 (Continued).

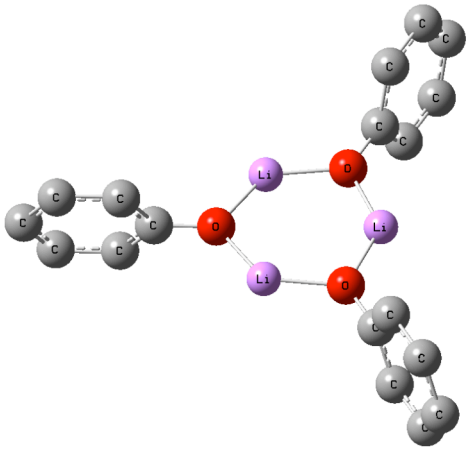


S3
G = -628.804731
(-90 ºC)
see pg S96

Atom	X	Y	Z	Atom	X	Y	Z
C	2.713146	0.000509	0.000435	C	4.833768	1.201606	-0.003630
C	3.435852	1.209164	0.002346	C	3.439119	1.209620	-0.001352
C	4.830537	1.204857	0.003476	H	2.887009	2.146919	-0.001753
C	5.540441	0.001723	0.001880	H	5.372221	2.146784	-0.005970
C	4.832447	1.202517	0.000898	H	6.626783	0.005519	-0.004626
C	3.437751	1.209021	0.002053	H	5.364091	2.152981	0.000871
H	2.884704	2.145773	0.004202	H	2.878994	2.143860	0.004929
H	5.369848	2.148295	0.002191	Li	0.000978	0.000689	1.169437
H	6.626779	0.002594	0.002781	C	2.713147	0.001881	0.001741
H	5.366470	2.151466	0.005659	C	3.434511	1.208559	0.002524
H	2.881265	2.145007	0.003576	C	4.829227	1.205765	0.000225
O	1.369205	0.001554	0.001536	C	5.540448	0.003442	-0.002857
Li	0.000795	0.004256	-1.164322	C	4.833768	1.201606	-0.003630
O	1.369236	0.004566	0.003817	C	3.439119	1.209620	-0.001352
Li	0.000978	0.000689	1.169437	H	2.887009	2.146919	-0.001753
C	2.713147	0.001881	0.001741	H	5.372221	2.146784	-0.005970
C	3.434511	1.208559	0.002524	H	6.626783	0.005519	-0.004626
C	4.829227	1.205765	0.000225	H	5.364091	2.152981	0.000871
C	5.540448	0.003442	-0.002857	H	2.878994	2.143860	0.004929

Table S1 (Continued).



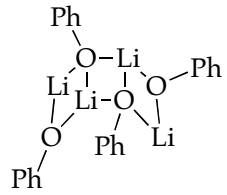


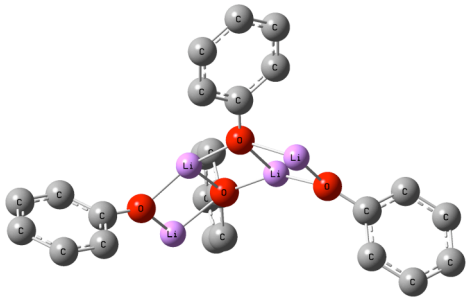
S4
G = -943.237654
(-90 ºC)
see pg S96

Atom	X	Y	Z
C	2.069417	-2.495842	0.017862
C	2.418869	-3.169197	-1.169423
C	3.310709	-4.241647	-1.141474
C	3.875780	-4.667942	0.062716
C	3.535784	-4.005369	1.244339
C	2.643711	-2.932657	1.228016
H	2.372608	-2.419180	2.148011
H	3.966417	-4.325587	2.190274
H	4.570300	-5.502921	0.079868
H	3.566246	-4.746298	-2.070351
H	1.982065	-2.831663	-2.106865
O	1.205011	-1.456935	-0.004029
Li	1.654226	0.280478	-0.026645
O	0.655702	1.772306	-0.050969
Li	-1.074472	1.293896	-0.045560
O	-1.865682	-0.316009	-0.020829
Li	-0.585361	-1.573845	-0.001484
C	-3.198099	-0.543881	-0.012336
C	-3.909870	-0.620892	1.201018
C	-5.285232	-0.855515	1.203589

Atom	X	Y	Z
C	-5.983235	-1.018257	0.004698
C	-5.285275	-0.943464	-1.202888
C	-3.909988	-0.709375	-1.216986
H	-3.364301	-0.649606	-2.156194
H	-5.814197	-1.067955	-2.144993
H	-7.054020	-1.200472	0.011295
H	-5.814110	-0.911327	2.152234
H	-3.364252	-0.494477	2.133645
C	1.126315	3.039005	-0.034540
C	1.607624	3.644876	-1.211907
C	2.093883	4.952305	-1.190335
C	2.111889	5.686874	-0.002368
C	1.635945	5.094367	1.169513
C	1.149073	3.786855	1.159490
H	0.787238	3.320343	2.073368
H	1.644480	5.652400	2.102956
H	2.490830	6.704747	0.009974
H	2.459522	5.399845	-2.111623
H	1.583949	3.074199	-2.137805

Table S1 (Continued).



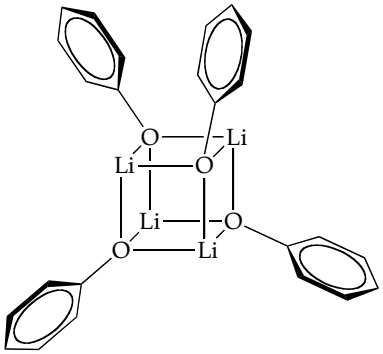


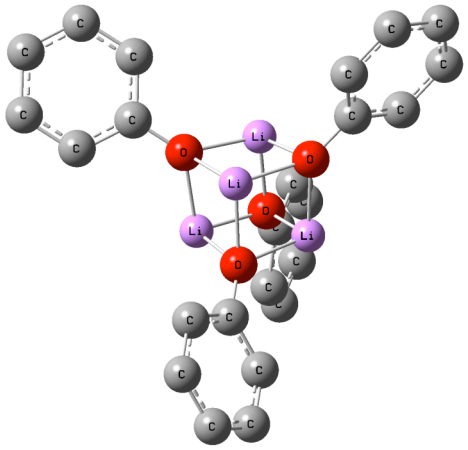
S5
G = -1257.654764
(-90 ºC)
see pg S96

Atom	X	Y	Z
Li	1.235419	-0.039225	-0.341376
O	-0.021377	-1.419237	-0.488498
C	0.208946	-2.594839	-1.114897
C	1.401766	-3.319474	-0.899971
C	1.594450	-4.557802	-1.507304
C	0.608020	-5.117535	-2.327957
C	-0.576934	-4.415749	-2.541693
C	-0.780274	-3.165833	-1.946691
H	-1.686388	-2.597738	-2.154629
H	-1.349369	-4.830658	-3.184374
H	0.766359	-6.085341	-2.794221
H	2.522762	-5.095878	-1.332313
H	2.161704	-2.898341	-0.245224
Li	-1.332043	0.118995	-0.350148
Li	-1.502374	-2.184017	0.399579
O	-2.636224	-0.834169	0.504556
C	-3.825872	-0.546433	1.057318
C	-3.956027	-0.376784	2.450838
C	-5.194405	-0.081762	3.020767
C	-6.333013	0.052932	2.222951
C	-6.214293	-0.112441	0.840801
C	-4.980947	-0.409088	0.261316
H	-4.890011	-0.546427	-0.813983
H	-7.091113	-0.012074	0.204867
H	-7.295857	0.283202	2.670239
H	-5.268231	0.045096	4.098675

Atom	X	Y	Z
H	-3.067206	-0.474040	3.070992
O	-0.062453	1.485038	-0.415535
Li	1.338291	2.189915	0.646873
O	2.489934	0.852677	0.649136
C	3.683347	0.512329	1.162390
C	3.781563	-0.078604	2.438735
C	5.023128	-0.434157	2.965805
C	6.196387	-0.211906	2.241025
C	6.109579	0.374401	0.975883
C	4.873203	0.734005	0.439630
H	4.804623	1.194209	-0.543590
H	7.013441	0.555890	0.398438
H	7.161492	-0.490205	2.654919
H	5.072478	-0.888718	3.952925
H	2.867167	-0.251154	3.002366
C	-0.168689	2.669639	-1.055564
C	0.041364	2.786416	-2.445797
C	-0.003346	4.034105	-3.062698
C	-0.247794	5.196088	-2.320961
C	-0.461020	5.094418	-0.947769
C	-0.427178	3.845801	-0.316650
H	-0.665434	3.757635	0.744227
H	-0.671481	5.983897	-0.359449
H	-0.277871	6.163945	-2.812117
H	0.159960	4.102286	-4.135376
H	0.244275	1.886569	-3.021449

Table S1 (Continued).

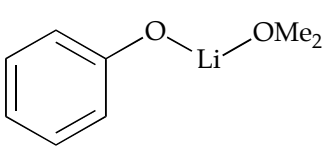


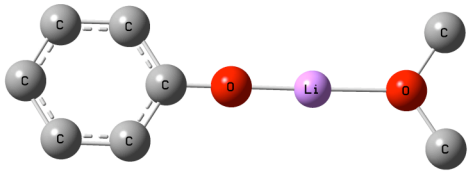


S6
G = -1257.674112
(-90 ºC)
see pg S96

Atom	X	Y	Z	Atom	X	Y	Z
O	0.088214	1.491101	0.770560	H	-2.932011	-2.447042	-1.217086
Li	1.373229	0.127329	0.440394	H	-5.206008	-2.678587	-2.168751
O	0.290501	-1.362177	0.924284	H	-6.530747	-0.656534	-2.773193
Li	-0.167909	-1.334068	-0.943993	C	0.503313	-2.464637	1.674106
O	-1.679740	-0.164416	-0.786702	C	-0.571169	-3.151924	2.272697
Li	-1.073143	-0.016324	1.022406	C	-0.347450	-4.288065	3.050956
Li	-0.355293	1.188570	-1.078662	C	0.947491	-4.771203	3.250084
O	1.064461	-0.001989	-1.482919	C	2.019267	-4.101561	2.655221
C	2.258902	0.100391	-2.100888	C	1.804701	-2.965488	1.875281
C	2.932860	1.338141	-2.168333	H	2.643978	-2.452584	1.408175
C	4.180110	1.439285	-2.786900	H	3.033921	-4.466144	2.796801
C	4.787537	0.316411	-3.351814	H	1.118906	-5.655377	3.857016
C	4.128662	-0.914370	-3.289506	H	-1.194465	-4.798720	3.502908
C	2.882895	-1.026066	-2.673554	H	-1.584547	-2.785411	2.115070
H	2.373222	-1.986780	-2.630922	C	0.066606	2.640296	1.478916
H	4.587197	-1.798339	-3.726086	C	-1.142615	3.333342	1.691212
H	5.757210	0.398347	-3.833967	C	-1.166527	4.517817	2.428387
H	4.676384	2.405926	-2.828426	C	0.008479	5.043328	2.969561
H	2.460533	2.219383	-1.736879	C	1.212249	4.365877	2.761742
C	-2.926194	-0.290606	-1.288671	C	1.245494	3.181363	2.026640
C	-3.691394	0.843813	-1.624372	H	2.188085	2.660338	1.866722
C	-4.974345	0.709010	-2.155018	H	2.136882	4.761587	3.175146
C	-5.531860	-0.555019	-2.359210	H	-0.013040	5.965288	3.543138
C	-4.786203	-1.686358	-2.021308	H	-2.112666	5.032484	2.578330
C	-3.502449	-1.560402	-1.490364	H	-2.061033	2.930714	1.266382

Table S1 (Continued).

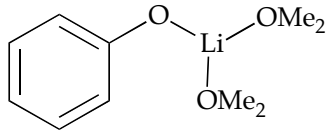


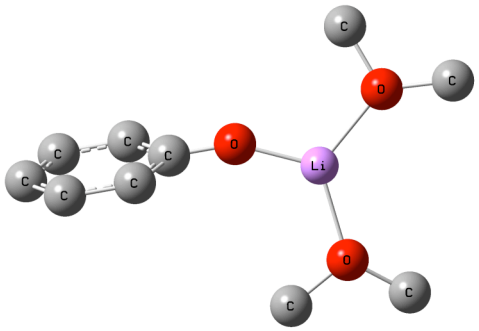


S7
G = -469.347775
(-90 ºC)
see pg S97

Atom	X	Y	Z	Atom	X	Y	Z
C	4.351507	1.196603	0.095597	H	-3.958030	-2.143218	0.089626
O	3.581022	-0.002253	-0.011255	H	-5.213485	0.009985	0.012596
Li	1.682009	-0.018204	-0.018163	H	-3.942248	2.153322	-0.076413
O	0.034879	-0.010253	-0.011751	H	-1.460458	2.139462	-0.087722
C	-1.283336	-0.005237	-0.005636	C	4.382918	-1.183275	-0.077852
C	-2.016337	1.204860	-0.048709	H	4.989554	-1.286687	0.830461
C	-3.409160	1.204585	-0.042190	H	5.039041	-1.151696	-0.956570
C	-4.126696	0.005752	0.007524	H	3.702280	-2.033281	-0.160858
C	-3.418014	-1.198595	0.050464	H	3.648636	2.031199	0.141252
C	-2.025180	-1.209604	0.044275	H	5.002007	1.313101	-0.780189
H	-1.476238	-2.148465	0.078162	H	4.961492	1.180414	1.007354

Table S1 (Continued).

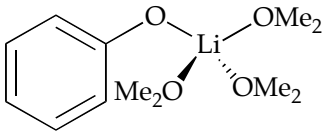


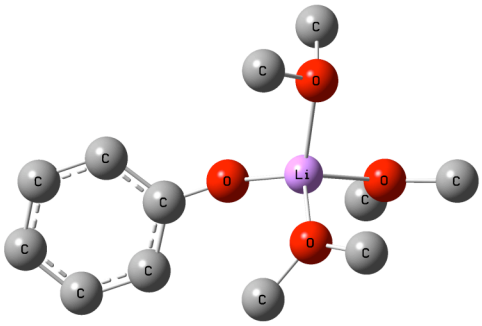


S8
G = -624.322348
(-90 ºC)
see pg S97

Atom	X	Y	Z
C	-2.036714	-2.716516	0.056135
O	-2.676744	-1.432393	0.069995
Li	-1.358918	-0.006364	0.012776
O	-1.786714	1.886260	-0.067205
C	-0.622547	2.719530	0.008805
H	-0.451744	3.220631	-0.952857
H	0.219672	2.066349	0.239726
H	-0.749083	3.473430	0.796912
C	-2.962748	2.605313	-0.406501
H	-3.786167	1.888363	-0.450502
H	-2.855008	3.093268	-1.385072
H	-3.187074	3.368289	0.351498
O	0.269833	-0.539376	0.038572
C	1.576679	-0.395502	0.027430
C	2.351632	-0.728124	-1.114208
C	3.734658	-0.568621	-1.122235
C	4.409985	-0.074351	-0.000962
C	3.666214	0.256348	1.135141
C	2.281291	0.100494	1.155595
H	1.708430	0.343988	2.048870
H	4.172032	0.638288	2.020739
H	5.489873	0.047348	-0.012530
H	4.295899	-0.834035	-2.016946
H	1.830926	-1.115667	-1.987612
C	-4.081578	-1.508358	0.249068
H	-4.469594	-0.486729	0.254437
H	-4.329723	-1.993390	1.203382
H	-4.551597	-2.070038	-0.570114
H	-0.968341	-2.516965	-0.047677
H	-2.407908	-3.313645	-0.787324
H	-2.236074	-3.247600	0.996253

Table S1 (Continued).

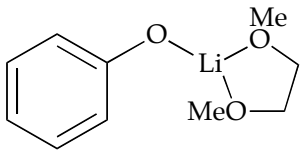


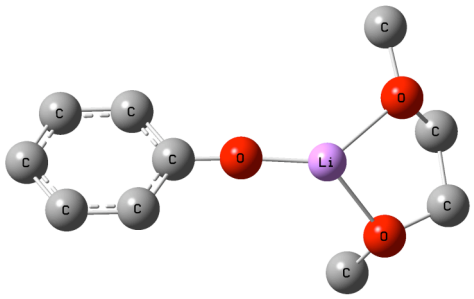


S9
G = -779.286249
(-90 ºC)
see pg S97

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.055463	0.045891	-0.020149	H	4.001234	-1.097933	-2.353457
O	-0.604407	0.053448	-0.603313	H	4.044316	-0.757084	-0.600365
C	-1.902492	0.002595	-0.422181	O	1.300760	-0.640954	1.853878
C	-2.590512	-1.234802	-0.284417	C	2.504820	-0.835568	2.576737
C	-3.968877	-1.286000	-0.086393	H	2.401185	-0.487008	3.614393
C	-4.730399	-0.115781	-0.019546	H	2.794198	-1.896514	2.588066
C	-4.077114	1.113482	-0.159581	H	3.281695	-0.250848	2.078174
C	-2.700492	1.177337	-0.357438	C	0.186039	-1.328181	2.424850
H	-2.203715	2.138503	-0.478482	H	-0.011171	-0.958067	3.440470
H	-4.651735	2.037738	-0.116287	H	-0.671633	-1.132073	1.780823
H	-5.805311	-0.159584	0.134334	H	0.381340	-2.409052	2.467839
H	-4.456565	-2.254810	0.013601	O	1.937402	1.875556	0.056900
H	-2.006823	-2.151703	-0.351012	C	1.907951	2.459843	-1.245415
O	2.174005	-0.968342	-1.364326	H	2.414000	3.435167	-1.240411
C	1.396254	-1.635970	-2.361633	H	2.435403	1.774559	-1.911106
H	1.462858	-2.725682	-2.233907	H	0.872940	2.576821	-1.590573
H	0.370163	-1.296617	-2.209778	C	1.266138	2.688759	1.018782
H	1.753845	-1.368739	-3.365993	H	0.212497	2.825331	0.743408
C	3.542266	-1.332697	-1.381935	H	1.323868	2.163211	1.973364
H	3.669754	-2.406840	-1.182859	H	1.757696	3.667774	1.104111

Table S1 (Continued).



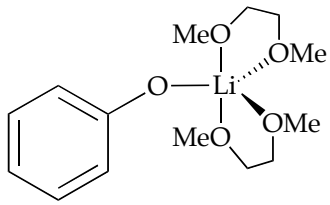


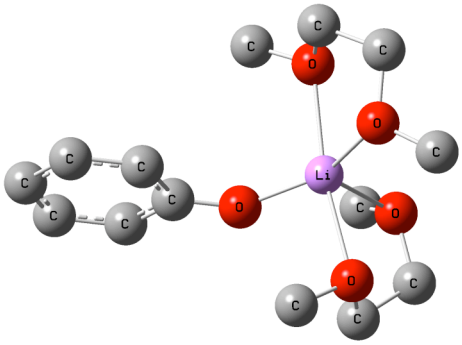
S10
G = -623.133974
(-90 ºC)
see pg S97

Atom	X	Y	Z
C	-3.538729	0.507852	0.383835
O	-2.663246	1.162153	-0.534217
Li	-1.092465	-0.058173	-0.788494
O	0.541695	0.057311	-0.444543
C	1.838410	0.059337	-0.227766
C	2.444620	1.007805	0.634262
C	3.817852	1.001612	0.866947
C	4.646547	0.056455	0.254761
C	4.067618	-0.886636	-0.600283
C	2.695801	-0.889624	-0.840097
H	2.249965	-1.623500	-1.508838
H	4.695041	-1.630723	-1.088724
H	5.717732	0.055306	0.438646
H	4.248264	1.745586	1.535748
H	1.804099	1.746407	1.112607

Atom	X	Y	Z
O	-2.332468	-1.509627	-0.206336
C	-3.637752	-0.942627	-0.068236
H	-4.100364	-0.990710	-1.059067
H	-4.248648	-1.526950	0.631330
C	-1.835643	-2.190672	0.954448
H	-1.890027	-1.555483	1.847537
H	-0.790009	-2.422685	0.749546
H	-2.406058	-3.112520	1.120955
C	-2.433826	2.539636	-0.228580
H	-2.003635	2.648813	0.775072
H	-1.724408	2.912887	-0.968394
H	-3.371215	3.106588	-0.293558
H	-4.531770	0.980749	0.375022
H	-3.128804	0.583221	1.402634

Table S1 (Continued).

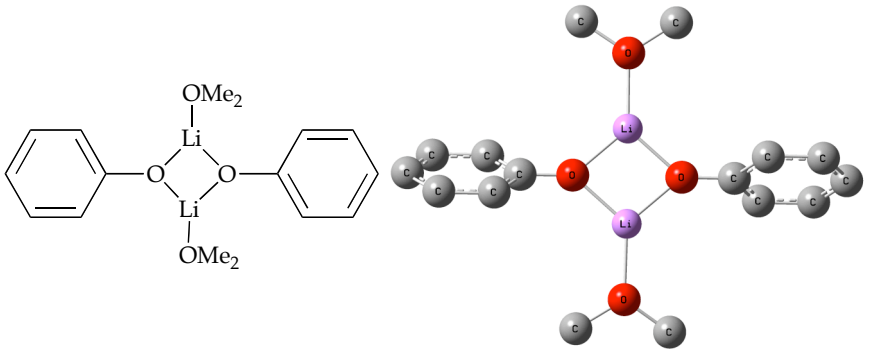




S11
G = -931.878286
(-90 ºC)
see pg S97

Atom	X	Y	Z
Li	-0.893184	0.064374	0.090176
O	0.784302	-0.592885	0.242668
C	2.050183	-0.376311	-0.011097
C	2.478565	0.516874	-1.034935
C	3.829651	0.743682	-1.292098
C	4.822013	0.097386	-0.549841
C	4.427405	-0.788092	0.459750
C	3.081851	-1.022169	0.726691
H	2.786378	-1.714876	1.512669
H	5.183820	-1.304047	1.049669
H	5.874467	0.275473	-0.753677
H	4.111465	1.434039	-2.086257
H	1.713839	1.018705	-1.627525
O	-0.618005	2.006240	1.126157
C	-0.893252	2.991687	0.145150
C	-2.226272	2.652466	-0.485378
O	-2.131860	1.342757	-1.034034
C	-3.342845	0.910007	-1.645271
H	-3.179800	-0.118636	-1.964818
H	-4.175153	0.945033	-0.927645
H	-3.588285	1.543486	-2.509240
H	-3.025359	2.681971	0.270803
H	-2.465017	3.382483	-1.273795
H	-0.944364	3.995166	0.597266
H	-0.099419	2.997474	-0.617693
C	0.643332	2.210101	1.766774
H	0.786356	1.380583	2.458550
H	0.637916	3.161601	2.317804
H	1.459581	2.201154	1.035774
O	-1.540155	-1.710317	-1.233024
C	-1.491976	-2.702284	-0.211583
C	-2.457906	-2.268362	0.877564
O	-2.070762	-1.032402	1.485877
C	-1.233854	-1.185704	2.639207
H	-0.237438	-1.539679	2.355925
H	-1.704711	-1.866599	3.361198
H	-1.147291	-0.193162	3.085696
H	-2.549223	-3.053955	1.640227
H	-3.447166	-2.097012	0.439796
H	-0.467495	-2.775223	0.175051
H	-1.801229	-3.681621	-0.613074
C	-0.583592	-1.945954	-2.266183
H	0.431546	-1.896839	-1.860662
H	-0.762933	-2.920878	-2.742548
H	-0.718913	-1.154868	-3.007682

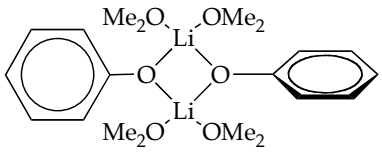
Table S1 (Continued).

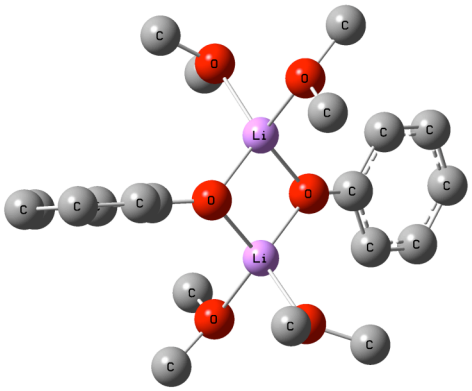


S12
G = -938.765067
(-90 ºC)
see pg S97

Atom	X	Y	Z	Atom	X	Y	Z
C	1.135185	-3.906757	-0.162174	C	-1.166091	3.899007	-0.141923
O	-0.034913	-3.110241	0.012836	H	-2.005121	3.203186	-0.207688
Li	0.000189	-1.199756	0.099909	H	-1.273664	4.524158	0.754643
O	1.383594	-0.004592	0.061397	H	-1.148361	4.541469	-1.032529
Li	0.013563	1.206414	0.007050	C	2.712800	-0.013818	0.043961
O	-1.371116	0.011779	0.061393	C	3.429504	-0.528898	-1.062014
C	-2.699614	0.013209	0.044743	C	4.823934	-0.537121	-1.074503
C	-3.420241	0.517418	-1.064125	C	5.553102	-0.034714	0.006633
C	-4.814619	0.518090	-1.075686	C	4.859464	0.478813	1.105994
C	-5.540504	0.017327	0.008488	C	3.465356	0.491532	1.129934
C	-4.843327	-0.485809	1.110423	H	2.927030	0.875461	1.994168
C	-3.449141	-0.489555	1.134143	H	5.410239	0.870934	1.958807
H	-2.908756	-0.863671	2.001469	H	6.639439	-0.042871	-0.007292
H	-5.391312	-0.876269	1.965789	H	5.346518	-0.936881	-1.941456
H	-6.626861	0.019046	-0.005019	H	2.863437	-0.903610	-1.912546
H	-5.339793	0.909890	-1.944698	C	-1.247650	-3.859604	-0.013504
H	-2.857132	0.889632	-1.917871	H	-2.067020	-3.152479	0.130924
O	0.024175	3.117148	-0.066705	H	-1.364158	-4.367520	-0.980183
C	1.217398	3.893866	0.010779	H	-1.256694	-4.605665	0.792461
H	1.198285	4.540600	0.898194	H	1.094539	-4.443273	-1.119926
H	2.052757	3.194309	0.084626	H	1.990871	-3.228446	-0.158625
H	1.332806	4.514053	-0.888140	H	1.234426	-4.632695	0.655641

Table S1 (Continued).



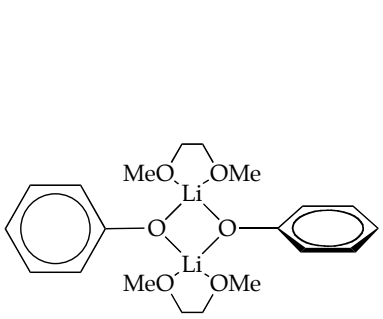


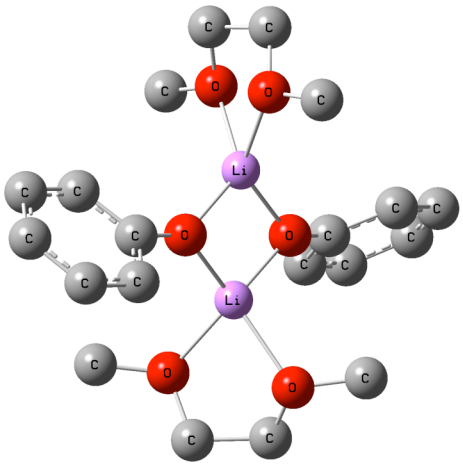
S13
G = -1248.688008
(-90 ºC)
see pg S97

Atom	X	Y	Z	Atom	X	Y	Z
C	0.712005	2.348694	-2.488717	H	0.711332	-3.014334	-3.168872
O	0.052675	2.673072	-1.268433	H	1.172849	-1.459897	-2.408000
Li	0.080046	1.282401	0.199056	C	-1.175158	-3.502813	-1.353063
O	1.421497	-0.029965	0.050047	H	-2.058337	-3.016962	-1.788696
Li	0.006549	-1.249657	0.220751	H	-1.393482	-3.806125	-0.327580
O	-1.353603	0.055344	0.364053	H	-0.911815	-4.389085	-1.947608
C	-2.626378	0.067943	0.003651	C	2.725180	-0.084700	-0.154282
C	-3.667535	0.202271	0.957272	C	3.538030	1.077545	-0.107292
C	-5.007994	0.209199	0.573851	C	4.912328	1.014122	-0.329757
C	-5.372992	0.084694	-0.769537	C	5.541185	-0.202736	-0.608522
C	-4.363633	-0.046098	-1.727643	C	4.759828	-1.360451	-0.661316
C	-3.019803	-0.054988	-1.355091	C	3.384528	-1.308647	-0.441680
H	-2.238138	-0.154703	-2.105933	H	2.786054	-2.216461	-0.494713
H	-4.625560	-0.141738	-2.780087	H	5.227381	-2.319297	-0.878787
H	-6.418970	0.091086	-1.063174	H	6.612979	-0.247500	-0.780547
H	-5.778351	0.315458	1.335566	H	5.501093	1.928702	-0.282643
H	-3.393900	0.307998	2.005004	H	3.061761	2.030462	0.115601
O	-0.072037	-2.505366	1.810642	C	-1.196404	3.330441	-1.472101
C	1.121202	-2.981043	2.422053	H	-1.598612	3.560241	-0.483706
H	0.987253	-4.008607	2.789198	H	-1.052142	4.261788	-2.037571
H	1.905711	-2.958445	1.664219	H	-1.900699	2.679027	-2.005217
H	1.414120	-2.334713	3.261281	H	0.926785	3.261255	-3.062503
C	-1.161479	-2.412678	2.720594	H	1.646053	1.850213	-2.224534
H	-2.001669	-1.983043	2.173955	H	0.093768	1.677842	-3.101827
H	-1.429130	-3.406676	3.106869	O	0.066508	2.559243	1.772124
H	-0.908223	-1.758090	3.566967	C	-0.312044	1.952116	3.002671
O	-0.077860	-2.598371	-1.289081	H	-1.000288	1.146099	2.744934
C	0.354783	-2.162190	-2.573127	H	-0.809377	2.681847	3.657407
H	-0.461989	-1.663872	-3.114447	H	0.566005	1.541427	3.521714

Atom	X	Y	Z
C	1.022167	3.597698	1.935839
H	1.234758	3.992728	0.940736
H	0.619767	4.399727	2.571109
H	1.948883	3.213478	2.384846

Table S1 (Continued).





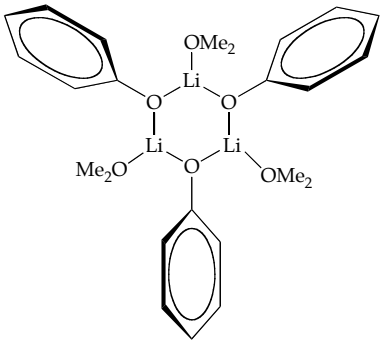
S14
G = -1246.326605
(-90 ºC)
see pg S98

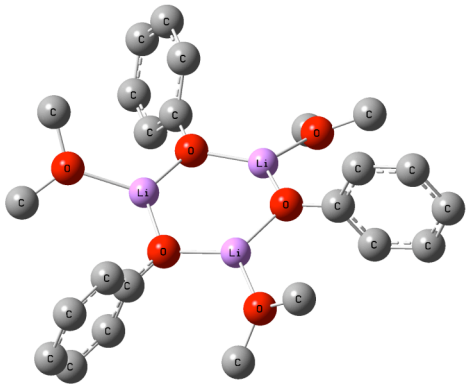
Atom	X	Y	Z
Li	0.006243	-1.242034	0.194769
O	-0.262288	-2.783350	-1.143046
C	-0.129667	-4.032806	-0.476716
C	0.958394	-3.876735	0.565856
O	0.559213	-2.824066	1.437518
C	1.527798	-2.529811	2.444334
H	1.691905	-3.407399	3.084648
H	2.475831	-2.211072	1.994986
H	1.121019	-1.712136	3.040748
H	1.081136	-4.817086	1.124034
H	1.916455	-3.623484	0.087685
H	-1.081155	-4.303172	0.005572
H	0.139627	-4.827141	-1.189106
C	-1.369904	-2.730126	-2.040891
H	-2.310890	-2.922542	-1.510224
H	-1.243334	-3.460461	-2.851697
H	-1.394061	-1.719623	-2.449207
O	-1.386718	-0.017096	0.095462
C	-2.707322	-0.069493	0.039121
C	-3.442153	0.698609	-0.898713
C	-4.833711	0.636182	-0.970658
C	-5.522171	-0.201612	-0.102014
C	-4.848128	-0.974539	0.835511
C	-3.456459	-0.906630	0.904173
H	-2.918577	-1.496391	1.643382
H	-5.414625	-1.617105	1.503745
H	-6.880171	-0.266530	-0.171263

Atom	X	Y	Z
H	-5.388604	1.226842	-1.694250
H	-2.890605	1.342308	-1.580848
Li	-0.047593	1.281600	0.159552
O	1.347151	0.055556	0.281737
C	2.653889	0.063483	0.074390
C	3.231027	-0.577159	-1.052134
C	4.609246	-0.577073	-1.270129
C	5.441203	0.065586	-0.361813
C	4.924282	0.706302	0.757724
C	3.545909	0.702397	0.972122
H	3.128871	1.193607	1.848233
H	5.601239	1.198997	1.450035
H	6.786120	0.067497	-0.571768
H	5.043215	-1.067569	-2.137039
H	2.567029	-1.069735	-1.759373
O	0.427216	2.817139	-1.127871
C	-0.286189	3.988018	-0.754605
C	-0.175008	4.111929	0.753115
O	-0.637810	2.888982	1.309303
C	-0.636040	2.860444	2.731002
H	-1.298141	3.637954	3.135663
H	-1.009969	1.877803	3.022934
H	0.378739	3.004807	3.127919
H	-0.786997	4.955372	1.106268
H	0.870984	4.288337	1.046632
H	-1.340758	3.901200	-1.057672
H	0.146567	4.877840	-1.235666

Atom	X	Y	Z
C	0.501494	2.598224	-2.531819
H	-0.500551	2.474648	-2.966333
H	1.081158	1.684394	-2.671067
H	1.011951	3.434960	-3.027632

Table S1 (Continued).



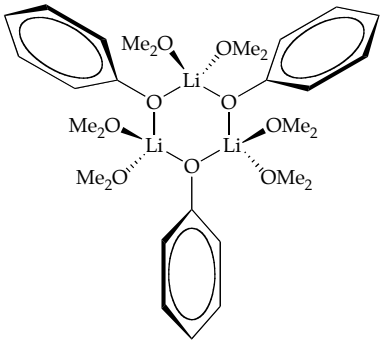


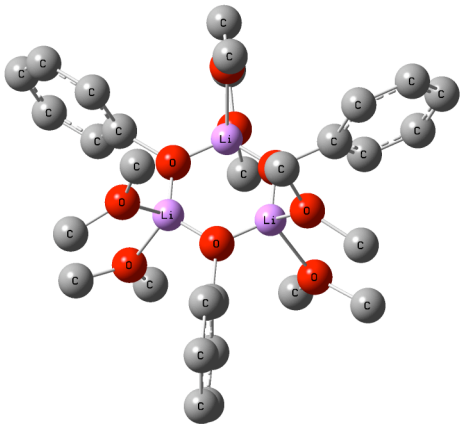
S15
G = -1408.154899
(-90 ºC)
see pg S98

Atom	X	Y	Z
C	-3.757886	2.899576	-0.248735
O	-3.295118	1.621730	-0.679487
Li	-1.597124	0.783585	-0.124085
O	-0.123660	1.853349	0.151508
Li	1.491670	0.990841	-0.035007
O	1.670435	-0.837822	-0.154004
Li	0.113257	-1.774394	0.145378
O	-1.576152	-1.053595	0.001706
C	-2.684602	-1.794954	-0.031971
C	-3.635229	-1.743322	1.014932
C	-4.795247	-2.517211	0.973023
C	-5.049835	-3.369309	-0.105110
C	-4.119691	-3.433594	-1.146570
C	-2.957842	-2.662084	-1.116513
H	-2.238629	-2.708594	-1.931765
H	-4.300856	-4.090116	-1.995314
H	-5.954009	-3.970928	-0.133050
H	-5.506671	-2.454689	1.794162
H	-3.436717	-1.084661	1.858040
O	0.221930	-3.639802	0.784373
C	-0.685245	-4.150060	1.758686
H	-1.131243	-5.091988	1.413341
H	-0.166470	-4.322657	2.712230
H	-1.475735	-3.410160	1.889374
C	1.268920	-4.558252	0.478796
H	0.850945	-5.489184	0.071403
H	1.857564	-4.787674	1.377029
H	1.915494	-4.084462	-0.260539
C	2.860842	-1.434569	-0.235834
C	3.692968	-1.581188	0.899038
C	4.937155	-2.203610	0.802716
C	5.397075	-2.703090	-0.419689
C	4.586517	-2.568346	-1.549901
C	3.339808	-1.945737	-1.465677
H	2.710186	-1.837712	-2.346451
H	4.926996	-2.950652	-2.510167
H	6.366795	-3.187900	-0.489252
H	5.553951	-2.301290	1.693963
H	3.334322	-1.197656	1.851818
O	3.126129	2.092249	-0.112473
C	3.326772	3.262421	0.677031
H	2.399615	3.456756	1.217579
H	4.152472	3.108177	1.385712
H	3.554198	4.125176	0.037185
C	4.265193	1.765849	-0.905311
H	4.036872	0.845859	-1.444671
H	5.143814	1.596530	-0.269275
H	4.480200	2.576388	-1.615530
C	-0.219435	3.180316	0.253462
C	-0.119169	4.017888	-0.882580
C	-0.219442	5.403777	-0.765333
C	-0.424075	6.005775	0.480120
C	-0.526618	5.192938	1.612006
C	-0.426246	3.804343	1.506931
H	-0.503954	3.171911	2.388896
H	-0.685881	5.642780	2.590016
H	-0.502153	7.085938	0.566091
H	-0.138367	6.020709	-1.658134

Atom	X	Y	Z
H	0.036184	3.550937	-1.852714
C	-4.172299	1.011680	-1.623311
H	-5.175702	0.889601	-1.194964
H	-3.766493	0.027257	-1.859096
H	-4.237945	1.622358	-2.534757
H	-4.734973	2.804205	0.244994
H	-3.022077	3.295632	0.452012
H	-3.847996	3.585713	-1.101234

Table S1 (Continued).



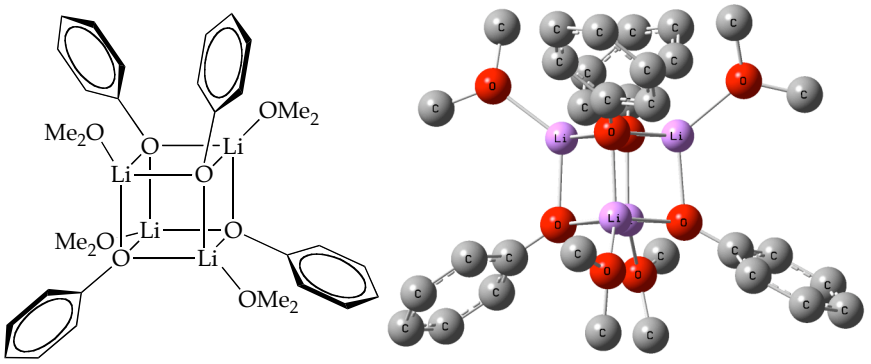


S16
G = -1873.024545
(-90 ºC)
see pg S98

Atom	X	Y	Z	Atom	X	Y	Z
Li	-3.018404	1.912134	-0.001678	C	-7.348989	0.703398	1.206322
Li	-0.925925	0.703703	0.000000	H	-5.404546	0.701421	2.159293
Li	-3.018623	-0.504047	0.000000	C	-7.348199	0.706405	-1.209858
C	-0.853911	-1.837983	0.001841	H	-5.402949	0.707226	-2.161619
C	-0.505715	-2.440833	1.210375	C	-8.046085	0.705576	-0.001816
C	-0.504575	-2.443442	-1.205883	H	-7.898973	0.702410	2.158508
C	0.190762	-3.649711	1.211942	H	-7.898096	0.707707	-2.162268
H	-0.781192	-1.964126	2.162270	H	-9.145689	0.706214	-0.002259
C	0.192150	-3.651792	-1.204238	O	-1.623579	1.912212	-0.001199
H	-0.779172	-1.967900	-2.158643	O	-3.716005	0.703928	-0.000682
C	0.539514	-4.255192	0.004750	O	-1.623463	-0.504047	0.000000
H	0.464800	-4.125067	2.164876	C	1.768816	0.704332	1.479852
H	0.467619	-4.129211	-2.155901	C	1.771354	0.702866	-1.475220
H	1.088603	-5.207888	0.005802	C	-0.397071	0.701984	-3.028516
C	-0.853075	3.245600	-0.001281	C	-0.402275	0.704990	3.029420
C	-0.501975	3.848365	-1.209016	H	0.374056	0.670780	-3.769656
C	-0.505783	3.850647	1.207239	H	-1.027799	-0.155928	-3.133717
C	0.195364	5.056748	-1.208992	H	-0.979238	1.590547	-3.156721
H	-0.775840	3.371984	-2.161540	H	-0.590764	1.712935	3.335065
C	0.191804	5.058500	1.207187	H	-1.324064	0.162365	3.001794
H	-0.782669	3.375171	2.159370	H	0.264560	0.240084	3.725187
C	0.542074	5.661817	-0.001005	H	2.172326	-0.169084	1.948065
H	0.471692	5.532037	-2.161297	H	2.172314	1.578218	1.947199
H	0.465663	5.535594	2.159477	H	2.175668	-0.171013	-1.941872
H	1.091842	6.614121	-0.000802	H	2.175656	1.576288	-1.942739
C	-5.256005	0.704184	-0.000934	O	0.238743	0.702780	-1.625897
C	-5.953829	0.702361	1.206650	O	0.235948	0.704395	1.627896
C	-5.953374	0.705847	-1.209607	O	-3.568283	-1.456924	-1.536879

Atom	X	Y	Z
O	-3.568283	-1.455188	1.537954
C	-4.430106	-2.530484	-1.150056
C	-4.450174	-2.513651	1.154777
H	-4.216925	-3.529275	-1.469225
H	-5.018756	-2.374940	-2.029941
H	-4.091820	-3.438994	1.555058
H	-5.430608	-2.316354	1.535202
C	-3.181949	-1.151456	-2.879390
C	-3.164563	-1.161660	2.878010
H	-2.394700	-0.426882	-2.867887
H	-4.022271	-0.756702	-3.411299
H	-2.839800	-2.042216	-3.363518
H	-2.152904	-1.478453	3.023223
H	-3.802259	-1.678960	3.564046
H	-3.236443	-0.107935	3.049462
O	-3.568595	2.865717	1.534573
O	-3.567539	2.862573	-1.540254
C	-4.249413	4.056093	-1.145975
C	-4.247663	4.059876	1.137395
H	-3.885897	5.013682	1.460318
H	-4.864946	3.998850	2.009254
H	-3.730757	4.907856	-1.533785
H	-5.247545	4.040437	-1.531186
C	-3.340934	2.456232	2.885644
C	-3.336755	2.451579	-2.890337
H	-2.323420	2.664759	-3.159793
H	-3.998451	2.982094	-3.542727
H	-3.515710	1.400356	-2.978692
H	-2.753115	1.562189	2.893129
H	-4.279342	2.270118	3.364865
H	-2.819998	3.229991	3.409880
H	2.027606	0.703383	-0.436358
H	2.026852	0.703818	0.441432
H	-4.280150	4.113041	-0.077934
H	-4.487971	-2.577604	0.087359
H	-5.288170	-2.335013	-0.541437
H	-5.117554	3.999567	0.517272

Table S1 (Continued).

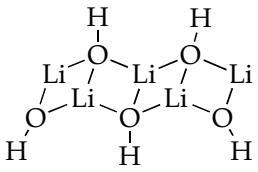


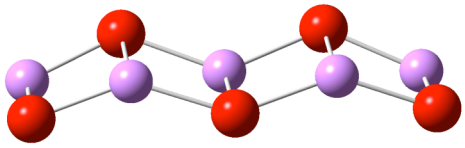
S17
G = -1877.563983
(-90 ºC)
see pg S99

Atom	X	Y	Z	Atom	X	Y	Z
O	0.735744	0.150809	1.573617	H	5.157250	0.150038	-0.735138
Li	-0.017001	-1.448312	0.740469	C	3.849996	0.017080	-1.945639
O	-1.695349	-0.581158	0.196583	H	4.759334	1.552106	-1.776617
Li	-0.745702	-0.163833	-1.465126	H	3.887956	1.985545	0.698766
O	-0.024207	1.540155	-0.840074	H	4.692678	1.493015	1.258957
Li	-0.849327	1.053843	0.880420	C	4.271105	2.906038	0.237750
O	-1.796917	2.475885	1.877358	C	3.072861	2.224806	1.382987
C	-1.246558	3.792034	1.919375	C	-0.086855	2.720876	-1.452231
H	-1.459989	4.263700	2.887901	C	1.090128	3.423597	-1.797994
H	-0.166947	3.695068	1.792759	C	0.996948	4.653385	-2.432424
H	-1.651272	4.407918	1.107140	C	-0.215079	5.251637	-2.760649
C	-3.209780	2.463345	2.076127	H	-1.379983	4.556418	-2.424567
H	-3.535103	1.422875	2.026161	H	-1.329320	3.317515	-1.784561
H	-3.459625	2.880874	3.060853	H	-2.245264	2.790086	-1.528694
H	-3.717343	3.047192	1.296464	O	-2.346781	4.990880	-2.668129
Li	1.498159	0.474023	-0.207360	C	-0.233568	6.214964	-3.257430
O	0.846870	-1.204713	-0.996767	H	2.147226	5.299751	-2.746138
C	1.614960	-2.001632	-1.737338	H	2.061367	2.998906	-1.566874
C	2.162888	-3.189951	-1.201027	H	-1.571199	-0.448846	-3.240446
C	2.956013	-4.002237	-1.998333	C	-1.417477	0.467617	-4.322966
C	3.258522	-3.708716	-3.323933	H	-0.554558	0.194142	-4.945538
C	2.725881	-2.530169	-3.852921	H	-2.322157	0.476781	-4.945658
C	1.921701	-1.687243	-3.085250	H	-1.262383	1.457089	-3.889555
H	1.516442	-0.772134	-3.510415	C	-1.794704	-1.788371	-3.678772
H	2.944229	-2.264714	-4.884759	C	-1.962875	-2.394304	-2.786582
H	3.884163	-4.377859	-3.903772	C	-2.684255	-1.836052	-4.320844
O	3.459032	-5.137382	-1.454012	C	-0.921824	-2.169839	-4.223165
C	1.964006	-3.465274	-0.170206	C	-2.942473	-0.980349	0.438134
H	3.361561	1.111041	-0.297515	C	-3.915794	-0.990536	-0.587601
H	4.344057	0.687785	-1.240599	H	-5.205791	-1.416412	-0.307075

Atom	X	Y	Z
H	-5.612124	-1.838804	0.954341
H	-4.654677	-1.818908	1.972062
O	-3.346129	-1.399496	1.730835
C	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
H	-6.112054	-1.418770	-1.315682
C	-3.655156	-0.659195	-1.587531
H	-0.087743	-3.230405	1.587431
H	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
C	-0.739019	-4.053244	-0.156392
C	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
C	0.388471	-4.380480	3.253585
C	0.544499	-2.607314	3.419761
C	-1.079476	-3.368106	3.417819
H	1.352599	0.184225	2.754704
H	0.861372	0.987474	3.808956
H	1.526453	1.004317	5.026471
F	2.673442	0.259171	5.278606
F	3.156961	-0.539318	4.238279
F	2.517961	-0.584212	2.999185
F	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
H	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table S1 (Continued).

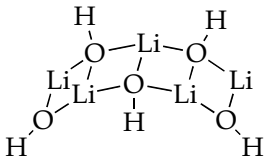


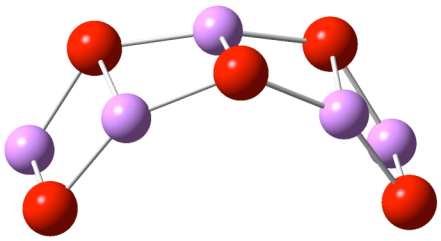


S18
G = -417.175865
(-90 °C)
see pg S99

Atom	X	Y	Z
O	1.736811	1.329447	0.042905
Li	-0.000032	0.792012	-0.411985
O	-0.000060	-1.060908	0.076784
Li	1.766318	-0.652129	0.514006
O	3.479635	-0.916966	-0.035349
Li	3.380869	0.758009	-0.488110
H	3.977151	-1.713672	-0.242117
Li	-1.766408	-0.652347	0.514272
O	-1.736709	1.329533	0.042958
Li	-3.380578	0.757988	-0.488474
O	-3.479686	-0.916889	-0.035345
H	-3.977312	-1.713512	-0.242180
H	-1.698768	2.078380	0.653734
H	0.000081	-1.854186	-0.477399
H	1.698419	2.078655	0.653207

Table S1 (Continued).

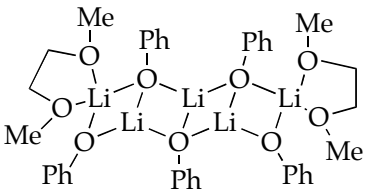


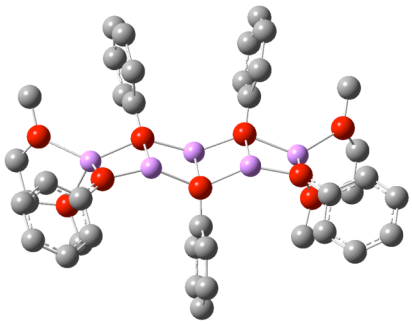


S19
G = -417.173551
(-90 °C)
see pg S99

Atom	X	Y	Z
O	1.798560	-1.321300	-0.329324
Li	0.000106	-1.305359	0.203534
O	0.000041	0.115904	1.534593
Li	1.663005	0.442922	0.758107
O	2.741305	1.362086	-0.374109
Li	2.763191	-0.117660	-1.287542
H	2.888212	2.306443	-0.483625
Li	-1.662780	0.443058	0.758015
O	-1.798250	-1.321423	-0.329517
Li	-2.763344	-0.117880	-1.287384
O	-2.741716	1.361833	-0.373908
H	-2.888638	2.306172	-0.483588
H	-2.269470	-2.094631	0.010934
H	0.000073	-0.035459	2.489222
H	2.269776	-2.094567	0.010990

Table S1 (Continued).



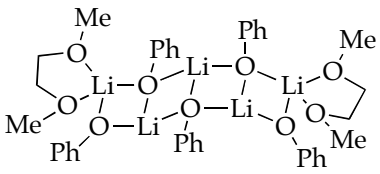


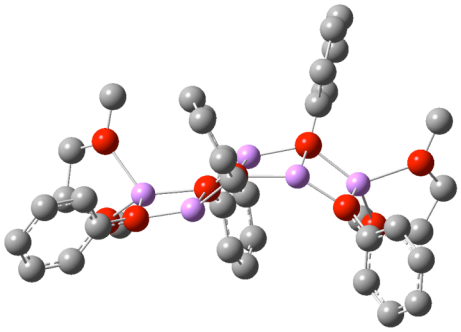
S20
G = -2189.592569
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.016066	0.745896	0.390569	C	5.629962	2.857525	-0.086052
O	-1.796734	1.197841	-0.001729	H	6.697166	2.966467	-0.321510
Li	-1.757762	-0.553401	-0.904184	H	5.324431	3.634368	0.625148
O	-0.010667	-1.053992	-0.340113	H	5.035743	2.956596	-0.994333
Li	1.730179	-0.522626	-0.904651	C	2.007018	2.497210	-0.122515
O	1.788058	1.181109	0.085890	C	2.147461	3.383649	0.966769
Li	3.651571	0.468399	0.332463	C	2.385621	4.742532	0.756288
O	3.475753	-0.913282	-0.904437	C	2.494056	5.255285	-0.538938
C	4.363037	-1.844181	-1.249540	C	2.354162	4.386988	-1.624910
C	5.608360	-1.489616	-1.819890	C	2.116891	3.026544	-1.425505
C	6.543973	-2.463610	-2.167681	H	2.006614	2.353888	-2.273093
C	6.276994	-3.820143	-1.962516	H	2.426169	4.770910	-2.639928
C	5.048991	-4.186100	-1.405061	H	2.673693	6.314443	-0.699890
C	4.105479	-3.221359	-1.051695	H	2.482911	5.405682	1.613222
H	3.150268	-3.514137	-0.621408	H	2.065112	2.982767	1.974998
H	4.819362	-5.237495	-1.242814	C	0.005416	-2.230870	0.326152
H	7.007739	-4.575901	-2.237238	C	0.004275	-3.458134	-0.366007
H	7.490538	-2.158516	-2.610065	C	0.019523	-4.667965	0.328834
H	5.811648	-0.435672	-1.995221	C	0.036330	-4.691652	1.726135
O	5.371947	1.556827	0.441234	C	0.037762	-3.481977	2.423215
C	6.044420	1.301213	1.669141	C	0.022843	-2.265937	1.736403
C	5.758941	-0.134217	2.059881	H	0.024761	-1.325687	2.286621
O	4.342955	-0.291969	2.120439	H	0.050399	-3.480283	3.511003
C	3.951126	-1.626332	2.458802	H	0.047906	-5.636621	2.261414
H	4.337860	-2.343298	1.725105	H	0.018189	-5.600634	-0.230004
H	4.314848	-1.883652	3.462884	H	-0.008119	-3.443444	-1.453144
H	2.860644	-1.652700	2.445919	O	-3.506410	-0.934835	-0.840546
H	6.178051	-0.824452	1.313933	Li	-3.643840	0.498541	0.347316
H	6.212363	-0.350773	3.038815	O	-4.262422	-0.221684	2.182564
H	7.128775	1.442007	1.549002	C	-5.677869	-0.049721	2.176119
H	5.684857	1.995611	2.443645	C	-5.964227	1.382763	1.775948

Atom	X	Y	Z
O	-5.341384	1.613514	0.517067
C	-5.611221	2.908491	-0.019216
H	-5.060554	2.986591	-0.956456
H	-5.265736	3.693327	0.664745
H	-6.687527	3.024971	-0.204349
H	-5.565065	2.084235	2.524305
H	-7.051039	1.534188	1.699096
H	-6.094135	-0.247171	3.175410
H	-6.133202	-0.746267	1.457717
C	-3.871877	-1.554070	2.530035
H	-2.782921	-1.592731	2.478257
H	-4.200907	-1.789703	3.551272
H	-4.292128	-2.279661	1.823885
C	-4.407055	-1.872470	-1.127447
C	-5.681384	-1.528200	-1.637189
C	-6.631310	-2.508438	-1.923085
C	-6.350577	-3.861554	-1.713941
C	-5.094359	-4.217520	-1.216047
C	-4.136206	-3.246457	-0.924987
H	-3.159738	-3.531885	-0.539705
H	-4.854049	-5.266164	-1.051498
H	-7.092615	-4.622376	-1.940104
H	-7.600304	-2.211012	-2.319788
H	-5.896488	-0.477107	-1.816184
C	-2.022548	2.466229	-0.407446
C	-2.026953	3.531029	0.518036
C	-2.271703	4.839515	0.100693
C	-2.525584	5.124906	-1.243500
C	-2.524794	4.078476	-2.169334
C	-2.279348	2.766165	-1.762138
H	-2.282660	1.954413	-2.486572
H	-2.714067	4.282414	-3.220843
H	-2.711629	6.145642	-1.565191
H	-2.259497	5.643240	0.833510
H	-1.832455	3.308942	1.565090

Table S1 (Continued).



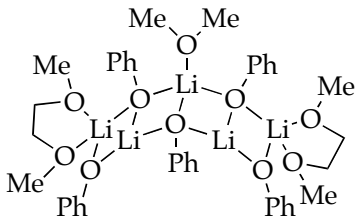


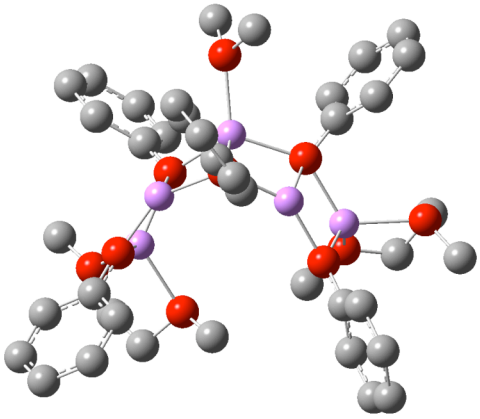
S21
G = -2189.593152
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
O	1.382046	-1.071584	-0.190871	H	7.249066	2.013004	-2.999219
Li	-0.007207	-0.313570	0.825823	H	5.198872	0.622301	-2.783252
O	0.246714	1.538169	0.406525	Li	-1.674026	1.470725	0.319502
Li	1.660633	0.876982	-0.641248	O	-1.864834	-0.361787	1.103552
O	3.436222	0.811312	-0.853859	Li	-3.343565	-0.349183	-0.162206
Li	3.354454	-0.942896	-0.277457	O	-3.129995	1.410764	-0.711075
O	4.658176	-2.285294	-1.176784	C	-3.846902	2.058206	-1.626727
C	5.856738	-2.032279	-0.439032	C	-3.670135	1.809943	-3.008258
C	5.618806	-2.181984	1.058321	C	-4.435925	2.480851	-3.962333
O	4.485494	-1.381224	1.374066	C	-5.400042	3.416296	-3.578355
C	4.179851	-1.322364	2.760175	C	-5.584815	3.672389	-2.216428
H	3.300297	-0.684415	2.863603	C	-4.826138	3.007780	-1.253826
H	3.957364	-2.322290	3.158767	H	-4.971842	3.205956	-0.194266
H	5.013522	-0.884213	3.324771	H	-6.329135	4.399914	-1.898353
H	5.426407	-3.227974	1.342735	H	-5.992591	3.938465	-4.324633
H	6.504350	-1.834072	1.610776	H	-4.272729	2.272569	-5.018105
H	6.132685	-0.999327	-0.671391	H	-2.910439	1.091560	-3.308523
H	6.664684	-2.699004	-0.769952	O	-5.239692	-0.898832	0.375504
C	4.406716	-3.663200	-1.454282	C	-5.797954	-1.842437	-0.529316
H	3.473317	-3.704832	-2.016147	C	-5.023925	-1.711549	-1.835225
H	5.223066	-4.080030	-2.058994	O	-3.614455	-1.784935	-1.609302
H	4.297505	-4.253880	-0.535562	C	-3.089871	-3.107461	-1.492613
C	4.521074	1.574670	-0.975394	H	-3.286367	-3.674958	-2.411655
C	5.428167	1.387084	-2.044263	H	-3.519239	-3.644876	-0.636521
C	6.573174	2.176531	-2.161844	H	-2.013263	-3.008166	-1.353797
C	6.853547	3.174473	-1.225353	H	-5.342818	-2.481336	-2.551505
C	5.962662	3.373273	-0.166139	H	-5.196508	-0.724884	-2.275307
C	4.816502	2.590490	-0.036995	H	-6.862976	-1.629118	-0.706471
H	4.123747	2.750873	0.786092	H	-5.719079	-2.855776	-0.105997
H	6.160762	4.150569	0.569352	C	-5.878037	-0.865321	1.648072
H	7.744262	3.789347	-1.321799	H	-6.923591	-0.545429	1.545964

Atom	X	Y	Z
H	-5.840265	-1.851137	2.130424
H	-5.329614	-0.147748	2.259321
C	-2.183789	-0.837001	2.322848
C	-2.464097	0.032156	3.399938
C	-2.799895	-0.472377	4.657044
C	-2.867848	-1.850073	4.880682
C	-2.587436	-2.720899	3.824526
C	-2.249089	-2.227608	2.563101
H	-2.028155	-2.905651	1.741704
H	-2.630439	-3.796617	3.981667
H	-3.129656	-2.237596	5.861112
H	-3.009651	0.220767	5.468555
H	-2.409658	1.105949	3.233574
C	0.441177	2.693687	1.084888
C	0.043988	3.925722	0.526087
C	0.217351	5.116571	1.234012
C	0.791251	5.111679	2.506859
C	1.192867	3.895815	3.066381
C	1.020908	2.699933	2.369549
H	1.333564	1.754104	2.807442
H	1.643867	3.875702	4.055866
H	0.927590	6.040422	3.053310
H	-0.094571	6.054128	0.780371
H	-0.387171	3.933008	-0.473072
C	1.057020	-2.218395	-0.814758
C	0.878835	-3.415146	-0.084594
C	0.566424	-4.611477	-0.732350
C	0.423753	-4.654902	-2.122383
C	0.592663	-3.476050	-2.856136
C	0.902403	-2.274151	-2.217870
H	1.035395	-1.361599	-2.794106
H	0.481834	-3.488973	-3.938024
H	0.185162	-5.588254	-2.624442
H	0.437507	-5.517551	-0.144196
H	0.996798	-3.385073	0.996532

Table S1 (Continued).



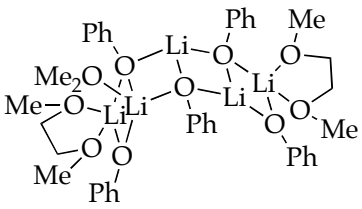


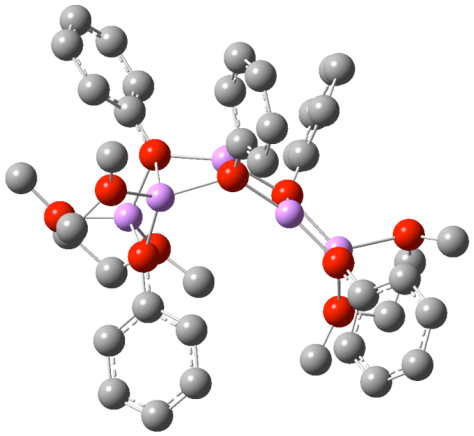
S22
G = -2344.557559
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.492577	-1.601194	0.991045	C	1.572923	2.137293	-1.903099
O	0.192599	-0.086309	2.110527	H	1.342080	2.860874	-2.696101
Li	1.831211	-0.481460	1.253009	H	0.683109	1.968910	-1.294362
O	1.159093	-1.720255	-0.091340	H	2.385124	2.520608	-1.275821
Li	2.450189	-0.621122	-1.135119	C	1.404776	-2.977170	-0.488035
O	3.235522	0.185947	0.345647	C	2.349425	-3.793138	0.176681
C	4.204232	1.092997	0.424529	C	2.592159	-5.100556	-0.246927
C	4.011302	2.327448	1.089371	C	1.909869	-5.638121	-1.342869
C	5.027960	3.280010	1.147142	C	0.975290	-4.842247	-2.011943
C	6.268748	3.043936	0.548643	C	0.724661	-3.533260	-1.596921
C	6.477892	1.826887	-0.105792	H	-0.004702	-2.914218	-2.114578
C	5.469090	0.865871	-0.169231	H	0.432440	-5.244207	-2.865073
H	5.640227	-0.088328	-0.662791	H	2.100761	-6.657337	-1.666537
H	7.441319	1.618784	-0.567946	H	3.321302	-5.705423	0.287773
H	7.057824	3.789327	0.597479	H	2.882461	-3.380808	1.030344
H	4.846592	4.218570	1.667095	Li	-1.149418	0.832603	1.156113
H	3.048406	2.517516	1.559006	O	-2.081516	-0.621897	0.296431
O	1.936674	0.874184	-2.484155	Li	-2.497377	0.841009	-0.943069
C	3.090093	0.968545	-3.317964	O	-1.521563	2.153690	-0.055431
H	2.899023	1.646052	-4.164200	C	-1.580742	3.480690	-0.120363
H	3.937343	1.359093	-2.737124	C	-1.443670	4.165381	-1.351732
C	3.401707	-0.420979	-3.834927	C	-1.518228	5.556493	-1.418549
O	3.567745	-1.276098	-2.710042	C	-1.732475	6.318321	-0.267380
C	3.972402	-2.599523	-3.054404	C	-1.870758	5.659075	0.957304
H	4.955662	-2.580761	-3.543650	C	-1.798875	4.269194	1.034327
H	4.028630	-3.167552	-2.125838	H	-1.915326	3.764833	1.991917
H	3.238721	-3.072122	-3.719604	H	-2.037939	6.233467	1.866137
H	4.323341	-0.392847	-4.435045	H	-1.787253	7.401844	-0.322263
H	2.583811	-0.794743	-4.470291	H	-1.403613	6.050718	-2.381567

Atom	X	Y	Z
H	-1.266665	3.579214	-2.251225
O	-4.465594	1.329150	-1.279606
C	-4.897661	2.691831	-1.257259
H	-4.519025	3.124494	-0.331075
H	-4.492750	3.263905	-2.100795
H	-5.994424	2.737731	-1.271454
C	-4.825417	0.602861	-2.454396
H	-4.868423	-0.447877	-2.153342
H	-5.815966	0.909692	-2.816703
C	-3.777608	0.787282	-3.543318
O	-2.517751	0.450500	-2.968177
C	-1.425654	0.573239	-3.873834
H	-0.513014	0.351870	-3.318179
H	-1.534067	-0.135980	-4.705945
H	-1.367437	1.594008	-4.277591
H	-3.750647	1.825198	-3.908953
H	-4.000533	0.128522	-4.396322
C	-3.200806	-1.360356	0.367477
C	-3.414900	-2.436928	-0.523586
C	-4.579752	-3.204545	-0.458328
C	-5.568418	-2.923634	0.488625
C	-5.372828	-1.856680	1.371048
C	-4.211668	-1.085705	1.315446
H	-4.069314	-0.252760	2.000474
H	-6.133156	-1.619390	2.112042
H	-6.473747	-3.522081	0.537450
H	-4.713570	-4.029861	-1.154887
H	-2.645894	-2.656173	-1.260640
C	0.416324	0.220361	3.404417
C	0.216908	1.531500	3.887076
C	0.451244	1.843866	5.225870
C	0.898505	0.867839	6.120122
C	1.112871	-0.429936	5.651967
C	0.876371	-0.755038	4.315120
H	1.036390	-1.769842	3.956559
H	1.467056	-1.201623	6.331850
H	1.083651	1.116817	7.161040
H	0.292075	2.863458	5.569408
H	-0.100456	2.306678	3.191483
O	-0.991313	-3.218385	2.095466
C	-1.191999	-4.528035	1.563879
H	-0.923881	-5.285253	2.313380
H	-2.238461	-4.663590	1.262422
H	-0.539639	-4.630359	0.696724
C	-1.773696	-2.995480	3.268922
H	-1.510595	-3.729627	4.042998
H	-2.844211	-3.066788	3.041176
H	-1.537466	-1.993927	3.629994

Table S1 (Continued).



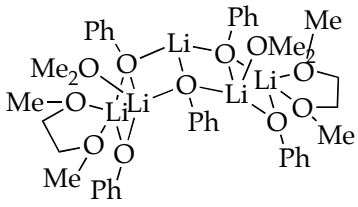


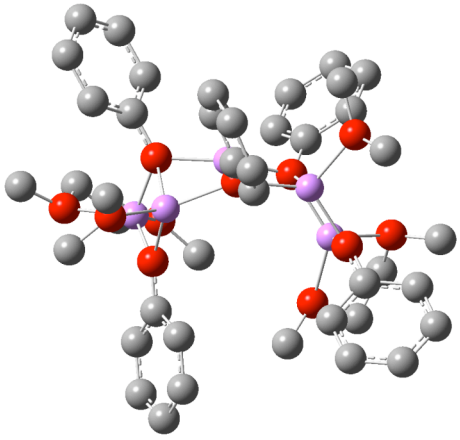
S23
G = -2344.563093
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.391799	-1.008202	-0.590160	O	3.381045	1.585371	2.223298
O	-0.289811	-1.380076	-1.319307	C	3.519012	2.807127	1.494917
Li	-1.672727	0.006652	-1.646733	H	2.638091	2.904932	0.858322
O	-2.549468	-0.309106	0.224236	H	3.576533	3.660081	2.184477
Li	-0.871125	-1.070883	0.490448	H	4.416086	2.781867	0.864392
O	0.881375	-0.783074	1.316262	H	5.421626	1.302371	2.456458
Li	2.735560	-0.162681	1.323296	H	4.601236	2.060301	3.845869
O	3.105301	-0.468682	-0.465190	C	0.635576	-1.608345	2.355033
C	4.174646	-0.288663	-1.237965	C	0.383189	-1.097387	3.648370
C	4.549203	0.997172	-1.694484	C	0.105571	-1.953749	4.713522
C	5.681742	1.177761	-2.488976	C	0.063022	-3.338789	4.526503
C	6.478767	0.091531	-2.858881	C	0.303380	-3.856577	3.252538
C	6.116099	-1.186845	-2.424573	C	0.587088	-3.009273	2.178914
C	4.987187	-1.378613	-1.629042	H	0.789086	-3.421844	1.192207
H	4.703897	-2.375726	-1.299141	H	0.276083	-4.931062	3.087610
H	6.718534	-2.047115	-2.709471	H	-0.156339	-4.001329	5.358773
H	7.358444	0.236553	-3.479746	H	-0.084855	-1.533712	5.698886
H	5.939774	2.179239	-2.827999	H	0.399154	-0.019890	3.792488
H	3.918825	1.841468	-1.427870	Li	-2.431003	1.588231	0.369072
O	4.010087	-1.047864	2.667427	O	-1.399686	1.808519	-1.161128
C	5.184788	-1.665519	2.133543	C	-0.638190	2.825094	-1.541389
H	4.844137	-2.377235	1.381999	C	0.702371	2.638106	-1.964013
H	5.849070	-0.938069	1.651591	C	1.493591	3.718505	-2.354136
H	5.725590	-2.194215	2.929121	C	0.991473	5.024159	-2.335399
C	4.252421	-0.069417	3.676953	C	-0.329500	5.226997	-1.927888
H	3.346450	-0.044738	4.289909	C	-1.132410	4.153453	-1.540578
H	5.098968	-0.364139	4.311820	H	-2.168603	4.315832	-1.249263
C	4.500623	1.297916	3.058176	H	-0.745544	6.232960	-1.918987

Atom	X	Y	Z
H	1.611471	5.861352	-2.643862
H	2.513168	3.532778	-2.685976
H	1.103763	1.627481	-1.984952
O	-1.628162	2.533587	2.024059
C	-2.365610	3.740509	2.178768
H	-2.127303	4.217882	3.141448
H	-2.111747	4.438945	1.368073
C	-3.836510	3.381285	2.138176
O	-4.086130	2.694539	0.915891
C	-5.439487	2.256576	0.790754
H	-6.116748	3.120117	0.742348
H	-5.505452	1.678590	-0.130980
H	-5.718092	1.610938	1.632708
H	-4.446415	4.295294	2.196666
H	-4.095459	2.731977	2.987444
C	-0.213116	2.734053	2.047975
H	0.093959	3.155569	3.015521
H	0.243670	1.752834	1.908735
H	0.093857	3.404441	1.236072
C	-3.706084	-0.878937	0.599728
C	-4.691222	-1.223084	-0.351751
C	-5.901071	-1.793240	0.046055
C	-6.168197	-2.039048	1.395899
C	-5.197408	-1.710508	2.346210
C	-3.983795	-1.138808	1.960221
H	-3.228594	-0.886797	2.701664
H	-5.382731	-1.903559	3.400687
H	-7.110254	-2.486228	1.700337
H	-6.641791	-2.050012	-0.708420
H	-4.481990	-1.033797	-1.402025
O	-2.699520	-0.068333	-3.364422
C	-2.967451	-1.168222	-4.229298
H	-2.410705	-1.064586	-5.170158
H	-4.042712	-1.226543	-4.452474
H	-2.645728	-2.074458	-3.715101
C	-3.067555	1.184574	-3.936649
H	-4.143630	1.202325	-4.160622
H	-2.822997	1.949027	-3.199479
H	-2.504349	1.366425	-4.862500
C	-0.389258	-2.513941	-2.040767
C	0.453801	-2.741605	-3.149956
C	0.353440	-3.917335	-3.894765
C	-0.587983	-4.896011	-3.563213
C	-1.430779	-4.679918	-2.470489
C	-1.338517	-3.507514	-1.716985
H	-2.004649	-3.344955	-0.872210
H	-2.171139	-5.428710	-2.197848
H	-0.662211	-5.810276	-4.145120
H	1.016549	-4.066299	-4.743890
H	1.177172	-1.975490	-3.420637

Table S1 (Continued).



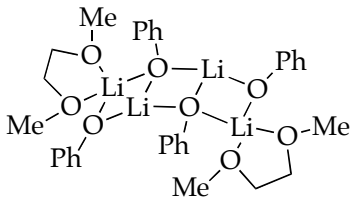


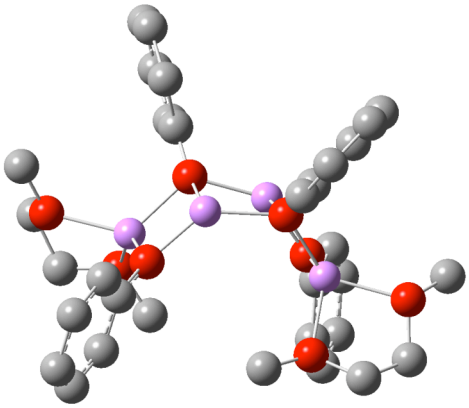
S24
G = -2499.523053
(-90 °C)
see pg S100

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.647308	1.072248	-1.037436	O	2.458367	-2.856719	0.751810
O	-0.048857	1.740842	-0.203628	C	2.402922	-2.519462	2.145139
Li	-1.508728	1.192720	1.106410	H	1.514122	-1.908317	2.297505
O	-2.507190	0.116624	-0.358067	H	2.326117	-3.430841	2.752005
Li	-0.762054	0.211559	-1.049527	H	3.291478	-1.948155	2.437461
O	0.780925	-0.680888	-1.655034	H	4.504987	-3.187244	0.750310
Li	2.342013	-1.341960	-0.692738	H	3.503746	-4.647569	0.949933
O	3.104965	0.254162	-0.203626	C	0.607332	-1.281336	-2.848922
C	4.031528	0.682022	0.643591	C	-0.375337	-2.281355	-3.022240
C	3.728422	0.946649	2.003003	C	-0.559363	-2.898420	-4.260977
C	4.708340	1.397746	2.885905	C	0.227264	-2.545778	-5.359531
C	6.023695	1.604845	2.458716	C	1.206461	-1.561195	-5.198612
C	6.340891	1.353021	1.121924	C	1.398010	-0.936095	-3.966745
C	5.369152	0.900145	0.228169	H	2.163260	-0.174290	-3.841467
H	5.621504	0.713155	-0.813346	H	1.830176	-1.274438	-6.042864
H	7.357604	1.512148	0.766859	H	0.080943	-3.027634	-6.322181
H	6.782625	1.957934	3.151482	H	-1.325931	-3.663810	-4.365958
H	4.439830	1.590671	3.923023	H	-0.988795	-2.561672	-2.168689
H	2.708439	0.785127	2.342345	Li	-2.564998	-1.268476	0.946593
O	3.560418	-2.642619	-1.764823	O	-1.444018	-0.408992	2.135097
C	4.861392	-2.127035	-2.052220	C	-0.832265	-0.770019	3.252996
H	4.708846	-1.194951	-2.596932	C	0.144848	0.056163	3.863747
H	5.428248	-1.913953	-1.138049	C	0.797712	-0.337297	5.031387
H	5.417112	-2.835416	-2.680899	C	0.507225	-1.561598	5.641302
C	3.553890	-3.891181	-1.075160	C	-0.463813	-2.383798	5.062234
H	2.626072	-4.393211	-1.367480	C	-1.123638	-2.000159	3.895712
H	4.401909	-4.514961	-1.389404	H	-1.887087	-2.642069	3.459179
C	3.574604	-3.679628	0.429428	H	-0.714867	-3.335548	5.527367

Atom	X	Y	Z
H	1.018419	-1.862901	6.551347
H	1.545299	0.321573	5.468659
H	0.383186	1.007938	3.393748
O	-2.210052	-3.183569	0.284845
C	-3.364083	-3.997347	0.459322
H	-3.399124	-4.786344	-0.306783
H	-3.337724	-4.473970	1.450862
C	-4.584497	-3.106500	0.344830
O	-4.444157	-2.074135	1.318769
C	-5.617331	-1.273658	1.470030
H	-6.464457	-1.897806	1.785441
H	-5.397291	-0.542930	2.250268
H	-5.862560	-0.750600	0.538775
H	-5.490157	-3.699111	0.541071
H	-4.660519	-2.665190	-0.659506
C	-0.987224	-3.880428	0.521485
H	-0.894796	-4.734178	-0.163522
H	-0.174369	-3.178314	0.338401
H	-0.938556	-4.233274	1.559941
C	-3.559132	0.436060	-1.126451
C	-4.478804	1.431597	-0.725557
C	-5.578360	1.754193	-1.521191
C	-5.799776	1.101090	-2.737244
C	-4.894897	0.119534	-3.148706
C	-3.791735	-0.213699	-2.360513
H	-3.086804	-0.973042	-2.692329
H	-5.044505	-0.394013	-4.096140
H	-6.656037	1.357744	-3.354651
H	-6.267457	2.527782	-1.188131
H	-4.302445	1.944143	0.217094
O	-2.515459	2.530833	2.274083
C	-2.572409	3.954795	2.235869
H	-2.084040	4.382334	3.122147
H	-3.617691	4.294511	2.203964
H	-2.052201	4.281248	1.336639
C	-3.181882	1.996525	3.415050
H	-4.250756	2.255628	3.390760
H	-3.048966	0.915544	3.378504
H	-2.740329	2.388752	4.341132
C	-0.101218	3.076659	-0.305207
C	0.806293	3.891038	0.411708
C	0.756531	5.281668	0.309770
C	-0.195396	5.908225	-0.501618
C	-1.101866	5.115581	-1.211912
C	-1.061402	3.722701	-1.118534
H	-1.778739	3.113626	-1.664209
H	-1.853061	5.583302	-1.845055
H	-0.230723	6.991472	-0.577082
H	1.467899	5.881316	0.873847
H	1.544430	3.406288	1.046856
O	2.289151	2.275464	-2.542191
C	1.441463	2.776489	-3.571712
H	2.023076	2.966285	-4.485241
H	0.695311	2.006491	-3.777394
H	0.941092	3.699589	-3.255058
C	3.351361	3.174375	-2.226596
H	3.977307	3.349690	-3.113261
H	3.949104	2.702814	-1.445066
H	2.955043	4.131531	-1.864044

Table S1 (Continued).



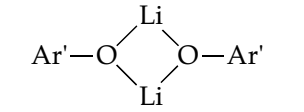


S25
G = -1875.179010
(-90 °C)
see pg S101

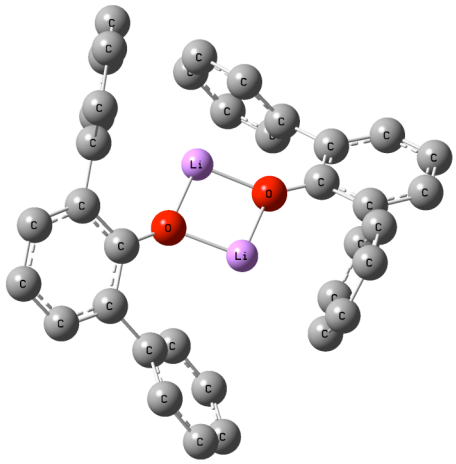
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.645265	1.213883	0.810355	H	4.395891	-2.505417	-0.001876
O	-1.206640	0.991174	1.180681	C	5.116109	0.033989	0.518091
Li	-0.635759	-0.881792	1.124715	H	6.166629	0.010762	0.199163
O	1.236051	-0.597271	1.192369	H	4.804853	1.069304	0.665847
Li	2.260416	-0.286838	-0.438329	H	4.998975	-0.526790	1.453908
O	1.661951	1.465729	-0.676260	C	1.876654	-1.306257	2.138901
C	2.089362	2.445160	-1.467353	C	2.390288	-0.687735	3.299123
C	2.150812	2.284544	-2.872023	C	3.056851	-1.433823	4.271593
C	2.592922	3.317306	-3.698372	C	3.232565	-2.812133	4.121449
C	2.988002	4.545206	-3.161661	C	2.725264	-3.437264	2.979540
C	2.935230	4.720473	-1.775900	C	2.057847	-2.700991	1.999056
C	2.497097	3.693965	-0.941070	H	1.667177	-3.186447	1.107776
H	2.468252	3.834570	0.138267	H	2.846300	-4.510507	2.848419
H	3.241906	5.668133	-1.337490	H	3.749268	-3.388549	4.883562
H	3.331105	5.347881	-3.808464	H	3.438520	-0.931401	5.157701
H	2.627446	3.160052	-4.774826	H	2.249272	0.383757	3.425191
H	1.838026	1.332100	-3.296295	O	-1.884317	-1.447679	-0.058835
O	4.275626	-0.496855	-0.505788	Li	-2.448643	0.344594	-0.136776
C	4.574358	-1.842981	-0.861143	O	-4.483743	0.486818	-0.130120
C	3.664811	-2.208213	-2.018682	C	-5.223434	-0.581976	0.462472
O	2.325913	-1.957208	-1.606416	H	-4.858463	-0.684510	1.485286
C	1.346082	-2.318483	-2.578968	H	-6.294644	-0.340807	0.479169
H	1.481629	-1.738806	-3.502877	H	-5.058155	-1.519401	-0.082383
H	1.411172	-3.389738	-2.809483	C	-4.876557	0.770313	-1.469970
H	0.368161	-2.105219	-2.146027	H	-4.771173	-0.133084	-2.088259
H	3.905109	-1.599296	-2.903293	H	-5.925214	1.101376	-1.502480
H	3.795332	-3.269568	-2.276523	C	-3.970801	1.872972	-1.981462
H	5.625845	-1.935603	-1.170834	O	-2.628801	1.418216	-1.847673

Atom	X	Y	Z
C	-1.652195	2.369869	-2.276525
H	-1.767599	3.317092	-1.733267
H	-0.672155	1.945466	-2.057982
H	-1.747254	2.555656	-3.354318
H	-4.202972	2.091441	-3.034419
H	-4.114401	2.791692	-1.393072
C	-2.228174	-2.507632	-0.779321
C	-2.493709	-2.401820	-2.167700
C	-2.858060	-3.519368	-2.919840
C	-2.972548	-4.778121	-2.324696
C	-2.715274	-4.899140	-0.955389
C	-2.352401	-3.790421	-0.193434
H	-2.161335	-3.890166	0.873282
H	-2.800871	-5.870675	-0.472581
H	-3.256094	-5.645958	-2.913657
H	-3.052454	-3.403756	-3.984731
H	-2.395888	-1.424915	-2.637398
C	-1.668201	1.775007	2.173878
C	-1.516564	3.177494	2.119351
C	-1.983422	3.988857	3.154639
C	-2.618189	3.431847	4.266812
C	-2.780259	2.045262	4.329113
C	-2.314783	1.225532	3.301535
H	-2.440901	0.145690	3.357185
H	-3.271710	1.594112	5.188286
H	-2.980492	4.066111	5.070810
H	-1.851978	5.066562	3.086778
H	-1.037379	3.617291	1.246090

Table S1 (Continued).



Ar' = 2,6-diphenylphenyl

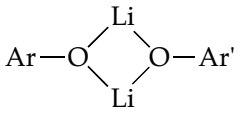


S27
G =-1552.739845
(-90 ºC)
see pg S101

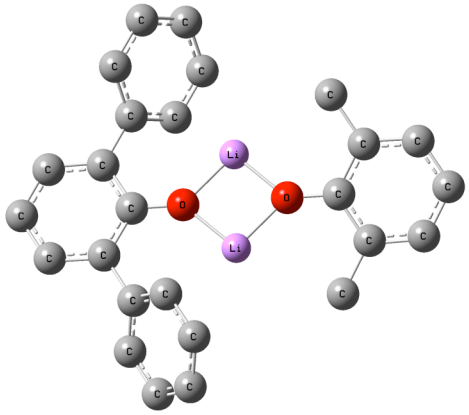
Atom	X	Y	Z	Atom	X	Y	Z
C	-2.664969	2.442608	0.296970	C	4.749091	-2.691575	0.712091
C	-2.371815	1.168845	-0.268623	H	5.654334	-3.268653	0.876347
C	-3.441076	0.421802	-0.848147	C	3.523630	-3.141035	1.202602
C	-4.737984	0.954374	-0.839545	C	2.348002	-2.416000	0.985417
C	-5.017099	2.196306	-0.274220	C	1.041940	-2.923473	1.491440
C	-3.976289	2.928913	0.294863	C	0.789837	-3.034865	2.867260
H	-4.173189	3.905746	0.730958	H	1.568467	-2.748854	3.569088
H	-6.027587	2.593925	-0.289412	C	-0.443536	-3.491449	3.338531
H	-5.538263	0.385515	-1.306893	C	-1.456900	-3.841929	2.445043
C	-3.201826	-0.923731	-1.432953	C	-1.221611	-3.753731	1.070229
C	-2.103124	-1.184676	-2.278454	H	-1.991272	-4.042220	0.360060
C	-1.913384	-2.445637	-2.847989	C	0.017977	-3.305544	0.601268
C	-2.817170	-3.480953	-2.592552	H	0.214528	-3.291400	-0.470520
C	-3.912738	-3.238888	-1.761050	H	-2.417442	-4.190582	2.813968
C	-4.096856	-1.980881	-1.184876	H	-0.614765	-3.565438	4.409487
H	-4.942904	-1.811006	-0.524626	H	3.466524	-4.081114	1.747036
H	-4.626378	-4.033104	-1.555507	H	5.741912	-1.124053	-0.381172
H	-2.672853	-4.459785	-3.041873	C	3.735569	0.558400	-0.959018
H	-1.066985	-2.612419	-3.509998	C	4.175279	0.568720	-2.291909
H	-1.414169	-0.378959	-2.511266	C	4.302644	1.764503	-3.001595
O	-1.147232	0.672765	-0.201904	C	3.997796	2.981144	-2.389979
Li	-0.481588	-1.025452	0.023675	C	3.567083	2.990209	-1.061041
O	1.278583	-0.475058	0.095085	C	3.430121	1.792174	-0.355506
Li	0.594304	1.214619	-0.024510	H	3.142986	1.810932	0.694788
C	2.386710	-1.174265	0.287254	H	3.365326	3.934540	-0.562797
C	3.643138	-0.720526	-0.202912	H	4.106142	3.913750	-2.937047
C	4.793478	-1.490679	0.005188	H	4.643380	1.744424	-4.033720

Atom	X	Y	Z
H	4.414755	-0.375958	-2.772731
C	-1.576467	3.237587	0.925698
C	-1.648819	3.612839	2.276320
C	-0.643894	4.381419	2.867810
C	0.458603	4.796640	2.119982
C	0.543873	4.440489	0.771321
C	-0.458229	3.664479	0.182564
H	-0.414144	3.439222	-0.882378
H	1.376220	4.789932	0.167221
H	1.236732	5.401781	2.576991
H	-0.723883	4.655921	3.916565
H	-2.502354	3.289030	2.865613

Table S1 (Continued).



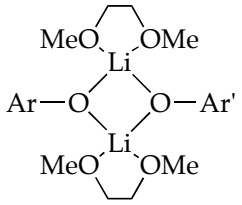
Ar' = 2,6-diphenylphenyl
Ar= 2,6-dimethylphenyl



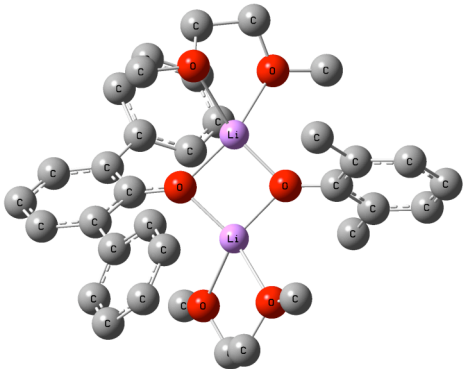
S28
G =-1169.361703
(-90 ºC)
see pg S101

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.169700	-2.425565	0.693442	C	2.350255	-3.543277	0.766719
C	-3.936463	-1.177658	0.334405	H	3.099602	-3.392299	1.539041
C	-3.220550	-0.001376	0.000083	C	1.646898	-4.749194	0.705420
C	-3.935775	1.175124	-0.334888	C	0.666486	-4.948019	-0.267579
C	-5.332280	1.155522	-0.331182	C	0.405407	-3.932601	-1.193526
C	-6.039692	-0.000885	-0.001201	H	-0.331788	-4.086032	-1.978125
C	-5.332939	-1.157552	0.329423	C	1.113771	-2.728871	-1.134733
H	-5.873827	-2.065748	0.590093	H	0.942614	-1.961918	-1.887299
H	-7.126094	-0.000736	-0.001685	H	0.119438	-5.885429	-0.313671
H	-5.872577	2.063936	-0.592332	H	1.862997	-5.533389	1.426415
C	-3.168208	2.422697	-0.693113	H	4.779953	-2.142230	-0.115769
H	-2.554473	2.787828	0.146726	H	4.777740	2.146459	0.113019
H	-2.491248	2.255997	-1.545270	C	2.095142	2.508629	0.146801
H	-3.841049	3.241127	-0.969424	C	2.345887	3.544895	-0.766867
O	-1.886575	-0.001487	0.000690	C	1.641448	4.750151	-0.704914
Li	-0.546837	-1.240470	0.023393	C	0.661752	4.948042	0.268985
O	0.793487	-0.000112	0.000971	C	0.402462	3.932350	1.195141
Li	-0.548194	1.239138	-0.021856	C	1.111887	2.729285	1.135687
C	2.112614	0.000672	0.000163	H	0.942096	1.962132	1.888352
C	2.839742	1.223574	0.074104	H	-0.334184	4.085073	1.980391
C	4.238748	1.203317	0.055886	H	0.113868	5.884938	0.315617
C	4.945501	0.002213	-0.001432	H	1.856159	5.534545	-1.426109
H	6.031397	0.002820	-0.002019	H	3.094664	3.394655	-1.539887
C	4.240006	-1.199674	-0.058008	H	-2.555181	-2.790879	-0.145730
C	2.841015	-1.221426	-0.074680	H	-2.493603	-2.259078	1.546292
C	2.097673	-2.507255	-0.146713	H	-3.843228	-3.243695	0.968961

Table S1 (Continued).



Ar = 2,6-diphenylphenyl
Ar'= 2,6-dimethylphenyl

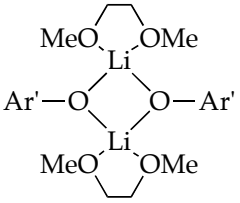


S29
G =-1786.854325
(-90 ºC)
see pg S101

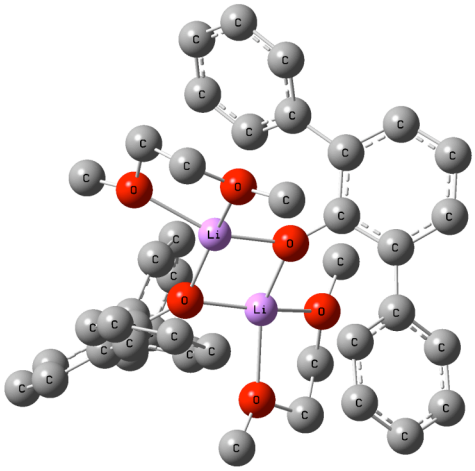
Atom	X	Y	Z	Atom	X	Y	Z
C	2.922316	0.881726	2.547005	C	1.811391	3.882882	0.189370
C	3.707459	0.889940	1.258510	H	1.524976	4.808744	0.327932
C	3.032446	0.631589	0.032396	H	2.559838	4.112587	0.959746
C	3.780214	0.643319	1.178697	H	2.243268	3.170374	0.511548
C	5.152898	0.906210	1.140702	C	2.192752	0.483567	0.013488
C	5.813195	1.163113	0.061665	C	3.171579	0.456398	0.461125
C	5.080262	1.152117	1.249462	C	4.523738	0.085865	0.521210
H	5.582971	1.350257	2.195272	C	4.959698	1.175595	0.128428
H	6.880421	1.367880	0.073119	H	6.012066	1.439385	0.181174
H	5.712416	0.909654	2.075292	C	4.020505	2.092951	0.334717
C	3.073869	0.362153	2.482730	C	2.655071	1.784690	0.412472
H	2.270967	1.084072	2.684234	C	1.728311	2.832195	0.920446
H	2.593961	0.626309	2.479730	C	1.927296	4.182608	0.570124
H	3.774317	0.395210	3.324620	H	2.713905	4.433694	0.136066
O	1.728396	0.390011	0.017323	C	1.137676	5.201052	1.104502
Li	0.652695	1.016296	0.621153	C	0.112951	4.899863	2.004487
O	0.920346	0.164964	0.078430	C	0.113545	3.565532	2.350202
Li	0.224422	1.237293	0.697256	H	0.902246	3.311729	3.054806
O	0.666922	3.262907	0.769247	C	0.675145	2.547896	1.811020
C	0.156298	3.970231	1.888403	H	0.483136	1.518656	2.087727
C	1.071337	3.235974	2.383002	H	0.497620	5.691813	2.430506
O	0.701638	1.879073	2.609739	H	1.325616	6.232926	0.816798
C	1.763241	1.116537	3.179464	H	4.353461	3.071613	0.671624
H	2.624303	1.068951	2.501709	H	5.243090	0.803099	0.909048
H	1.382122	0.108716	3.345580	C	2.799651	1.831532	0.894734
H	2.072346	1.550556	4.140906	C	3.622892	2.924951	0.558275
H	1.424866	3.699624	3.317048	C	3.344242	4.215782	1.009636
H	1.878481	3.286100	1.638745	C	2.226346	4.454846	1.811098
H	0.922660	4.016464	2.677610	C	1.392820	3.386376	2.147856
H	0.117633	4.998937	1.608584	C	1.670838	2.097444	1.692986

Atom	X	Y	Z
H	1.010351	1.282377	1.963340
H	0.520085	3.553817	2.774735
H	2.009318	5.457937	2.169173
H	4.003696	5.035307	0.733376
H	4.493130	2.756823	0.070801
O	2.073624	2.546096	0.946687
C	1.509448	3.623229	1.682715
C	0.738509	3.021167	2.839912
O	0.173803	2.072735	2.305300
C	1.046733	1.522526	3.284918
H	1.611918	2.319255	3.788101
H	1.742372	0.867488	2.760850
H	0.485482	0.950535	4.038004
H	0.199026	3.814302	3.379795
H	1.425643	2.526004	3.543870
H	2.302096	4.279001	2.074129
H	0.846621	4.217123	1.037884
C	3.031668	2.961455	0.024253
H	2.565281	3.606227	0.780100
H	3.854502	3.502991	0.462828
H	3.421852	2.055048	0.487332
H	2.472468	0.101489	2.739776
H	2.090865	1.599675	2.523278
H	3.562594	1.131912	3.400262

Table S1 (Continued).



Ar' = 2,6-diphenylphenyl

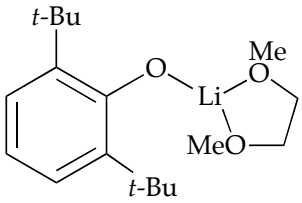


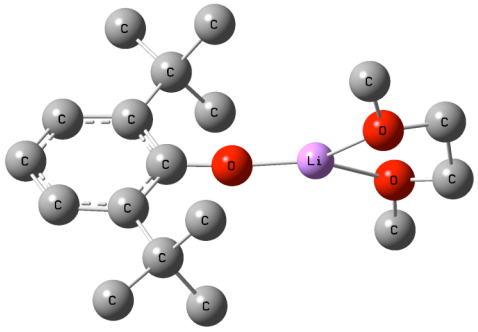
S30
G = -2170.22553
(-90 ºC)
see pg S101

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000543	-1.345001	-0.001585	C	1.630158	3.027726	-4.179925
O	-1.352142	0.001204	-0.000303	C	1.115672	1.772121	-3.846509
Li	0.000661	1.345772	0.003453	C	1.661894	1.038203	-2.792367
O	1.352585	-0.000337	0.002233	H	1.255828	0.063233	-2.550983
C	2.666593	-0.002825	0.002736	H	0.290270	1.354286	-4.418782
C	3.413854	0.732515	-0.980323	H	1.207880	3.595209	-5.005302
C	4.815891	0.710496	-0.954256	H	3.111785	4.516320	-3.684596
C	5.524303	-0.008822	0.003689	H	4.071573	3.217110	-1.819357
H	6.610534	-0.011108	0.004040	O	-1.083556	3.001697	-0.775687
C	4.812259	-0.725205	0.961157	C	-1.949784	2.977635	-1.905148
C	3.410158	-0.741312	0.986270	H	-1.377696	3.052991	-2.839130
C	2.740402	-1.537209	2.050994	H	-2.670068	3.806057	-1.851618
C	1.655853	-1.039711	2.797167	H	-2.489735	2.031330	-1.871561
H	1.254349	-0.062822	2.555905	C	-0.338576	4.208546	-0.668734
C	1.105826	-1.771542	3.850803	C	0.346926	4.206063	0.682090
C	1.614484	-3.029557	4.184046	O	1.087398	2.996279	0.787123
C	2.681419	-3.546301	3.446171	C	1.950909	2.965869	1.918499
H	3.089544	-4.524743	3.688946	H	2.674053	3.792049	1.869191
C	3.232099	-2.810770	2.395988	H	1.376787	3.040126	2.851337
H	4.056153	-3.229230	1.824555	H	2.487791	2.017877	1.883181
H	1.189261	-3.595368	5.009058	H	1.019664	5.074844	0.750791
H	0.282028	-1.350195	4.422811	H	-0.390728	4.264963	1.494915
H	5.351996	-1.272397	1.730426	H	0.399082	4.266329	-1.481618
H	5.358434	1.255331	-1.723217	H	-1.008073	5.079981	-0.735675
C	2.748294	1.530998	-2.045760	C	-2.666153	0.001926	-0.000744
C	3.245930	2.802134	-2.391041	C	-3.411663	-0.728414	-0.988887
C	2.699098	3.539820	-3.441718	C	-4.813723	-0.708833	-0.963469

Atom	X	Y	Z
C	-5.523820	0.003372	-0.001444
H	-6.610055	0.003867	-0.001682
C	-4.813492	0.715041	0.960790
C	-3.411417	0.733292	0.986797
C	-2.743515	1.524057	2.056547
C	-1.658564	1.023963	2.800374
C	-1.109951	1.750617	3.858305
C	-1.620461	3.006046	4.198382
H	-1.196325	3.567844	5.026690
C	-2.687872	3.525369	3.463031
H	-3.097486	4.501855	3.711105
C	-3.237166	2.794908	2.408583
H	-4.061626	3.215410	1.839229
H	-0.285783	1.327217	4.428266
H	-1.255505	0.049042	2.553801
H	-5.354549	1.256685	1.733056
H	-5.354963	-1.249761	-1.736108
C	-2.744090	-1.519036	-2.058954
C	-1.658268	-1.019333	-2.801787
C	-1.110214	-1.745278	-3.860495
C	-1.622162	-2.999630	-4.202373
H	-1.198509	-3.560800	-5.031353
C	-2.690363	-3.518646	-3.467927
C	-3.239126	-2.788867	-2.412718
H	-4.064292	-3.209084	-1.844175
H	-3.101286	-4.494184	-3.717579
H	-0.285335	-1.322153	-4.429637
H	-1.254032	-0.045269	-2.553764
O	-1.089695	-3.000002	0.772624
C	-0.347745	-4.208468	0.662742
C	0.338295	-4.204270	-0.687786
O	1.082110	-2.996188	-0.789310
C	1.947336	-2.965693	-1.919406
H	2.667271	-3.794757	-1.871521
H	2.487785	-2.019858	-1.880562
H	1.374269	-3.035069	-2.853243
H	1.008857	-5.074595	-0.758308
H	-0.399098	-4.259269	-1.501023
H	0.389363	-4.270130	1.475868
H	-1.019557	-5.078316	0.727229
C	-1.953844	-2.975891	1.903659
H	-1.380125	-3.054533	2.836381
H	-2.491414	-2.028122	1.872852
H	-2.676375	-3.802336	1.849822

Table S1 (Continued).

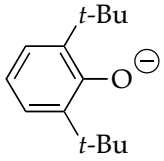


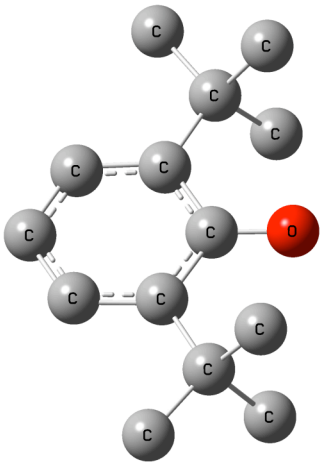


S31
G = -937.41487
(-90 ºC)
see pg S102

Atom	X	Y	Z
C	-4.350731	-0.082719	-0.843778
H	-4.398580	0.957869	-1.197646
H	-5.193713	-0.639529	-1.277073
C	-4.418833	-0.135722	0.670973
H	-5.302839	0.412851	1.025804
H	-4.487696	-1.176567	1.020459
O	-3.224416	0.463341	1.167771
Li	-1.688627	-0.083812	0.032261
O	-3.110567	-0.669183	-1.230942
C	-2.912675	-0.730110	-2.645393
H	-1.929067	-1.173475	-2.804529
H	-3.682588	-1.358087	-3.111071
H	-2.941525	0.274875	-3.086327
O	-0.003008	-0.032629	0.094986
C	1.312322	0.032060	0.026469
C	2.104217	-1.167517	0.074690
C	3.495980	-1.059609	-0.009240
H	4.108445	-1.954272	0.023109
C	4.136260	0.169804	-0.134200
H	5.220237	0.222565	-0.197684
C	3.370158	1.330993	-0.173376
C	1.974140	1.303143	-0.094571
C	1.163916	2.618695	-0.134325
C	2.062718	3.867977	-0.254459
H	2.751995	3.960713	0.592446
H	2.654808	3.863029	-1.176797
H	1.435591	4.768062	-0.269339
C	0.348567	2.784268	1.171626
H	1.022765	2.891982	2.029933
H	-0.283331	3.682266	1.124438
H	-0.283667	1.911345	1.346298
C	0.220693	2.635130	-1.362455
H	0.803612	2.604390	-2.290950
H	-0.446011	1.769873	-1.357039
H	-0.385316	3.551941	-1.374765
H	3.885790	2.280685	-0.267883
C	1.436160	-2.553821	0.218978
C	2.462079	-3.706604	0.266050
H	3.147621	-3.613637	1.116038
H	1.931887	-4.661109	0.373513
H	3.060801	-3.763242	-0.650250
C	0.626377	-2.624817	1.536765
H	1.296782	-2.540589	2.400592
H	-0.098239	-1.809830	1.591238
H	0.095550	-3.583998	1.615252
C	0.513894	-2.834181	-0.992580
H	1.100426	-2.866414	-1.918880
H	0.007199	-3.802809	-0.879693
H	-0.240199	-2.051197	-1.096167
C	-3.159645	0.538051	2.593421
H	-2.198632	0.991412	2.839248
H	-3.974245	1.163389	2.979802
H	-3.221643	-0.463418	3.039049

Table S1 (Continued).



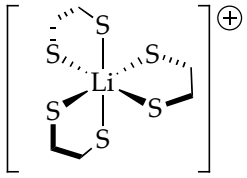


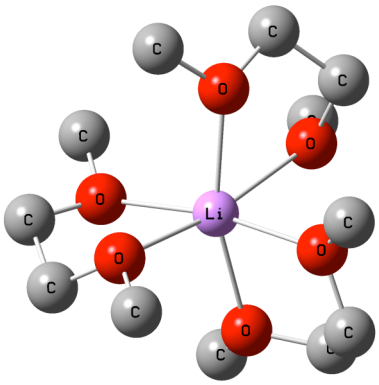
S32
G =-621.110315
(-90 ºC)
see pg S102

Atom	X	Y	Z
C	2.580348	-0.309132	-0.000034
C	1.242466	0.457692	0.000044
C	0.000004	-0.304851	0.000165
C	-1.242463	0.457686	0.000014
C	-1.201859	1.851771	0.000041
H	-2.131585	2.417662	0.000034
C	-0.000002	2.565204	0.000051
H	-0.000005	3.654006	0.000116
C	1.201859	1.851778	0.000033
H	2.131582	2.417673	-0.000005
C	-2.580347	-0.309135	-0.000033
C	-3.807362	0.623394	-0.000205
H	-3.832567	1.268693	-0.887531
H	-4.727406	0.022651	0.000160
H	-3.832304	1.269370	0.886640
C	-2.668588	-1.204111	-1.260747
H	-2.677805	-0.587119	-2.169346
H	-1.799633	-1.864740	-1.289379

Atom	X	Y	Z
H	-3.589815	-1.807391	-1.251249
C	-2.668761	-1.203950	1.260778
H	-2.677889	-0.586859	2.169310
H	-3.590084	-1.807085	1.251339
H	-1.799915	-1.864723	1.289505
O	0.000008	-1.590616	0.000210
C	3.807373	0.623385	-0.000277
H	3.832303	1.268977	-0.887400
H	3.832600	1.269068	0.886771
H	4.727410	0.022633	-0.000393
C	2.668514	-1.204149	-1.260723
H	2.677770	-0.587177	-2.169334
H	3.589694	-1.807502	-1.251218
H	1.799505	-1.864708	-1.289342
C	2.668815	-1.203913	1.260795
H	2.678247	-0.586779	2.169294
H	1.799829	-1.864489	1.289730
H	3.590012	-1.807240	1.251204

Table S1 (Continued).

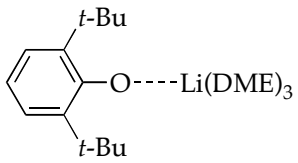


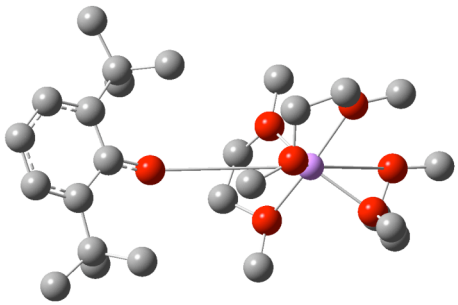


S33
G =-933.651556
(-90 ºC)
see pg S102

Atom	X	Y	Z
Li	-0.125337	0.042745	-0.039737
O	2.179459	-0.262614	0.727516
C	2.860212	-0.269250	-0.529438
C	2.234468	-1.276898	-1.477107
O	0.862027	-0.923565	-1.654213
C	0.186689	-1.771677	-2.582846
H	0.217591	-2.819117	-2.252420
H	-0.847654	-1.429629	-2.625929
H	0.645069	-1.699918	-3.577662
H	2.304910	-2.298297	-1.073272
H	2.758263	-1.256745	-2.444292
H	3.926666	-0.491477	-0.397471
H	2.764842	0.737682	-0.943257
C	2.846288	-1.004888	1.745565
H	2.221346	-0.955226	2.639720
H	2.987253	-2.057427	1.463143
H	3.826546	-0.565002	1.970343
O	-1.020854	-1.757358	0.875443
C	-2.335302	-2.006175	0.380178
C	-2.986415	-0.680012	0.060358
O	-2.150514	0.014659	-0.864280
C	-2.791408	1.171603	-1.401567
H	-3.038721	1.890761	-0.609475
H	-2.095998	1.625714	-2.107152
H	-3.710836	0.889883	-1.930447
H	-3.976780	-0.861579	-0.380558
H	-3.115961	-0.075254	0.969027
H	-2.280537	-2.633217	-0.521633
H	-2.933550	-2.539101	1.133467
C	-0.342451	-2.964434	1.216323
H	-0.887371	-3.508600	1.998685
H	-0.235086	-3.616159	0.338469
H	0.643826	-2.687901	1.587461
O	0.480389	1.978431	-0.755487
C	0.176309	3.018555	0.171671
C	0.293042	2.452503	1.570773
O	-0.512648	1.275952	1.649314
C	-0.609676	0.776853	2.983835
H	0.387186	0.595932	3.408142
H	-1.145667	1.489723	3.623136
H	-1.158972	-0.162814	2.931074
H	1.336387	2.193704	1.796149
H	-0.051756	3.202470	2.296522
H	0.882456	3.853447	0.058840
H	-0.838670	3.398211	-0.015752
C	0.640568	2.448856	-2.092070
H	1.503900	3.123284	-2.164520
H	0.804825	1.569293	-2.715599
H	-0.254294	2.984864	-2.435917

Table S1 (Continued).



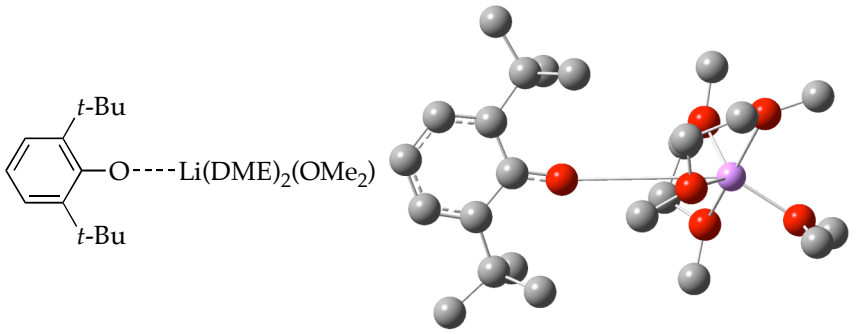


S34
G = -1554.847684
(-90 °C)
see pg S102

Atom	X	Y	Z	Atom	X	Y	Z
Li	2.288924	-0.056393	0.328573	H	-0.472963	-0.562858	3.211541
O	3.956190	-1.308135	0.754839	O	1.447783	-1.490807	-0.937720
C	4.888699	-1.925650	-0.129681	C	0.458322	-0.854485	-1.776403
C	4.814663	-1.276056	-1.504021	C	1.068534	0.431464	-2.287072
O	5.303394	0.057848	-1.537285	O	1.612883	1.143807	-1.172032
C	6.709075	0.152382	-1.695633	C	1.998416	2.472877	-1.509231
H	6.952537	1.216370	-1.745343	H	2.762101	2.468491	-2.299696
H	7.259874	-0.295795	-0.855158	H	1.126797	3.047660	-1.845829
H	7.037337	-0.332984	-2.627101	H	2.409352	2.919571	-0.604585
H	5.366330	-1.904791	-2.220708	H	1.873165	0.242861	-3.015317
H	3.767809	-1.238063	-1.816859	H	0.286098	1.029563	-2.771013
H	5.901512	-1.843119	0.293480	H	0.227601	-1.507209	-2.631083
H	4.654417	-2.997867	-0.224642	H	-0.463453	-0.665265	-1.208267
C	4.037800	-1.824384	2.080422	C	1.076161	-2.820229	-0.584050
H	5.019386	-1.606958	2.524855	H	1.078385	-3.468770	-1.471203
H	3.249701	-1.339222	2.657404	H	1.819993	-3.182169	0.130303
H	3.879721	-2.912305	2.087585	H	0.079043	-2.846325	-0.130705
O	1.202591	-0.013611	2.097403	O	-2.156028	-0.192782	-0.275912
C	1.133668	1.354219	2.500683	C	-3.426902	0.048462	-0.092748
C	2.554972	1.867402	2.601144	C	-4.378049	-1.025175	0.124060
O	3.196279	1.612441	1.356070	C	-3.930905	-2.498677	-0.001534
C	4.580074	1.940126	1.350236	C	-5.083326	-3.500417	0.216475
H	4.724783	3.021396	1.483522	H	-5.510452	-3.425133	1.223623
H	5.110720	1.408908	2.153491	H	-5.894093	-3.359507	-0.507504
H	4.972140	1.621695	0.383958	H	-4.705318	-4.523886	0.094026
H	3.095679	1.347686	3.407086	C	-2.838331	-2.827055	1.041509
H	2.554641	2.944799	2.824936	H	-3.221571	-2.690904	2.060955
H	0.644776	1.437013	3.481910	H	-2.502387	-3.870506	0.943890
H	0.549165	1.933036	1.775351	H	-1.994665	-2.153331	0.893056
C	-0.068396	-0.693539	2.199864	C	-3.372207	-2.744661	-1.424256
H	-0.786199	-0.337564	1.447954	H	-4.163685	-2.617793	-2.172907
H	0.141291	-1.751916	2.038305	H	-2.576648	-2.028808	-1.638870

Atom	X	Y	Z
H	-2.978140	-3.767436	-1.520566
C	-5.709190	-0.716581	0.413738
C	-6.176060	0.595447	0.469187
C	-5.290590	1.632580	0.183904
C	-3.945049	1.402808	-0.113250
C	-3.022290	2.578305	-0.502921
C	-3.745850	3.939948	-0.503624
H	-4.128653	4.202802	0.489744
H	-3.043794	4.728022	-0.806411
H	-4.586558	3.958101	-1.206476
C	-1.835716	2.690409	0.482312
H	-2.197898	2.869216	1.503034
H	-1.273636	1.755731	0.464404
H	-1.176059	3.527727	0.205490
C	-2.478052	2.343404	-1.933018
H	-3.294641	2.371877	-2.664573
H	-1.750787	3.122358	-2.210886
H	-2.000974	1.362318	-1.984051
H	-5.674595	2.648452	0.190699
H	-7.217091	0.803872	0.704454
H	-6.418436	-1.517505	0.599508

Table S1 (Continued).



S35
G = -1401.074951
(-90 °C)
see pg S102

Atom	X	Y	Z	Atom	X	Y	Z
Li	-2.757092	-0.217902	0.094217	H	-2.860418	2.373394	2.814684
O	-4.454943	-1.378406	-0.090207	H	-1.271123	2.825857	2.123277
C	-5.150116	-1.952763	1.010227	H	-2.718365	2.773967	1.074422
H	-4.600099	-1.681690	1.912373	H	-2.063527	0.033794	3.419725
H	-6.178905	-1.569993	1.066946	H	-0.493139	0.789827	3.017962
H	-5.181902	-3.047589	0.923073	H	-0.517329	-1.752127	2.846960
C	-5.012586	-1.736715	-1.348369	H	0.060986	-0.891198	1.382100
H	-6.036320	-1.349392	-1.452355	C	-1.580422	-2.997526	0.850797
H	-4.369375	-1.302408	-2.114923	H	-1.520128	-3.670848	1.717003
H	-5.034180	-2.829099	-1.466998	H	-2.394271	-3.320237	0.197078
O	-1.925184	-0.121408	-1.775978	H	-0.628704	-3.033584	0.308362
C	-1.932445	1.236853	-2.214154	O	1.602165	-0.187683	0.333357
C	-3.355705	1.743814	-2.123478	C	2.819920	0.093101	-0.047948
O	-3.804708	1.556524	-0.783915	C	3.765259	-0.948434	-0.401244
C	-5.159956	1.932053	-0.591187	C	3.413245	-2.433629	-0.162570
H	-5.307748	2.997995	-0.813673	C	4.556471	-3.393225	-0.549593
H	-5.831164	1.339493	-1.228964	H	4.798027	-3.337513	-1.617889
H	-5.400562	1.745770	0.457413	H	5.472643	-3.189499	0.016349
H	-4.008158	1.186496	-2.813294	H	4.256057	-4.426595	-0.332958
H	-3.393669	2.808913	-2.397108	C	2.173108	-2.845482	-0.988723
H	-1.591947	1.299331	-3.257873	H	2.362165	-2.717989	-2.062514
H	-1.256326	1.838954	-1.595347	H	1.918675	-3.901756	-0.814252
C	-0.652022	-0.770200	-2.000125	H	1.332582	-2.212617	-0.704400
H	0.122213	-0.390854	-1.318977	C	3.120092	-2.650431	1.342250
H	-0.817743	-1.832642	-1.816844	H	4.023079	-2.467233	1.937223
H	-0.350670	-0.633321	-3.046173	H	2.342942	-1.959121	1.674188
O	-1.884639	-1.670536	1.271637	H	2.793394	-3.683163	1.535044
C	-0.808115	-1.077429	2.028468	C	5.014833	-0.595634	-0.916739
C	-1.334665	0.214028	2.613779	C	5.411638	0.731861	-1.068192
O	-1.977228	0.952554	1.567999	C	4.548747	1.740083	-0.643606
C	-2.217857	2.310348	1.923897	C	3.283423	1.465036	-0.119475

Atom	X	Y	Z
C	2.397541	2.608512	0.420122
C	3.067072	3.993436	0.312601
H	3.272650	4.272209	-0.727893
H	2.399974	4.757226	0.733569
H	4.011144	4.036866	0.867468
C	1.064770	2.680547	-0.360920
H	1.254455	2.868496	-1.425920
H	0.542804	1.728124	-0.254013
H	0.431870	3.498115	0.018589
C	2.097623	2.355104	1.917876
H	3.020900	2.403473	2.507624
H	1.406543	3.114950	2.315266
H	1.659985	1.361623	2.039108
H	4.887450	2.768939	-0.723385
H	6.388250	0.974853	-1.480106
H	5.715446	-1.372712	-1.207906