Supporting Information

Solid-State and Solution Structures of Glycinimine-Derived Lithium Enolates

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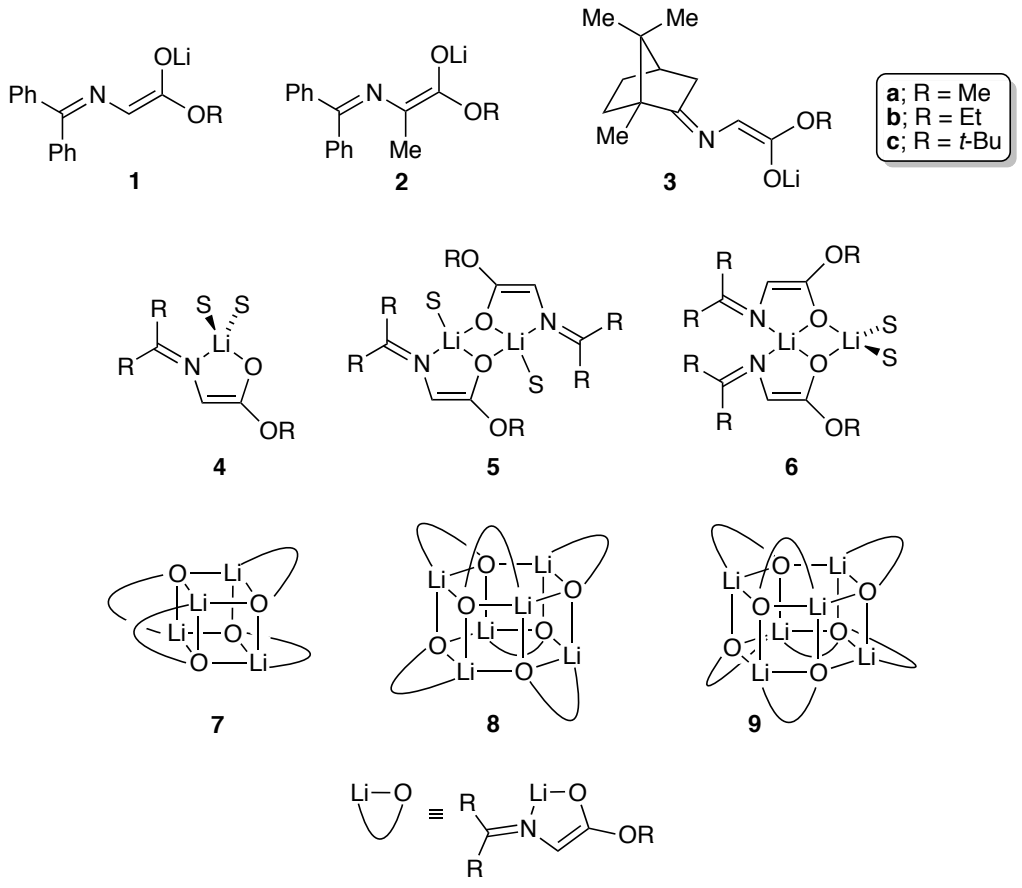
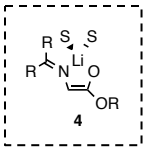
Structures



I. X-ray Crystal Structures



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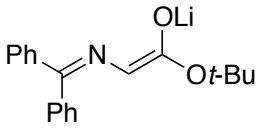


1c

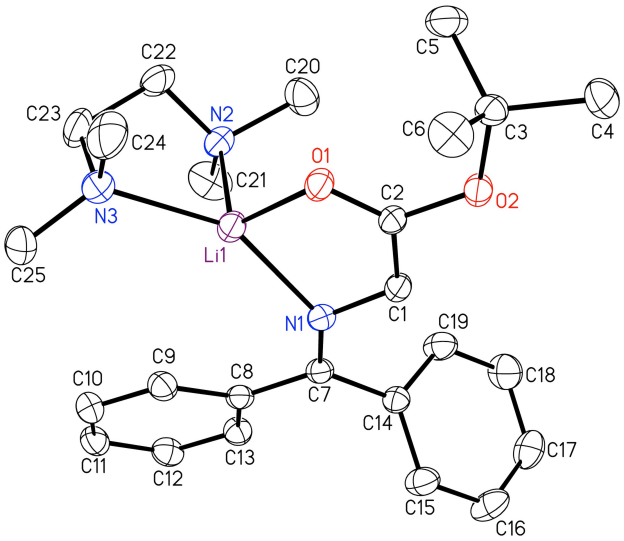


Figure 1. X-ray crystal structure and data of TMEDA-solvated monomer **4c**.

Table 1. Crystal data and structure refinement for **4c**.

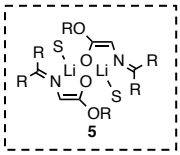
Identification code	4c	
Empirical formula	C25 H36 Li N3 O2	
Formula weight	417.51	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.532(3) Å	a= 90°.
	b = 8.758(3) Å	b= 97.382(12)°.
	c = 26.851(9) Å	g = 90°.
Volume	2456.2(13) Å^3	
Z	4	
Density (calculated)	1.129 Mg/m^3	

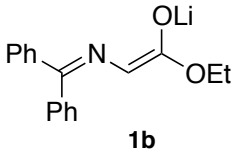
Absorption coefficient	0.071 mm^{-1}
F(000)	904
Crystal size	0.40 x 0.20 x 0.10 mm^3
Theta range for data collection	2.45 to 28.28°.
Index ranges	-13<=h<=14, -7<=k<=11, -35<=l<=31
Reflections collected	21418
Independent reflections	6028 [R(int) = 0.0285]
Completeness to theta = 28.28°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9929 and 0.9722
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6028 / 262 / 433
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1022
R indices (all data)	R1 = 0.0601, wR2 = 0.1127
Largest diff. peak and hole	0.231 and -0.176 e.$Å^{-3}$

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

	x	y	z	U(eq)
Li(1)	11169(2)	10676(2)	1618(1)	29(1)
O(1)	9923(1)	12017(1)	1832(1)	29(1)
O(2)	9012(1)	14277(1)	1541(1)	29(1)
N(1)	11876(1)	12513(1)	1263(1)	24(1)
C(1)	10902(1)	13543(1)	1267(1)	26(1)
C(2)	9955(1)	13190(1)	1566(1)	24(1)
C(3)	7910(1)	14108(1)	1814(1)	28(1)
C(4)	7125(1)	15524(2)	1655(1)	44(1)
C(5)	7151(1)	12681(2)	1647(1)	40(1)
C(6)	8340(2)	14116(2)	2373(1)	41(1)
C(7)	12781(1)	12658(1)	976(1)	25(1)

C(8)	13798(1)	11497(1)	1001(1)	25(1)
C(9)	14008(1)	10441(1)	1396(1)	30(1)
C(10)	14934(1)	9314(1)	1402(1)	35(1)
C(11)	15700(1)	9223(1)	1023(1)	35(1)
C(12)	15527(1)	10268(2)	635(1)	34(1)
C(13)	14589(1)	11386(1)	623(1)	30(1)
C(14)	12784(1)	13924(1)	603(1)	25(1)
C(15)	13689(1)	15082(2)	665(1)	37(1)
C(16)	13693(2)	16234(2)	309(1)	46(1)
C(17)	12802(1)	16236(2)	-111(1)	44(1)
C(18)	11887(1)	15105(2)	-178(1)	45(1)
C(19)	11879(1)	13962(2)	180(1)	37(1)
C(20)	9225(5)	9998(6)	762(2)	45(1)
C(21)	11187(7)	8674(8)	703(3)	53(1)
N(2)	10332(5)	9266(7)	1050(2)	32(1)
C(22)	9889(3)	8007(3)	1354(1)	44(1)
C(23)	10944(3)	7491(2)	1758(1)	45(1)
N(3)	11411(6)	8758(8)	2098(2)	33(1)
C(24)	10512(3)	9026(4)	2464(1)	55(1)
C(25)	12629(4)	8262(8)	2386(2)	42(1)
C(20')	9102(13)	9675(19)	907(6)	62(3)
C(21')	11091(15)	9100(20)	627(6)	52(3)
N(2')	10396(14)	9133(18)	1063(5)	37(3)
C(22')	10493(10)	7716(8)	1342(3)	55(2)
C(23')	10300(8)	7937(9)	1881(3)	57(2)
N(3')	11345(14)	8775(18)	2161(5)	30(2)
C(24')	10961(10)	9333(11)	2645(3)	55(2)
C(25')	12564(13)	7970(20)	2250(6)	67(4)





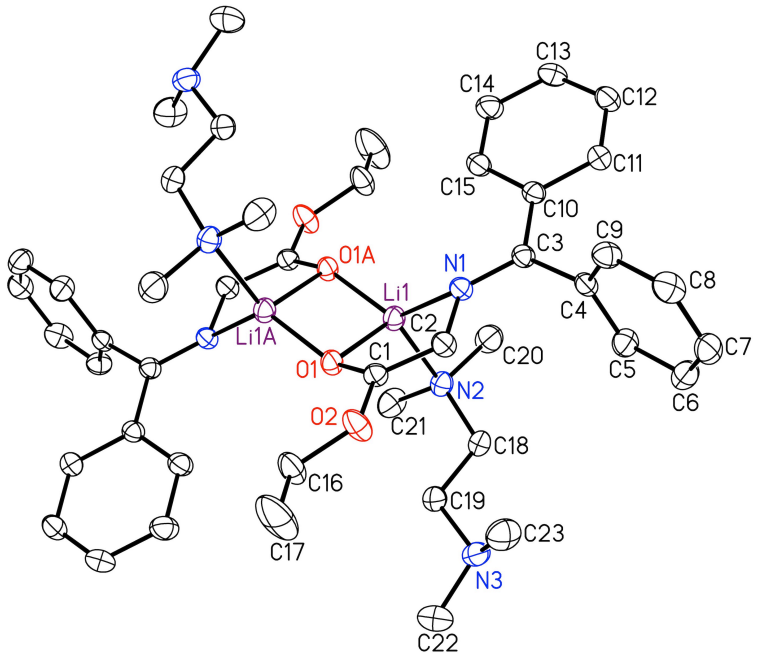


Figure 2. X-ray crystal structure and data of TMEDA-solvated dimer **5b**.

Table 3. Crystal data and structure refinement for **5b**.

Identification code	5b	
Empirical formula	C46 H64 Li2 N6 O4	
Formula weight	778.91	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.0340(4) Å	a= 106.481(2)°.
	b = 11.0213(6) Å	b= 91.063(2)°.
	c = 11.9901(7) Å	g = 101.589(2)°.
Volume	1117.79(10) $Å^3$	
Z	1	
Density (calculated)	1.157 Mg/m^3	

Absorption coefficient	0.073 mm^{-1}
F(000)	420
Crystal size	0.45 x 0.20 x 0.10 mm^3
Theta range for data collection	2.23 to 28.28°.
Index ranges	-12<=h<=12, -14<=k<=14, -15<=l<=15
Reflections collected	18543
Independent reflections	5460 [R(int) = 0.0226]
Completeness to theta = 28.28°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9927 and 0.9677
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5460 / 0 / 379
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.1036
R indices (all data)	R1 = 0.0522, wR2 = 0.1112
Largest diff. peak and hole	0.269 and -0.217 e.$Å^{-3}$

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

	x	y	z	U(eq)
Li(1)	4763(2)	5084(2)	3979(2)	28(1)
O(1)	4370(1)	3611(1)	4652(1)	26(1)
O(2)	3776(1)	1431(1)	3770(1)	38(1)
N(1)	5790(1)	3908(1)	2663(1)	25(1)
N(2)	2858(1)	5531(1)	3311(1)	30(1)
N(3)	-46(1)	2388(1)	2181(1)	36(1)
C(1)	4387(1)	2667(1)	3753(1)	25(1)
C(2)	4962(1)	2735(1)	2714(1)	27(1)
C(3)	6405(1)	4028(1)	1710(1)	25(1)
C(4)	6028(1)	2962(1)	582(1)	25(1)
C(5)	4675(1)	2811(1)	-59(1)	33(1)

C(6)	4244(1)	1812(1)	-1089(1)	38(1)
C(7)	5166(1)	947(1)	-1483(1)	38(1)
C(8)	6511(1)	1089(1)	-854(1)	38(1)
C(9)	6954(1)	2092(1)	173(1)	32(1)
C(10)	7477(1)	5236(1)	1742(1)	25(1)
C(11)	8130(1)	5410(1)	735(1)	30(1)
C(12)	9181(1)	6524(1)	763(1)	35(1)
C(13)	9605(1)	7501(1)	1800(1)	37(1)
C(14)	8975(1)	7346(1)	2809(1)	37(1)
C(15)	7939(1)	6232(1)	2790(1)	32(1)
C(16)	2954(2)	1272(1)	4737(1)	42(1)
C(17)	2529(3)	-129(2)	4617(2)	80(1)
C(18)	1726(1)	4484(1)	2494(1)	31(1)
C(19)	849(1)	3521(1)	3057(1)	33(1)
C(20)	3566(2)	6423(1)	2671(1)	44(1)
C(21)	2149(2)	6240(1)	4311(1)	43(1)
C(22)	-1243(2)	1714(2)	2717(2)	57(1)
C(23)	882(2)	1500(1)	1596(1)	49(1)

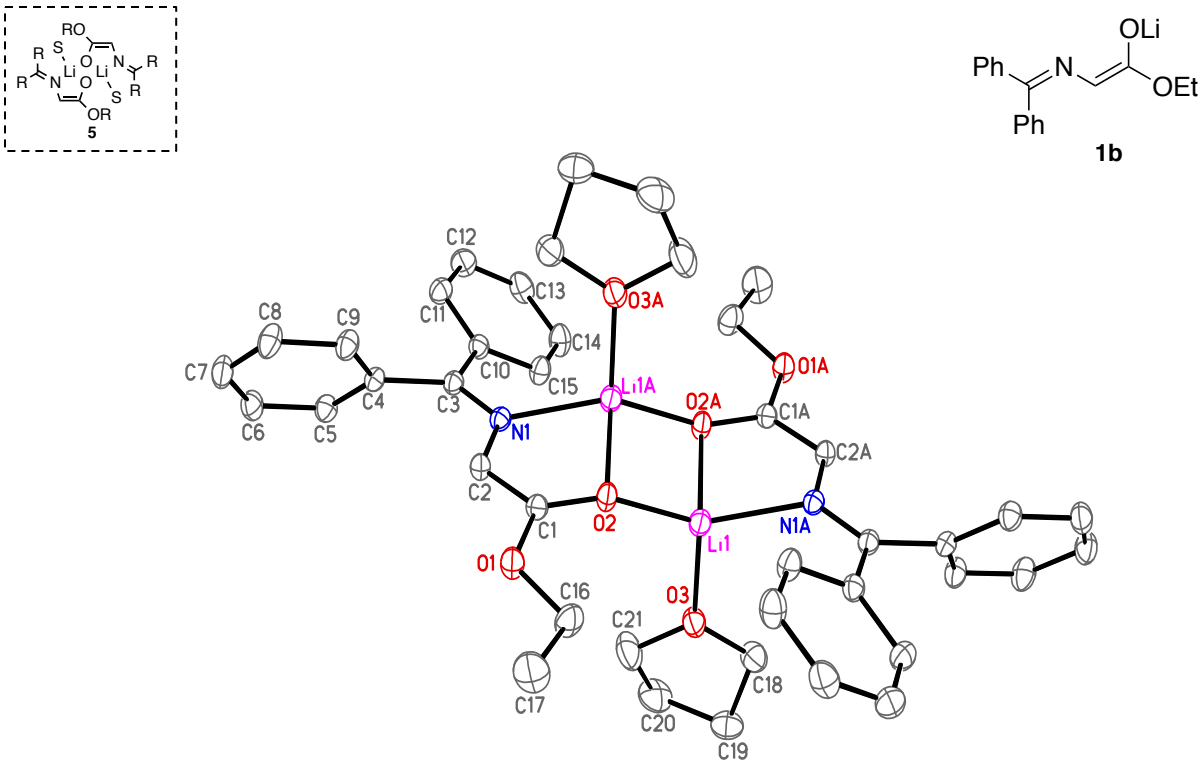


Figure 3. X-ray crystal structure of THF-solvated dimer **5b**.

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

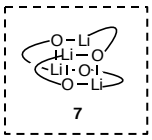
Identification code	5b	
Empirical formula	C42 H48 Li2 N2 O6	
Formula weight	690.70	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2312(5) Å	a= 88.233(3)°.
	b = 10.1683(7) Å	b= 85.265(3)°.
	c = 10.2843(7) Å	g = 79.988(3)°.
Volume	947.26(11) $Å^3$	
Z	1	
Density (calculated)	1.211 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	368	

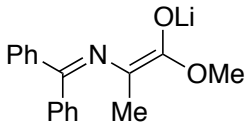
Crystal size	0.60 x 0.20 x 0.10 mm^3
Theta range for data collection	1.99 to 28.28°.
Index ranges	-11<=h<=12, -13<=k<=13, -13<=l<=13
Reflections collected	18039
Independent reflections	4671 [R(int) = 0.0196]
Completeness to theta = 28.28°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9921 and 0.9539
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4671 / 0 / 334
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0999
R indices (all data)	R1 = 0.0434, wR2 = 0.1050
Largest diff. peak and hole	0.260 and -0.227 e.$Å^{-3}$

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Li(1)	6032(2)	-248(2)	4012(2)	25(1)
O(1)	2229(1)	701(1)	2586(1)	28(1)
O(2)	3968(1)	141(1)	4051(1)	25(1)
O(3)	6879(1)	1097(1)	2992(1)	32(1)
N(1)	2206(1)	1837(1)	5834(1)	20(1)
C(1)	2719(1)	793(1)	3790(1)	20(1)
C(2)	1742(1)	1608(1)	4639(1)	22(1)
C(3)	1381(1)	2617(1)	6695(1)	21(1)
C(4)	-200(1)	3199(1)	6531(1)	21(1)
C(5)	-695(1)	4574(1)	6521(1)	26(1)
C(6)	-2170(1)	5100(1)	6363(1)	31(1)
C(7)	-3167(1)	4248(1)	6220(1)	33(1)
C(8)	-2689(1)	2877(1)	6226(1)	33(1)

C(9)	-1217(1)	2353(1)	6381(1)	28(1)
C(10)	2049(1)	2965(1)	7867(1)	22(1)
C(11)	1178(1)	3419(1)	8999(1)	29(1)
C(12)	1814(1)	3784(1)	10083(1)	35(1)
C(13)	3330(1)	3710(1)	10062(1)	35(1)
C(14)	4215(1)	3253(1)	8952(1)	34(1)
C(15)	3581(1)	2888(1)	7869(1)	28(1)
C(16)	3261(1)	59(1)	1587(1)	36(1)
C(17)	2444(2)	-99(2)	432(1)	50(1)
C(18)	8449(1)	1065(1)	2744(1)	35(1)
C(19)	8674(4)	2325(3)	2015(3)	38(1)
C(20)	7372(3)	3298(2)	2636(3)	49(1)
C(19')	8491(7)	2601(6)	2522(8)	45(1)
C(20')	7026(5)	3139(4)	1970(7)	49(1)
C(21)	6108(2)	2435(1)	2808(2)	49(1)





2a

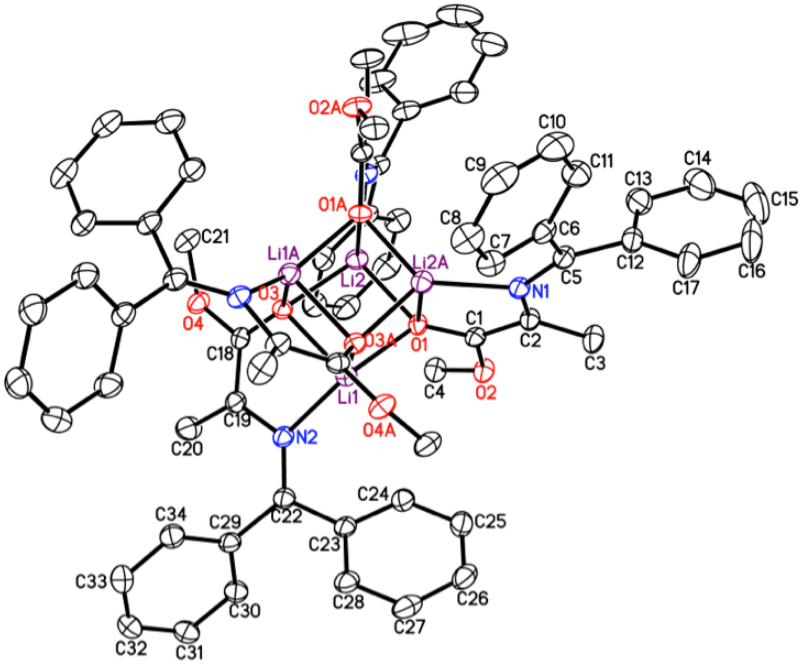


Figure 4. X-ray crystal structure of the unsolvated S_4 tetramer **7a**.

Table 7. Crystal data and structure refinement for **7a**.

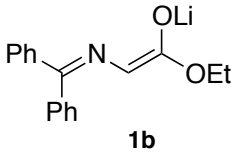
Identification code	7a	
Empirical formula	C68 H64 Li4 N4 O8	
Formula weight	1092.99	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 24.9263(16) Å	a= 90°.
	b = 12.4099(7) Å	b= 95.483(3)°.
	c = 22.9880(14) Å	g = 90°.
Volume	7078.4(7) $Å^3$	
Z	4	
Density (calculated)	1.026 Mg/m^3	
Absorption coefficient	0.066 mm^{-1}	

F(000)	2304
Crystal size	0.60 x 0.20 x 0.20 mm^3
Theta range for data collection	1.83 to 28.28°.
Index ranges	-33<=h<=33, -16<=k<=16, -30<=l<=30
Reflections collected	35462
Independent reflections	8788 [R(int) = 0.0308]
Completeness to theta = 28.28°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9869 and 0.9614
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8788 / 0 / 463
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1293
R indices (all data)	R1 = 0.0725, wR2 = 0.1404
Largest diff. peak and hole	0.248 and -0.221 e.$Å^{-3}$

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Li(1)	-54(1)	9671(2)	3074(1)	30(1)
Li(2)	530(1)	11232(2)	2623(1)	30(1)
O(1)	-51(1)	11255(1)	3128(1)	26(1)
O(2)	-49(1)	12015(1)	4028(1)	33(1)
O(3)	584(1)	9662(1)	2600(1)	27(1)
O(4)	1428(1)	8941(1)	2648(1)	35(1)
N(1)	-931(1)	12428(1)	2737(1)	28(1)
N(2)	340(1)	8449(1)	3515(1)	30(1)
C(1)	-264(1)	11941(1)	3463(1)	26(1)
C(2)	-696(1)	12598(1)	3303(1)	29(1)
C(3)	-913(1)	13347(1)	3741(1)	44(1)
C(4)	495(1)	11653(1)	4157(1)	35(1)

C(5)	-1296(1)	13029(1)	2454(1)	31(1)
C(6)	-1544(1)	12618(1)	1884(1)	32(1)
C(7)	-1571(1)	11513(1)	1772(1)	37(1)
C(8)	-1787(1)	11121(2)	1236(1)	48(1)
C(9)	-1988(1)	11824(2)	804(1)	53(1)
C(10)	-1972(1)	12907(2)	909(1)	54(1)
C(11)	-1752(1)	13316(2)	1443(1)	44(1)
C(12)	-1463(1)	14131(1)	2625(1)	38(1)
C(13)	-1084(1)	14961(1)	2689(1)	49(1)
C(14)	-1239(1)	15995(2)	2818(1)	73(1)
C(15)	-1772(2)	16204(2)	2891(1)	94(1)
C(16)	-2147(1)	15401(3)	2829(1)	87(1)
C(17)	-2001(1)	14356(2)	2689(1)	57(1)
C(18)	929(1)	8985(1)	2849(1)	28(1)
C(19)	841(1)	8311(1)	3304(1)	31(1)
C(20)	1286(1)	7604(1)	3581(1)	44(1)
C(21)	1467(1)	9319(1)	2069(1)	40(1)
C(22)	119(1)	7802(1)	3868(1)	31(1)
C(23)	-386(1)	8187(1)	4095(1)	32(1)
C(24)	-451(1)	9276(1)	4219(1)	37(1)
C(25)	-931(1)	9661(1)	4401(1)	46(1)
C(26)	-1351(1)	8966(1)	4466(1)	47(1)
C(27)	-1289(1)	7876(2)	4359(1)	45(1)
C(28)	-809(1)	7488(1)	4181(1)	37(1)
C(29)	299(1)	6693(1)	4036(1)	32(1)
C(30)	403(1)	6413(1)	4620(1)	36(1)
C(31)	567(1)	5377(1)	4774(1)	44(1)
C(32)	615(1)	4613(1)	4353(1)	46(1)
C(33)	498(1)	4869(1)	3772(1)	49(1)
C(34)	344(1)	5910(1)	3612(1)	42(1)



1b

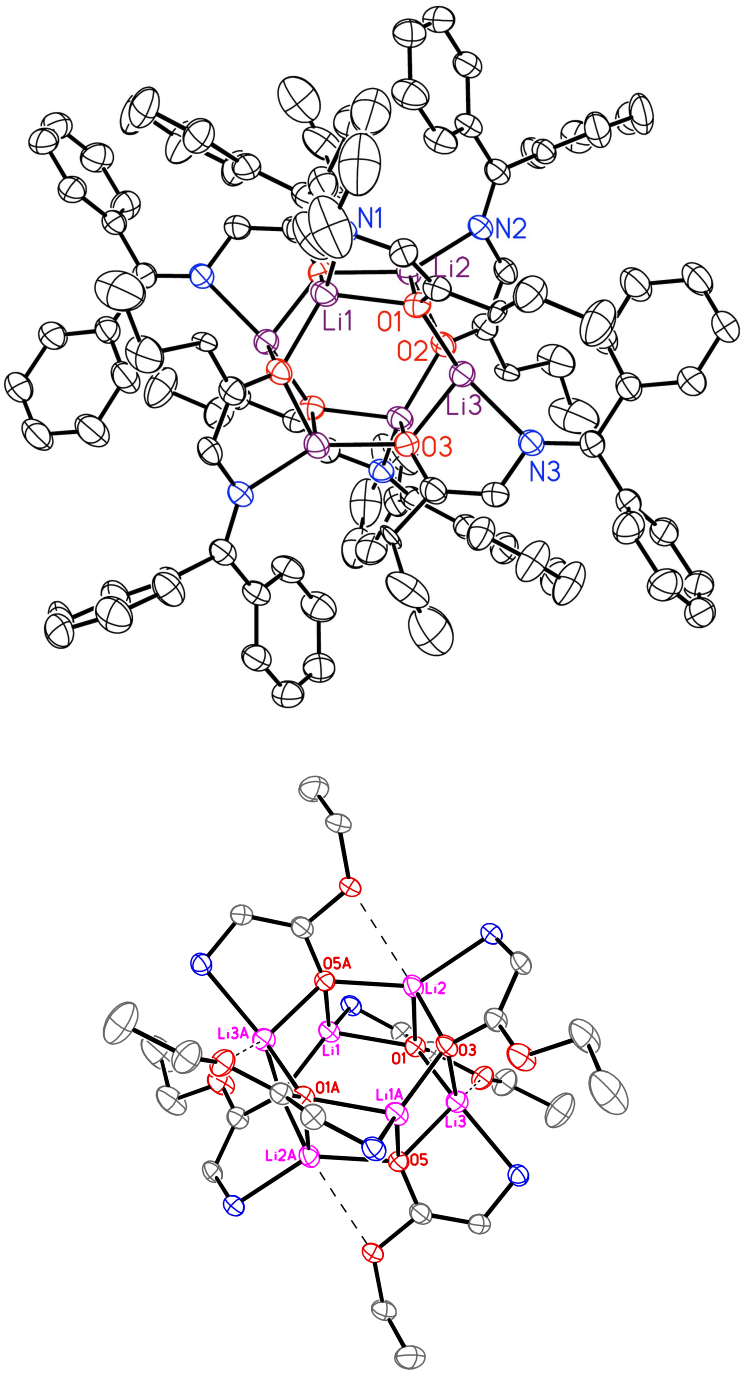


Figure 5. X-ray crystal structure of the core of unsolvated S_6 hexamer **8b**. Phenyl groups were removed from the bottom structure for clarity.

Table 9. Crystal data and structure refinement for **8b**.

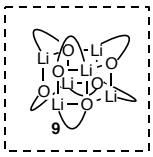
Identification code	8b	
Empirical formula	C102 H96 Li6 N6 O12	
Formula weight	1639.49	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.3105(6) Å	a= 90°.
	b = 16.9749(9) Å	b= 103.885(3)°.
	c = 25.2304(13) Å	g = 90°.
Volume	5118.3(5) $Å^3$	
Z	2	
Density (calculated)	1.064 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	1728	
Crystal size	0.50 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.71 to 24.77°.	
Index ranges	-14<=h<=14, -19<=k<=19, -29<=l<=29	
Reflections collected	66389	
Independent reflections	8740 [R(int) = 0.0304]	
Completeness to theta = 24.77°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9797 and 0.9665	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8740 / 247 / 699	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0505, wR2 = 0.1391	
R indices (all data)	R1 = 0.0675, wR2 = 0.1486	
Largest diff. peak and hole	0.229 and -0.197 e.$Å^{-3}$	

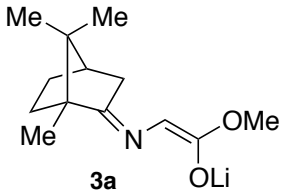
Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Li(1)	4700(2)	-3940(2)	423(1)	39(1)
Li(2)	6468(2)	-4266(2)	15(1)	39(1)
Li(3)	4799(2)	-4631(2)	-884(1)	39(1)
O(1)	4952(1)	-3819(1)	-324(1)	36(1)
O(3)	6239(1)	-5169(1)	-492(1)	36(1)
O(4)	7060(1)	-5851(1)	-1025(1)	56(1)
O(5)	3878(1)	-5482(1)	-709(1)	36(1)
N(1)	4445(1)	-2700(1)	370(1)	39(1)
N(2)	7841(1)	-4010(1)	-311(1)	36(1)
N(3)	3968(1)	-4861(1)	-1710(1)	38(1)
C(1)	4177(2)	-2586(1)	-190(1)	39(1)
C(2)	4468(1)	-3159(1)	-504(1)	36(1)
O(2)	4266(1)	-3109(1)	-1057(1)	45(1)
C(3)	3778(2)	-2384(2)	-1310(1)	60(1)
C(4)	3668(3)	-2447(2)	-1910(1)	89(1)
C(5)	4180(2)	-2175(1)	693(1)	43(1)
C(6)	3456(2)	-1488(1)	473(1)	53(1)
C(7)	2309(2)	-1604(2)	274(1)	80(1)
C(8)	1615(3)	-986(2)	61(2)	106(1)
C(9)	2073(4)	-245(2)	36(2)	106(1)
C(10)	3199(4)	-124(2)	215(1)	95(1)
C(11)	3906(3)	-743(1)	436(1)	71(1)
C(12)	4597(2)	-2263(1)	1289(1)	51(1)
C(13)	4205(2)	-1781(2)	1652(1)	67(1)
C(14)	4641(3)	-1869(2)	2212(1)	90(1)
C(15)	5426(3)	-2418(2)	2409(1)	105(1)
C(16)	5815(3)	-2893(2)	2059(1)	89(1)
C(17)	5418(2)	-2814(2)	1508(1)	65(1)
C(18)	7922(2)	-4650(1)	-639(1)	39(1)
C(19)	7092(2)	-5204(1)	-709(1)	39(1)
C(20)	7897(3)	-5907(3)	-1343(2)	75(1)
C(21)	7588(4)	-6621(3)	-1701(2)	129(2)

C(20')	7850(30)	-6330(30)	-1238(15)	69(10)
C(21')	7420(30)	-6010(30)	-1798(15)	77(12)
C(22)	8586(1)	-3449(1)	-223(1)	37(1)
C(23)	8431(2)	-2771(1)	119(1)	41(1)
C(24)	7379(2)	-2545(1)	183(1)	51(1)
C(25)	7261(2)	-1925(1)	518(1)	60(1)
C(26)	8180(2)	-1502(1)	793(1)	61(1)
C(27)	9229(2)	-1701(1)	730(1)	57(1)
C(28)	9354(2)	-2328(1)	394(1)	48(1)
C(29)	9588(1)	-3454(1)	-458(1)	40(1)
C(30)	10446(5)	-3997(6)	-301(4)	58(3)
C(31)	11340(8)	-3965(7)	-563(5)	60(2)
C(32)	11405(8)	-3410(6)	-942(4)	56(2)
C(33)	10585(6)	-2841(5)	-1073(3)	59(2)
C(34)	9671(7)	-2850(4)	-833(3)	47(1)
C(30')	10443(13)	-3969(9)	-281(8)	50(4)
C(31')	11400(20)	-4078(16)	-460(10)	62(4)
C(32')	11480(19)	-3668(15)	-906(10)	69(5)
C(33')	10629(14)	-3181(18)	-1122(8)	90(5)
C(34')	9698(14)	-3085(15)	-919(7)	73(5)
C(35)	3062(2)	-5302(1)	-1645(1)	45(1)
C(36)	3069(2)	-5568(1)	-1137(1)	44(1)
O(6)	2180(7)	-5886(4)	-968(3)	40(1)
C(37)	1114(4)	-5945(4)	-1353(3)	54(2)
C(38)	1060(6)	-6638(4)	-1724(3)	77(2)
O(6')	2277(11)	-6126(8)	-1074(5)	63(3)
C(37')	1357(10)	-6353(9)	-1510(4)	101(4)
C(38')	515(8)	-5675(9)	-1657(5)	149(6)
C(39)	4065(2)	-4638(1)	-2190(1)	39(1)
C(40)	3235(2)	-4858(1)	-2707(1)	41(1)
C(41)	3541(2)	-5390(1)	-3064(1)	50(1)
C(42)	2803(2)	-5592(1)	-3551(1)	59(1)
C(43)	1749(2)	-5270(1)	-3684(1)	62(1)
C(44)	1430(2)	-4743(2)	-3336(1)	63(1)
C(45)	2171(2)	-4536(1)	-2851(1)	54(1)

C(46)	5022(2)	-4143(1)	-2241(1)	43(1)
C(47)	5964(2)	-4063(2)	-1819(1)	64(1)
C(48)	6834(2)	-3571(2)	-1860(1)	83(1)
C(49)	6790(2)	-3154(2)	-2333(1)	75(1)
C(50)	5875(2)	-3235(2)	-2757(1)	69(1)
C(51)	5003(2)	-3722(1)	-2717(1)	56(1)





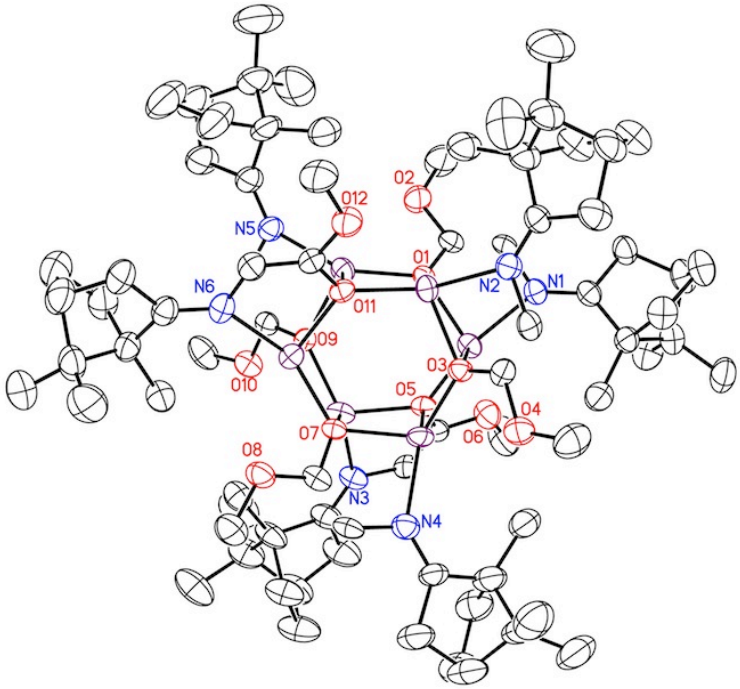


Figure 6. X-ray crystal structure of the unsolvated D_{3d} hexamer **9a**.

Table 11. Crystal data and structure refinement for **9a**.

Identification code	9a	
Empirical formula	C78 H120 Li6 N6 O12	
Formula weight	1375.44	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 14.4697(7) Å	a= 90°.
	b = 19.4187(8) Å	b= 101.333(2)°.
	c = 16.7250(8) Å	g = 90°.
Volume	4607.8(4) Å3	
Z	2	

Density (calculated)	0.991 Mg/m^3
Absorption coefficient	0.065 mm^{-1}
F(000)	1488
Crystal size	0.40 x 0.35 x 0.05 mm^3
Theta range for data collection	1.63 to 23.28°.
Index ranges	-16<=h<=16, -21<=k<=21, -18<=l<=17
Reflections collected	23935
Independent reflections	6836 [R(int) = 0.0317]
Completeness to theta = 23.28°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9968 and 0.9745
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6836 / 1 / 919
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0679, wR2 = 0.1796
R indices (all data)	R1 = 0.0788, wR2 = 0.1879
Absolute structure parameter	0(10)
Largest diff. peak and hole	0.298 and -0.217 $e.Å^{-3}$

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9012(2)	1680(2)	-99(2)	34(1)
O(2)	10408(3)	2052(2)	533(2)	63(1)
O(3)	7438(2)	978(2)	-1224(2)	38(1)
O(4)	6604(3)	525(2)	-2344(2)	61(1)
O(5)	7029(2)	2361(2)	-828(2)	39(1)
O(6)	7320(3)	3172(2)	-1662(2)	61(1)
O(7)	6095(2)	1300(2)	61(2)	36(1)
O(8)	5013(2)	798(2)	631(2)	54(1)
O(9)	7589(2)	2025(2)	1123(2)	36(1)

O(10)	7136(3)	2834(2)	1882(2)	52(1)
O(11)	8162(2)	615(2)	693(2)	39(1)
O(12)	8969(3)	-351(2)	869(2)	57(1)
N(1)	9298(3)	2033(2)	-1624(2)	44(1)
N(2)	9037(3)	208(2)	-1291(2)	45(1)
N(3)	5681(3)	3077(2)	-259(3)	50(1)
N(4)	4858(3)	1509(2)	-1412(3)	52(1)
N(5)	9228(3)	1744(2)	2237(3)	47(1)
N(6)	7392(3)	430(2)	2059(3)	50(1)
C(1)	9502(4)	2110(3)	-2336(3)	45(1)
C(2)	10441(4)	2310(3)	-2536(3)	59(1)
C(3)	10210(5)	2257(3)	-3474(4)	69(2)
C(4)	10148(5)	1471(3)	-3668(4)	74(2)
C(5)	9204(5)	1279(3)	-3428(4)	65(2)
C(6)	8834(4)	1977(3)	-3117(3)	51(1)
C(7)	9185(5)	2500(3)	-3702(4)	62(2)
C(8)	8741(5)	2402(4)	-4593(4)	79(2)
C(9)	9062(6)	3253(3)	-3459(5)	79(2)
C(10)	7788(4)	1973(4)	-3095(4)	66(2)
C(11)	9997(3)	2136(2)	-912(3)	39(1)
C(12)	9791(3)	1957(3)	-198(3)	42(1)
C(13)	11279(5)	2377(5)	516(5)	93(2)
C(14)	9782(4)	-101(3)	-1401(3)	48(1)
C(15)	10744(4)	-31(3)	-874(4)	60(2)
C(16)	11296(5)	413(3)	-1388(5)	74(2)
C(17)	11422(5)	-65(4)	-2101(5)	82(2)
C(18)	10936(5)	-720(3)	-1910(4)	69(2)
C(19)	9886(4)	-573(3)	-2104(4)	67(2)
C(20)	11183(5)	-752(3)	-977(4)	71(2)
C(21)	10662(8)	-1333(4)	-621(6)	110(3)
C(22)	12237(6)	-811(5)	-641(6)	121(4)
C(23)	10791(5)	246(4)	-25(4)	72(2)
C(24)	8179(4)	146(3)	-1888(3)	46(1)
C(25)	7457(4)	540(3)	-1802(3)	44(1)
C(26)	6557(5)	115(4)	-3055(4)	84(2)

C(27)	4960(4)	3395(3)	-100(4)	62(2)
C(28)	4504(5)	4035(4)	-467(6)	90(2)
C(29)	3654(5)	4090(4)	-39(6)	91(2)
C(30)	4048(5)	3810(4)	822(5)	82(2)
C(31)	4384(4)	3129(3)	495(4)	67(2)
C(32)	3468(5)	2852(4)	-93(5)	79(2)
C(33)	2974(5)	3538(5)	-438(6)	102(3)
C(34)	3241(6)	3712(4)	1298(7)	104(3)
C(35)	4826(7)	4246(4)	1302(7)	109(3)
C(36)	4834(4)	2606(3)	1109(4)	62(2)
C(37)	6130(4)	3354(3)	-874(3)	45(1)
C(38)	6799(3)	2958(3)	-1101(3)	41(1)
C(39)	7164(7)	3857(4)	-1987(6)	101(3)
C(40)	4229(4)	1674(3)	-2042(3)	55(1)
C(41)	4422(4)	2045(4)	-2767(4)	70(2)
C(42)	4015(5)	2779(4)	-2702(5)	87(2)
C(43)	2926(6)	2651(5)	-2887(6)	98(2)
C(44)	2864(5)	1879(5)	-3035(5)	89(2)
C(45)	3183(4)	1553(4)	-2192(4)	78(2)
C(46)	3693(5)	1714(5)	-3465(5)	89(2)
C(47)	3597(7)	2079(7)	-4300(5)	119(3)
C(48)	3832(7)	984(5)	-3576(5)	107(3)
C(49)	5454(5)	2062(5)	-2886(4)	81(2)
C(50)	4577(3)	1182(3)	-734(3)	48(1)
C(51)	5221(3)	1101(2)	-51(3)	43(1)
C(52)	4044(5)	636(4)	638(5)	77(2)
C(53)	9922(4)	1587(3)	2809(3)	57(1)
C(54)	10170(5)	1896(4)	3653(4)	78(2)
C(55)	10998(6)	1505(6)	4031(5)	102(3)
C(56)	11521(5)	1343(5)	3321(5)	95(3)
C(57)	10646(4)	1027(4)	2779(4)	73(2)
C(58)	10374(7)	474(5)	3335(5)	102(3)
C(59)	10646(9)	778(7)	4198(5)	127(4)
C(60)	11857(7)	2016(7)	2928(7)	135(4)
C(61)	12362(7)	844(7)	3542(7)	145(5)

C(62)	10717(5)	777(4)	1939(4)	72(2)
C(63)	8583(3)	2250(3)	2384(3)	42(1)
C(64)	7789(3)	2360(2)	1802(3)	40(1)
C(65)	7216(5)	3164(3)	2646(5)	75(2)
C(66)	7119(4)	351(3)	2736(3)	53(1)
C(67)	6523(4)	843(3)	3113(3)	58(1)
C(68)	7226(5)	1197(4)	3818(4)	75(2)
C(69)	7428(6)	621(5)	4453(5)	95(2)
C(70)	6876(5)	-10(4)	4028(4)	82(2)
C(71)	7343(5)	-237(4)	3332(4)	74(2)
C(72)	5964(5)	354(4)	3569(4)	75(2)
C(73)	5318(6)	-138(5)	2987(5)	96(2)
C(74)	5416(6)	705(5)	4141(5)	98(2)
C(75)	5965(5)	1378(3)	2512(4)	64(2)
C(76)	8025(4)	-55(3)	1831(3)	48(1)
C(77)	8364(3)	73(2)	1152(3)	40(1)
C(78)	9381(5)	-909(3)	1363(5)	77(2)
Li(1)	8103(5)	1902(4)	-1103(5)	40(2)
Li(2)	6565(5)	2266(4)	216(5)	45(2)
Li(3)	8758(6)	1535(4)	980(5)	42(2)
Li(4)	8542(5)	721(4)	-344(5)	38(2)
Li(5)	6333(5)	1482(4)	-1063(5)	42(2)
Li(6)	7043(5)	1070(4)	1017(5)	40(2)

II. NMR Spectroscopic Studies in Toluene

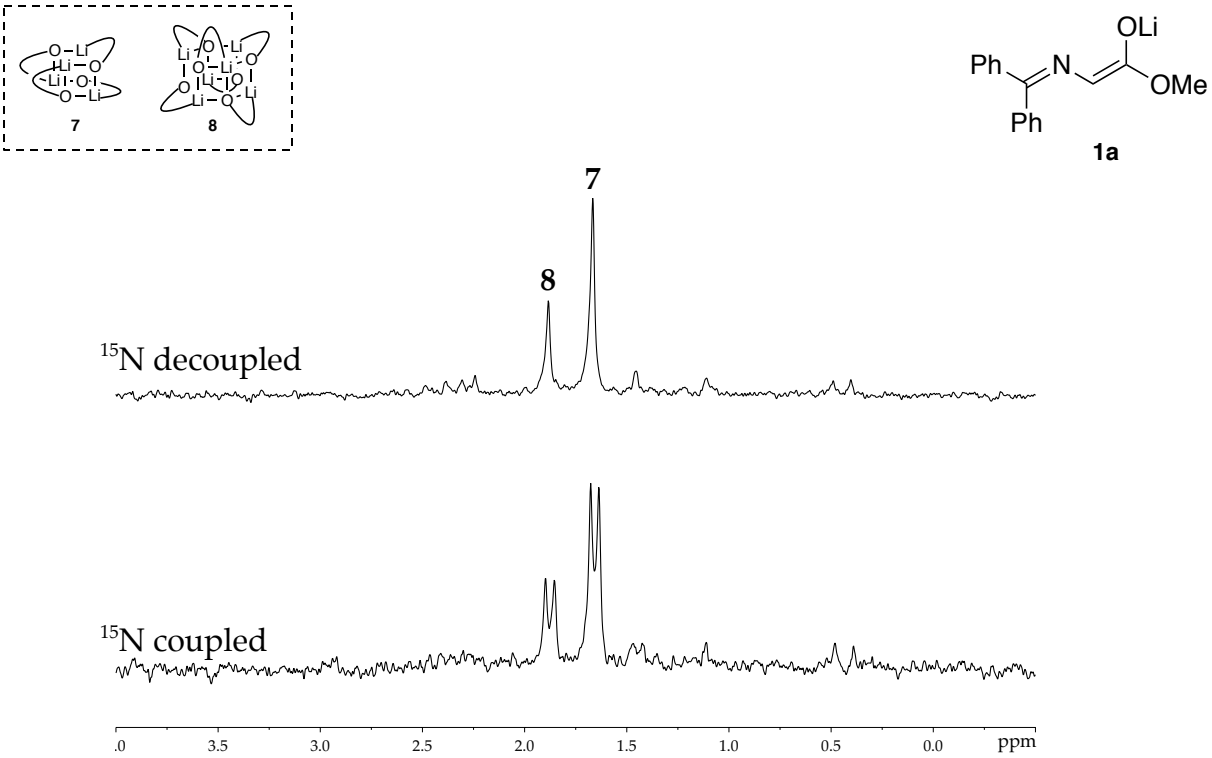


Figure 7. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**1a** in toluene at -80 °C showing the unsolvated tetramer **7** and hexamer **8** with J = 3.0 Hz for both aggregates.

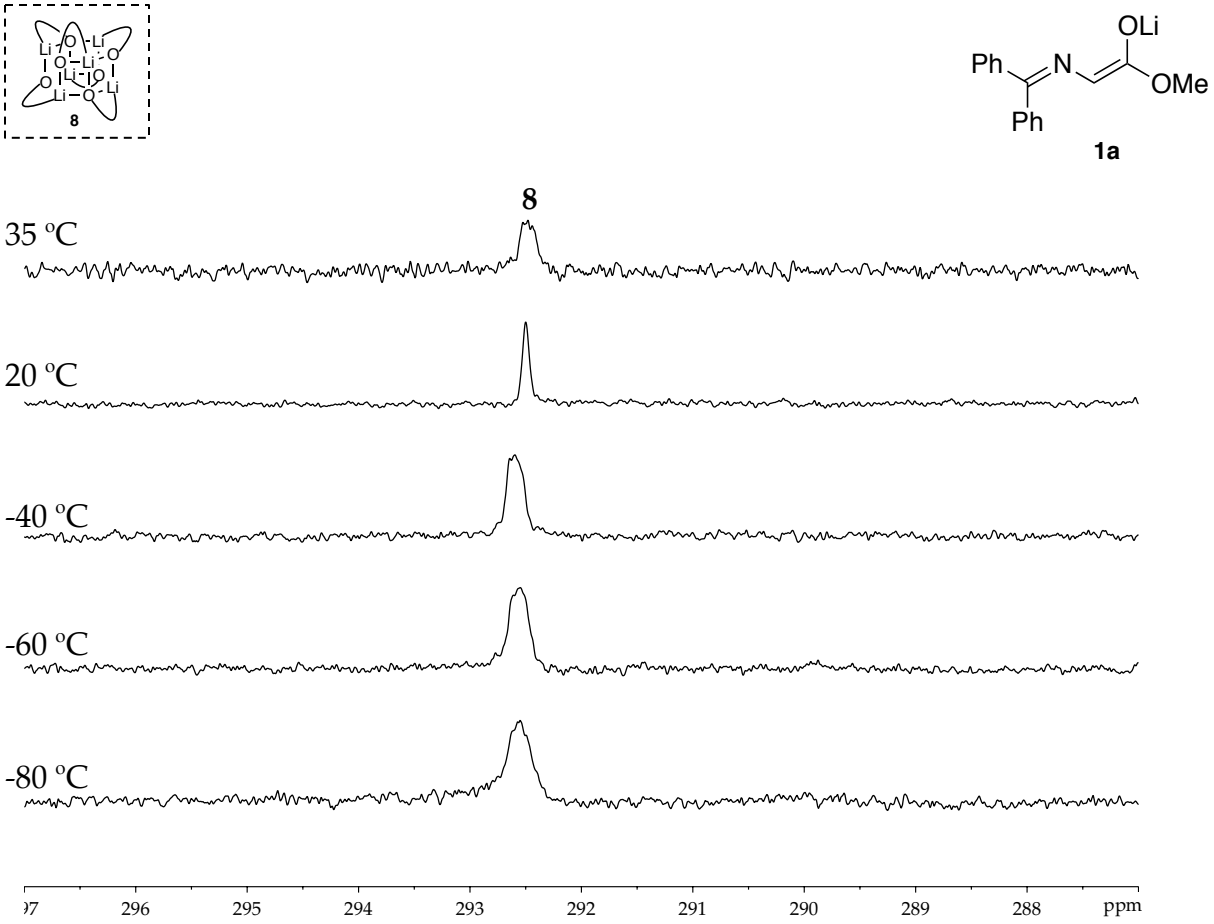
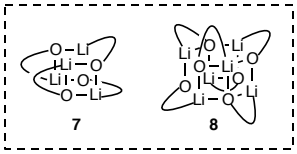
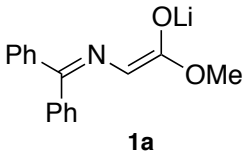


Figure 8. ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]**1a** in toluene at various temperatures showing indiscernible coupling.





1a

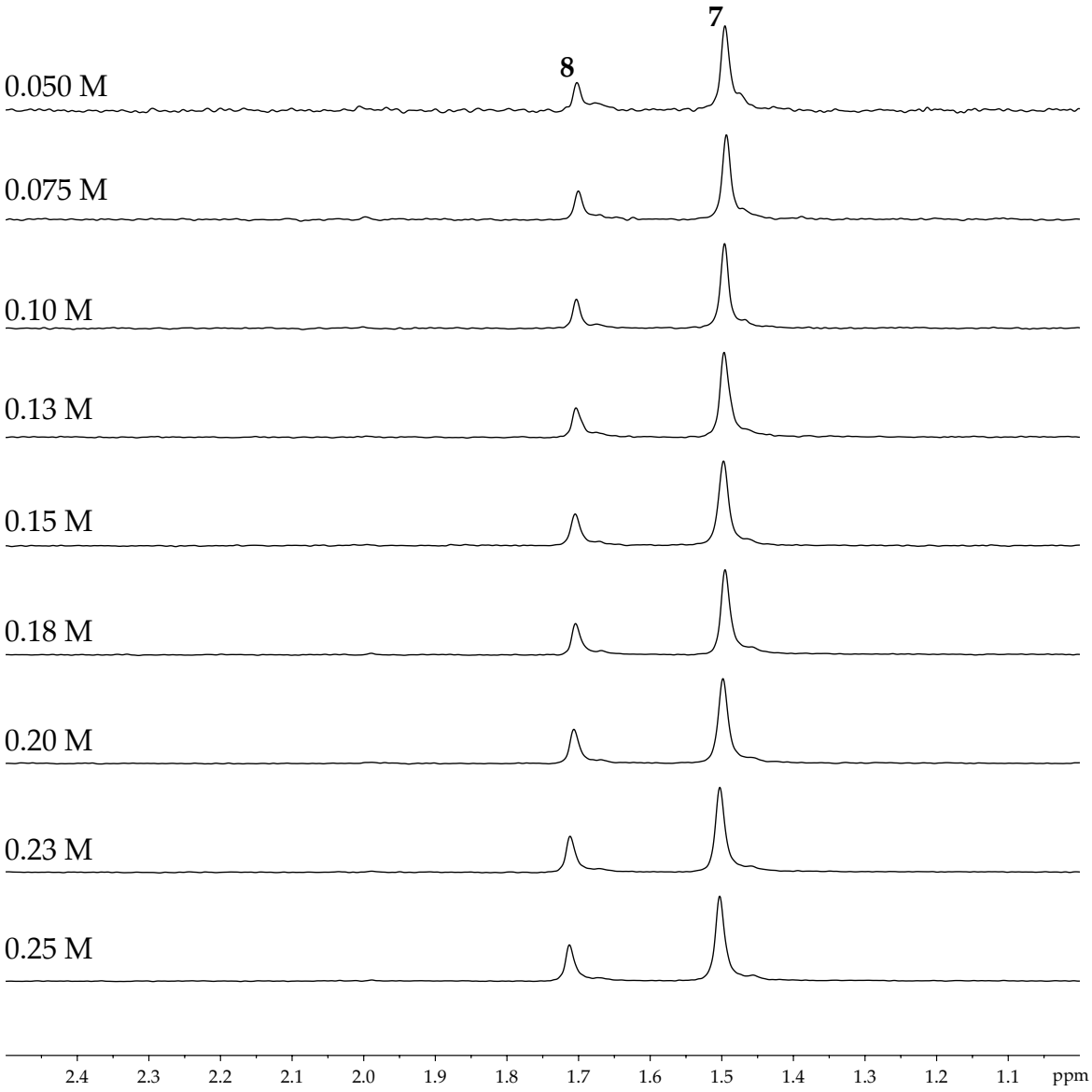
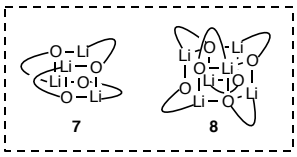
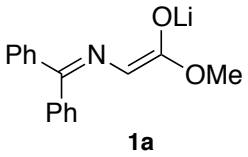


Figure 9. ^{6}Li NMR spectra of various concentrations of [^{6}Li]**1a** in toluene at -70 °C showing the unsolvated teramer **7** and hexamer **8**.





1a

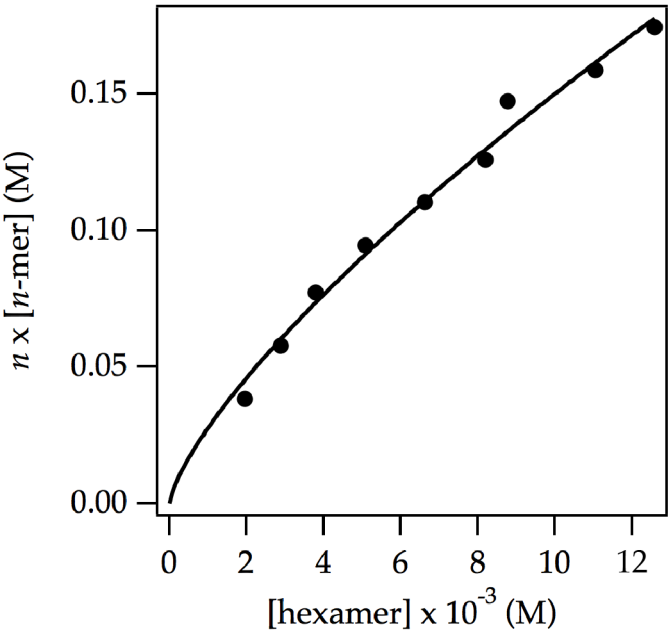


Figure 10. A plot of n[n-mer] vs. [**8**] for **1a** in toluene at -70 °C. n-mer corresponds to ^{6}Li resonance at 1.50 ppm, labeled as **7** in Figure 9. The best fit gives $n = 4.4 \pm 0.2$, confirming the lower aggregate n-mer as a tetramer. For derivations, see Derivation 1 on page S34. The plot was fitted to $y = n(K_{eq}^{1/6}x^{n/2})$. [$n = 4.4 \pm 0.2$, $K_{eq} = 1.0 \pm 0.8$]

n x [n-mer]	[hexamer] x 10^{-3}
0.175	12.6
0.159	11.1
0.147	8.77
0.126	8.19
0.110	6.63
0.0945	5.09
0.0773	3.78
0.0577	2.88
0.0382	1.96

Derivation 1. Derivation for the fitting equation of **Figure 10.**

Let $A_n \equiv$ Aggregate with aggregation number n
Let $A_6 \equiv$ Hexamer aggregate

$$n\ A_6 \leftrightharpoons 6\ A_n$$

$$\text{Therefore } K_{eq} = \frac{[A_n]^6}{[A_6]^n}$$

Let $\chi_{A_6} \equiv$ Mole fraction of A in hexamer aggregate
Let $\chi_{A_n} \equiv$ Mole fraction of A in aggregate with aggregation number n
Let $I_n \equiv$ NMR integration of peak of aggregate with aggregation number n
Let $I_H \equiv$ NMR integration of peak of hexamer aggregate

$$\text{Therefore } \chi_{A_6} = \frac{I_H}{I_H + I_n}$$

$$\text{and } \chi_{A_n} = \frac{I_n}{I_H + I_n}$$

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

$$\text{Therefore } [A_6] = \frac{I_H}{I_H + I_n}\left(\frac{C_{tot}}{6}\right)$$

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

Rearrange K_{eq} equation to give $[A_n] = {K_{eq}}^{1/6}\ [A_6]^{n/6}$

substitute integrations for concentrations $\frac{I_n}{I_H + I_n}\left(\frac{C_{tot}}{n}\right) = {K_{eq}}^{1/6}\left(\frac{I_H}{I_H + I_n}\left(\frac{C_{tot}}{6}\right)\right)^{n/6}$

multiply by n $\quad \frac{I_n\ C_{tot}}{I_H + I_n} = n * {K_{eq}}^{1/6}\left(\frac{I_H}{I_H + I_n}\left(\frac{C_{tot}}{6}\right)\right)^{n/6}$

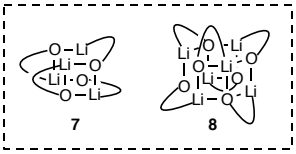
Plug in values for I_n, I_H, and C_{tot}

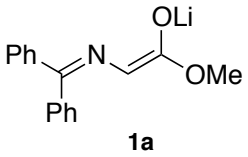
This gives you

$$Y = n * {K_{eq}}^{1/6}\ X^{n/6}$$

where

$Y = \frac{I_n\ C_{tot}}{I_H + I_n} = n * [A_n]$; $\quad X = \frac{I_H}{I_H + I_n}\left(\frac{C_{tot}}{6}\right) = [A_6]$





1a

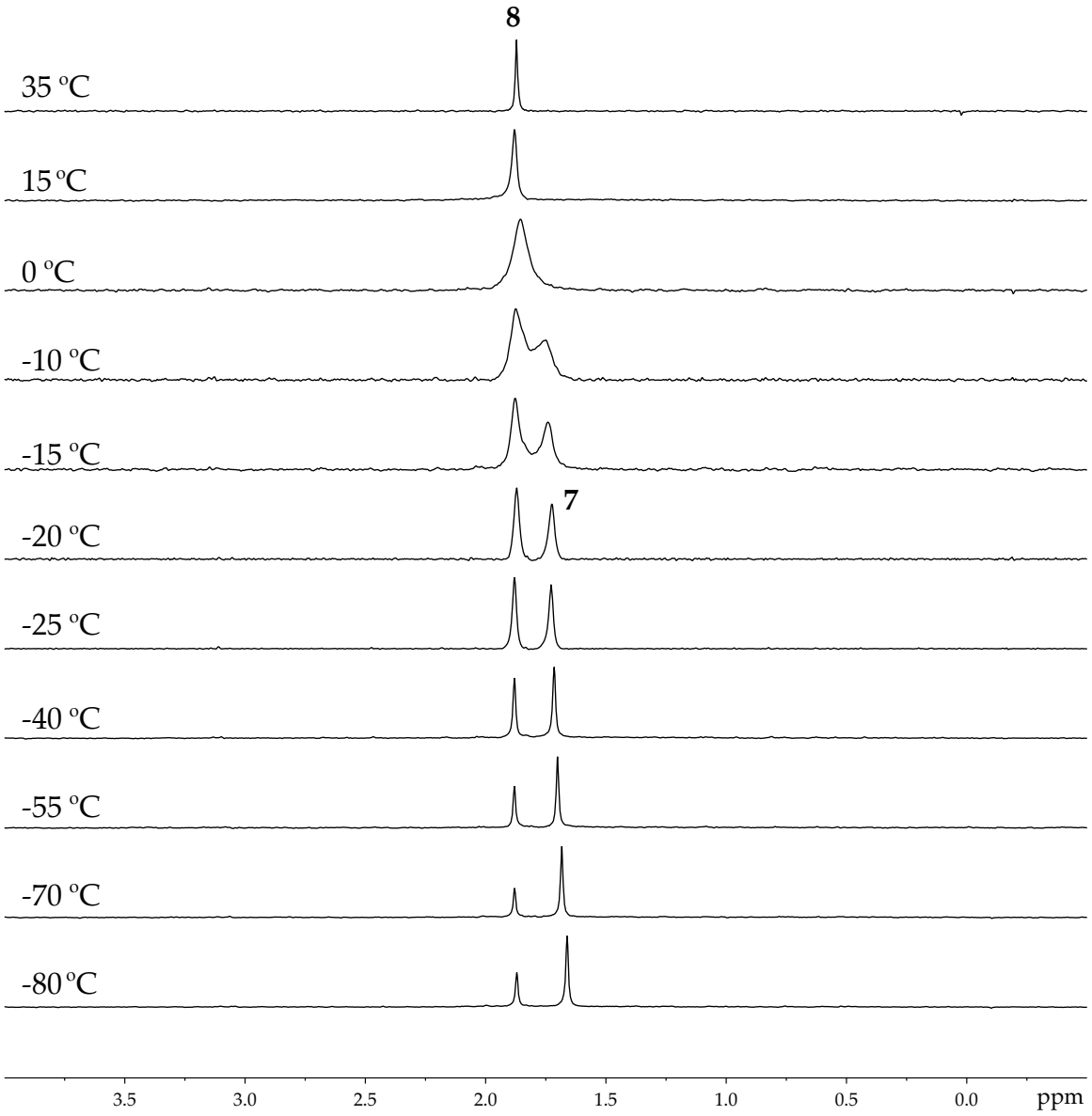


Figure 11. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** in toluene at various temperatures showing the unsolvated tetramer **7** and hexamer **8**.

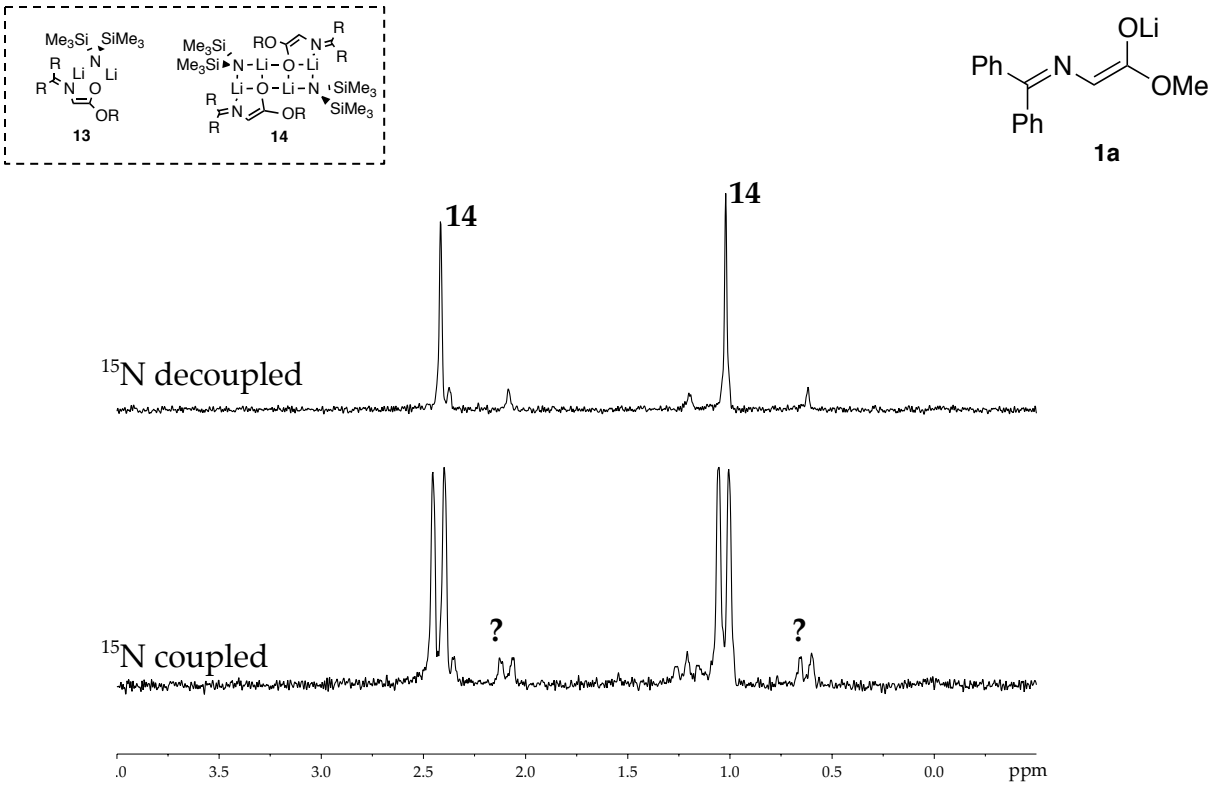


Figure 12. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** with 0.14 M excess [^{6}Li,^{15}N]LiHMDS in toluene at -75 °C showing dimer **13**, ladder **14**, or possibly both. J_{major} = 4.1 Hz, J_{minor} = 4.2 Hz.

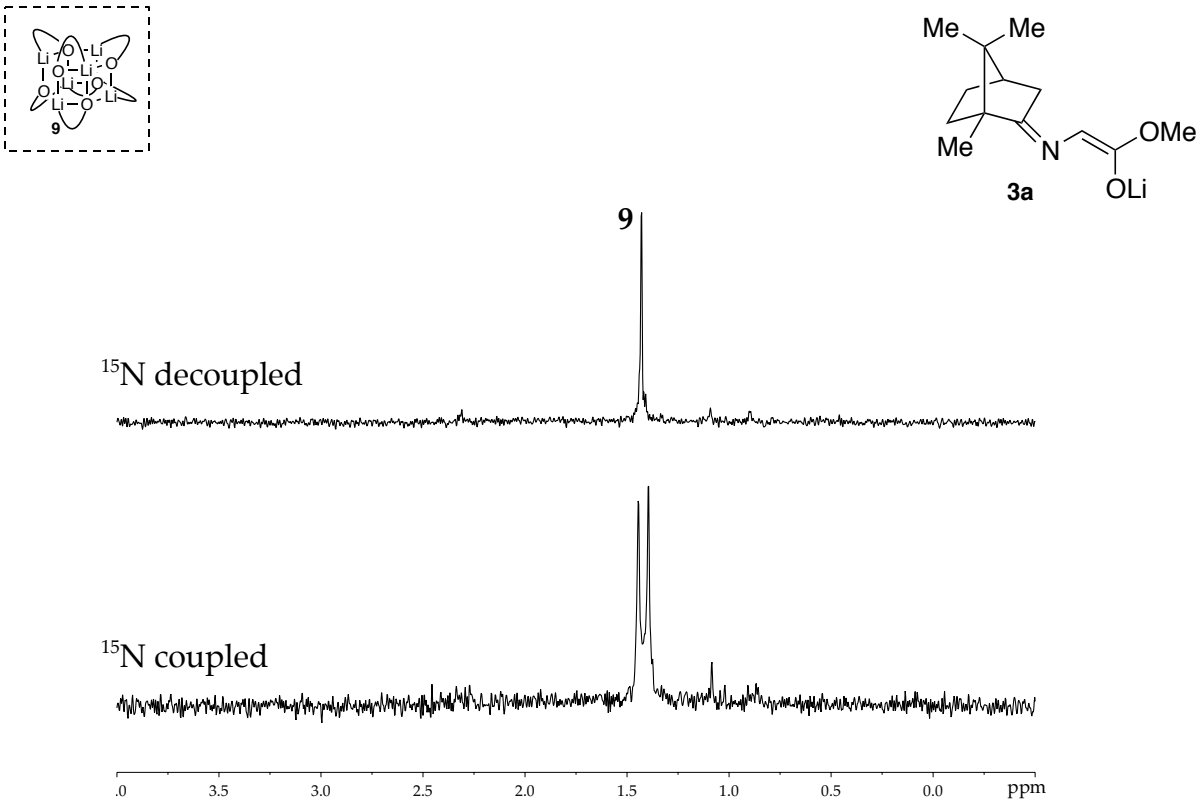


Figure 13. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**3a** in toluene at -80 °C showing the unsolvated hexamer **9** with J = 3.5 Hz.

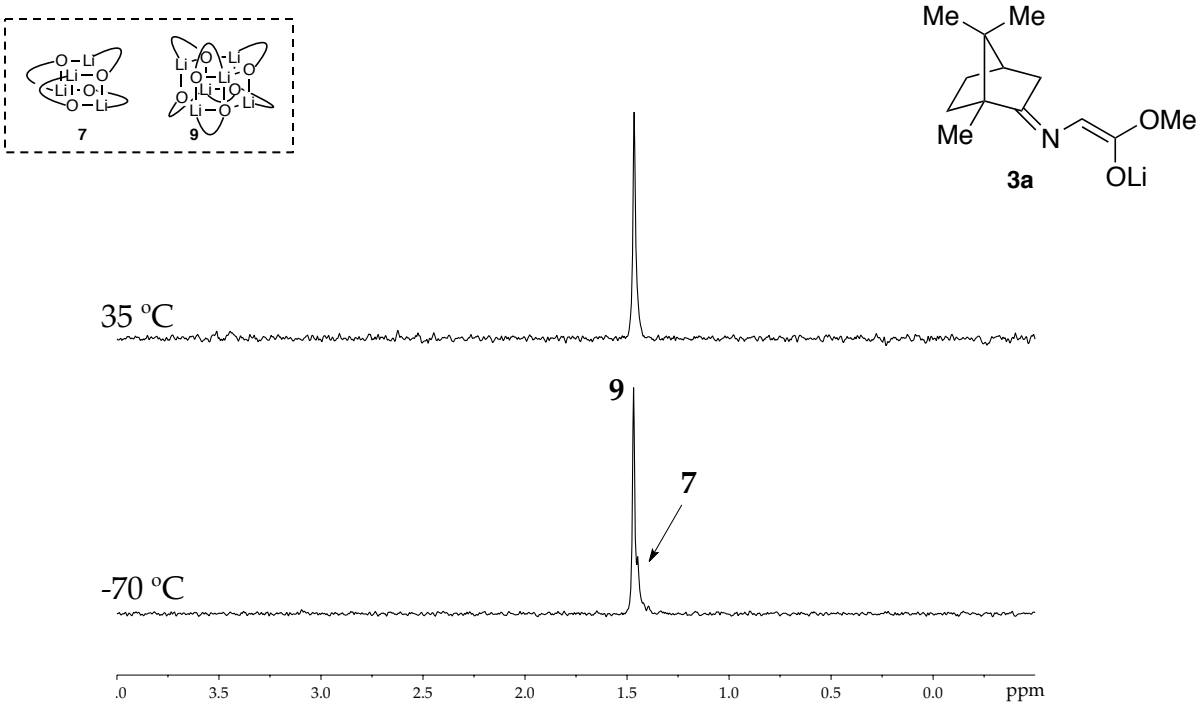


Figure 14. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3a** in toluene at various temperatures showing the unsolvated hexamer **9**. The unsolvated tetramer appears as a small shoulder at lower temperature.

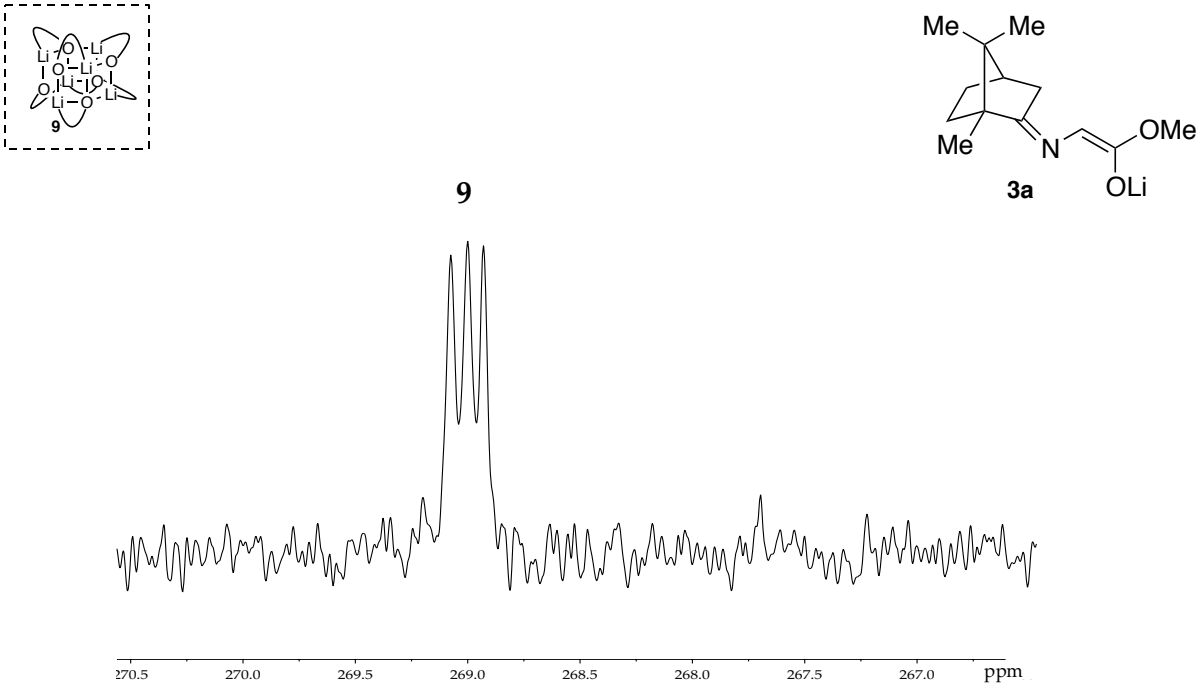


Figure 15. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3a** in toluene at -45 °C showing the unsolvated hexamer **9** with J = 3.6 Hz.

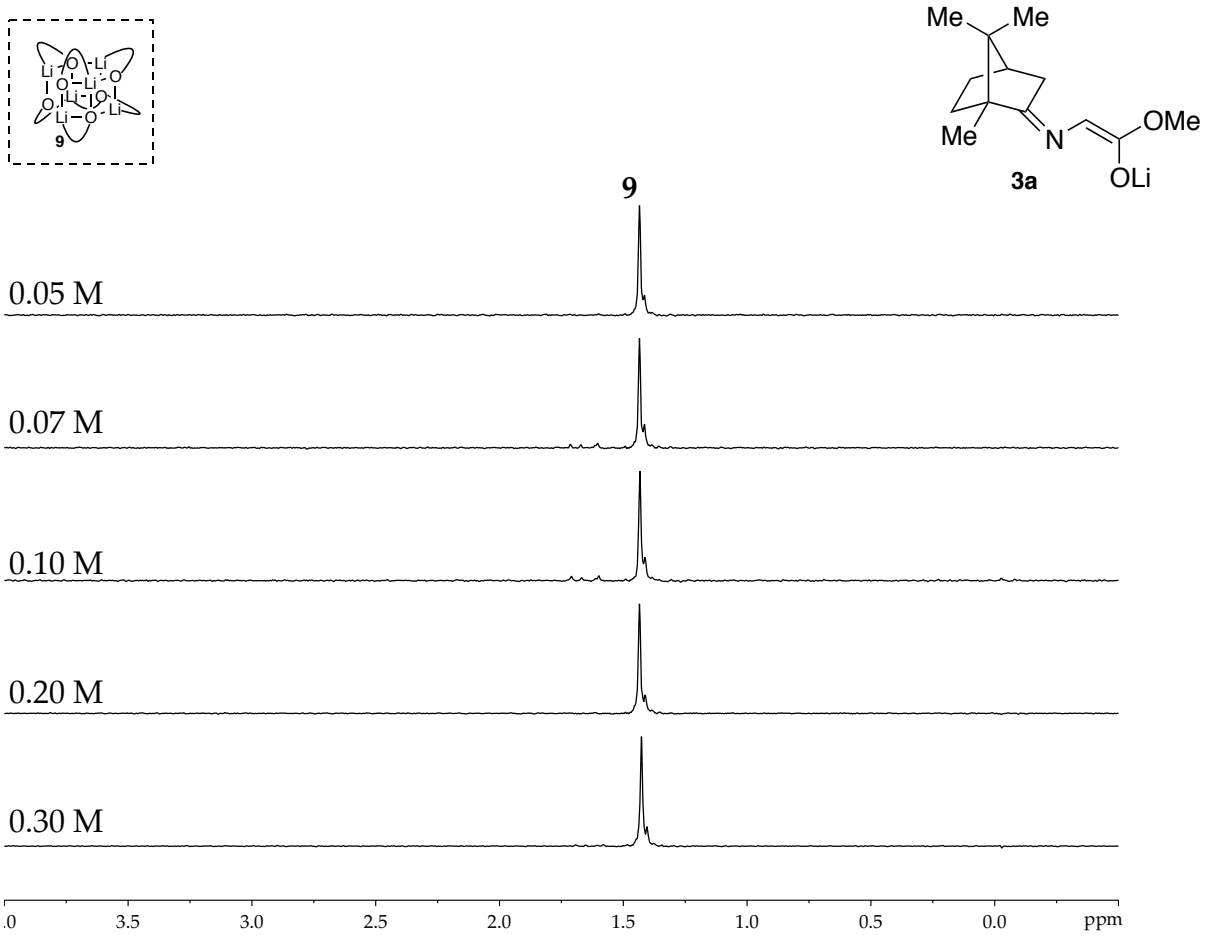
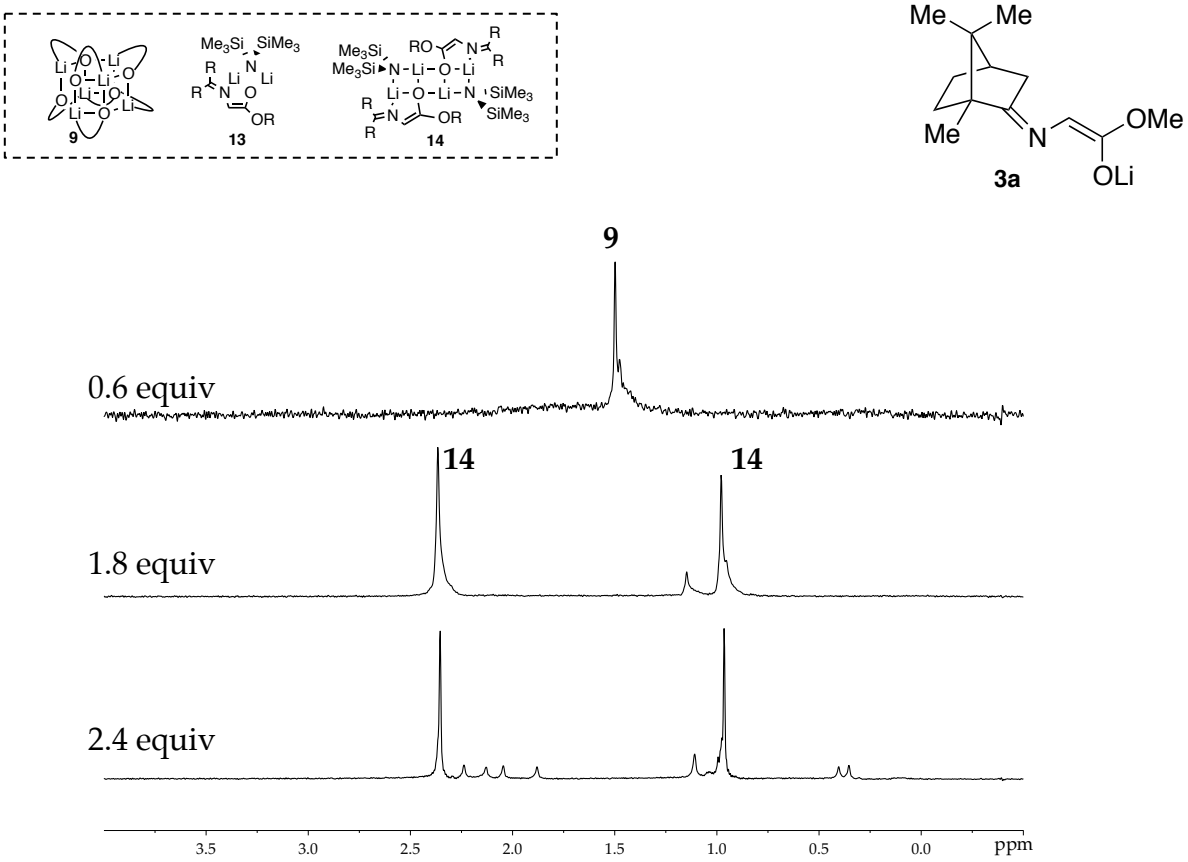


Figure 16. ^{6}Li NMR spectra of [^{6}Li]**3a** in toluene at -75 °C showing only one major aggregate, **9**. The enolate concentrations are as indicated.



Figurer 17. ^{6}Li NMR spectra of [^{6}Li]**3a** generated from 0.10 M **10a** with various equivalents of [^{6}Li]LiHMDS in toluene at -75 °C. The homoaggregate **9** is not observed in the presence of excess LiHMDS.

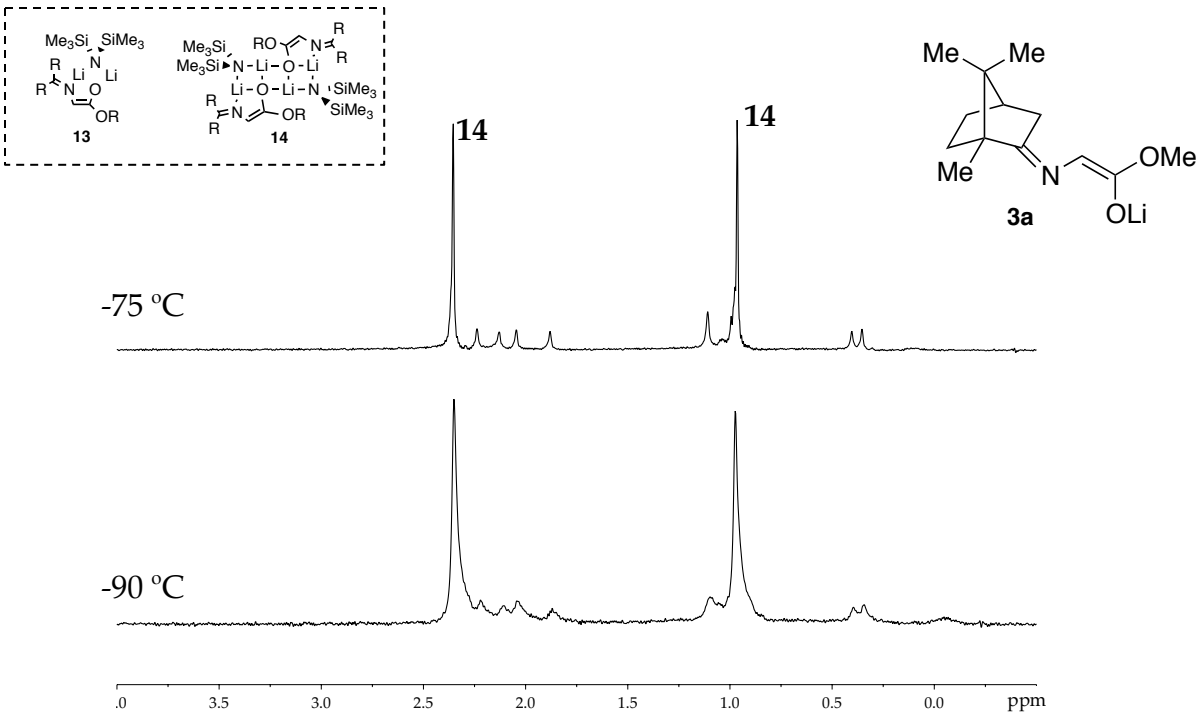


Figure 18. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3a** with 0.14 M [^{6}Li]LiHMDS in toluene at various temperatures showing mixed aggregates **13** or **14**.

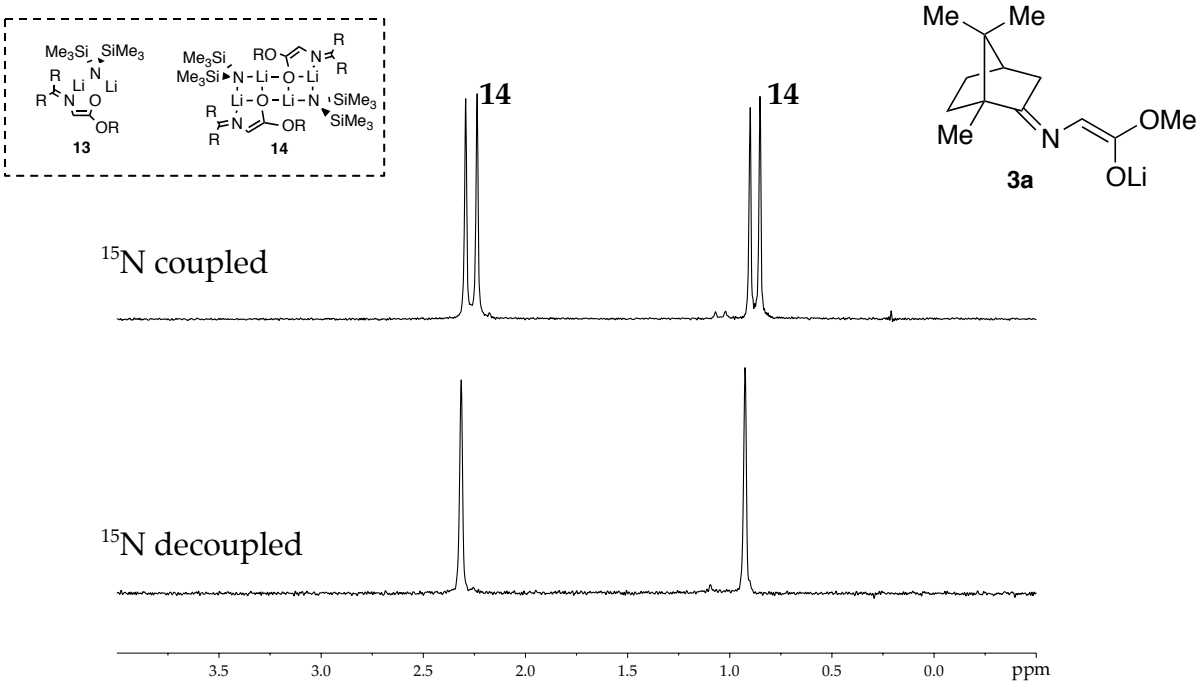


Figure 19. ^{6}Li NMR spectra of [^{6}Li]**3a** generated from 0.10 M **10a** with 0.12 M excess [^{6}Li,^{15}N]LiHMDS in toluene at -75 °C appearing as either mixed dimer **13** or ladder **14**. The coupling constant is 4.1 Hz.

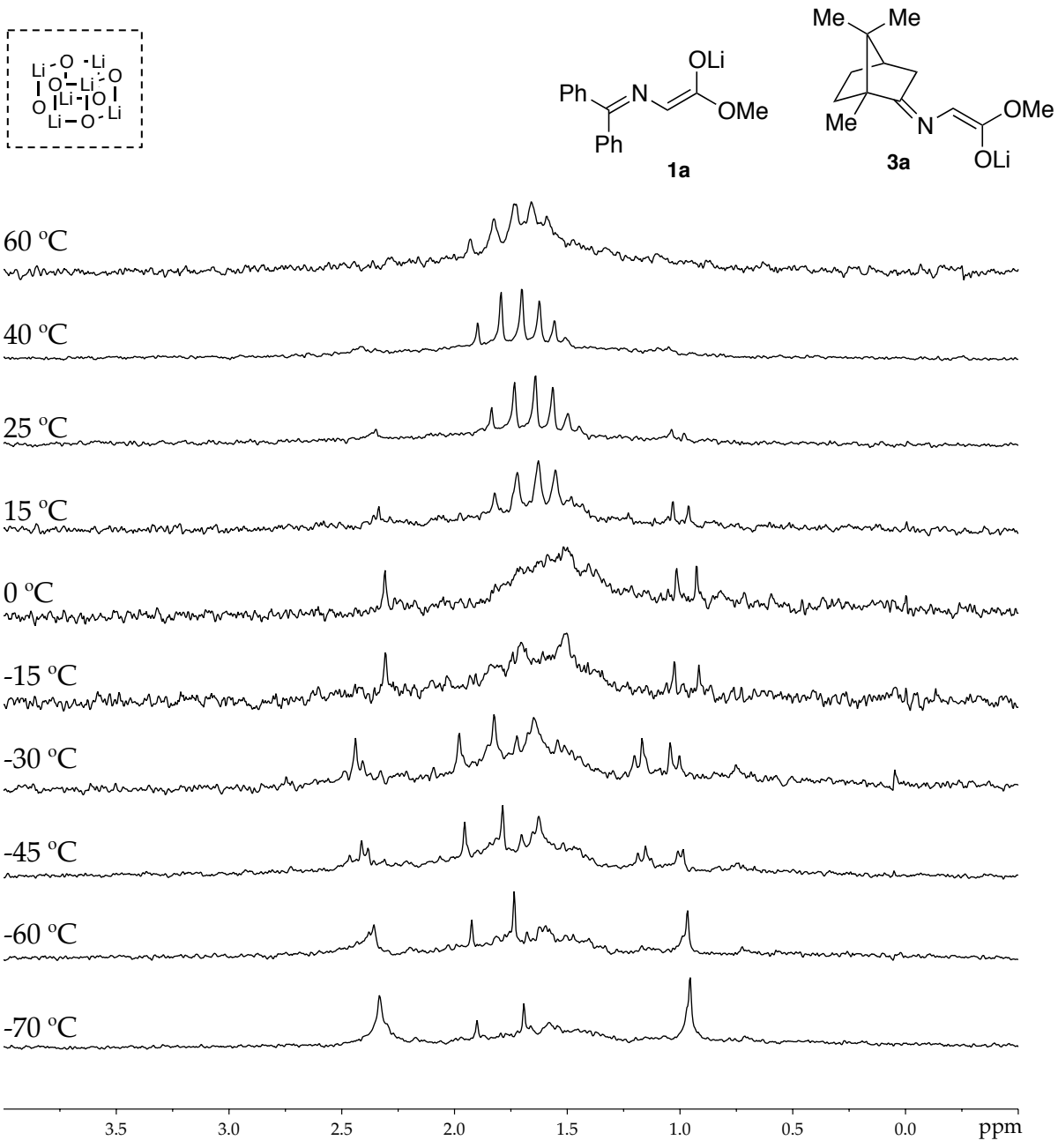


Figure 20. ^{6}Li NMR spectra of 0.050 M [^{6}Li]**1a** and 0.050 M [^{6}Li]**3a** in toluene at various temperatures showing an ensemble characteristic of hexameric enolates in the limit of rapid Li-Li and chelate exchange at high temperature (most visible at 25-40 °C). The low temperature spectra show complexity associated with positional isomerism.

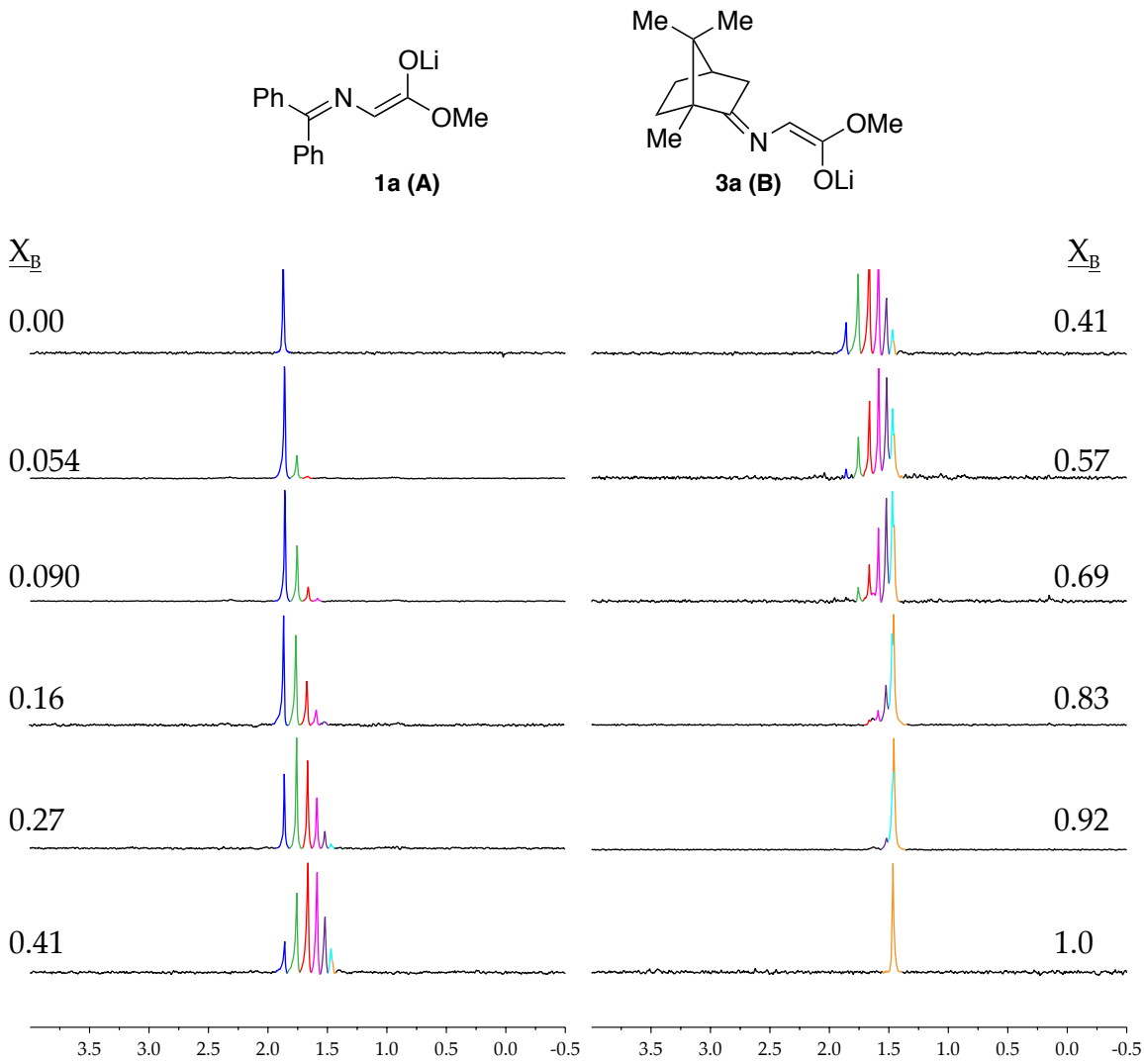


Figure 21. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** and [^{6}Li]**3a** mixtures in toluene at 35 °C. Baseline correction and line fitting are applied to all spectra. X_B indicates the measured mole fractions of **3a** (**B**). The ensembles are characteristic of hexamers in which Li-Li site exchanges and chelate exchanges are fast on NMR time scales.

Table 13. Resonance integrations for each aggregate in an ensemble of [^{6}Li]**1a** (**A**) and [^{6}Li]**3a** (**B**).

X_B	Resonance Integrations						
	$\mathbf{A_6}$	$\mathbf{A_5B_1}$	$\mathbf{A_4B_2}$	$\mathbf{A_3B_3}$	$\mathbf{A_2B_4}$	$\mathbf{A_1B_5}$	$\mathbf{B_6}$
0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
0.054	12278.60	3614.90	928.51	0.00	0.00	0.00	0.00
0.089	17430.33	10400.96	2416.34	418.06	0.00	0.00	0.00

0.16	4034.26	3982.14	1803.64	588.00	193.42	0.00	0.00
0.27	5027.30	9036.98	7862.71	4264.30	1314.00	394.83	0.00
0.41	1786.97	7628.34	13036.06	12981.62	5480.87	2042.75	374.61
0.57	168.59	1623.72	3063.78	5007.08	5861.88	3294.50	964.80
0.69	0.00	751.20	2342.64	4164.90	8425.58	8556.02	3305.85
0.83	0.00	0.00	282.66	1098.69	4548.01	7469.01	7674.40
0.92	0.00	0.00	0.00	0.00	774.73	4670.61	7544.16
1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00

Table 14. Relative integrations for each aggregate in an ensemble of [^{6}Li]**1a** (**A**) and [^{6}Li]**3a** (**B**).

X_B	Resonance Integrations						
	A_6	**A_5B_1**	**A_4B_2**	**A_3B_3**	**A_2B_4**	**A_1B_5**	**B_6**
0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
0.054	0.73	0.21	0.055	0.00	0.00	0.00	0.00
0.089	0.57	0.34	0.079	0.014	0.00	0.00	0.00
0.16	0.38	0.38	0.17	0.055	0.018	0.00	0.00
0.27	0.18	0.32	0.28	0.15	0.047	0.014	0.00
0.41	0.041	0.18	0.30	0.30	0.13	0.047	0.0086
0.57	0.0084	0.081	0.15	0.25	0.29	0.16	0.048
0.69	0.00	0.027	0.085	0.15	0.30	0.31	0.12
0.83	0.00	0.00	0.013	0.052	0.22	0.35	0.36
0.92	0.00	0.00	0.00	0.00	0.060	0.36	0.58
1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00

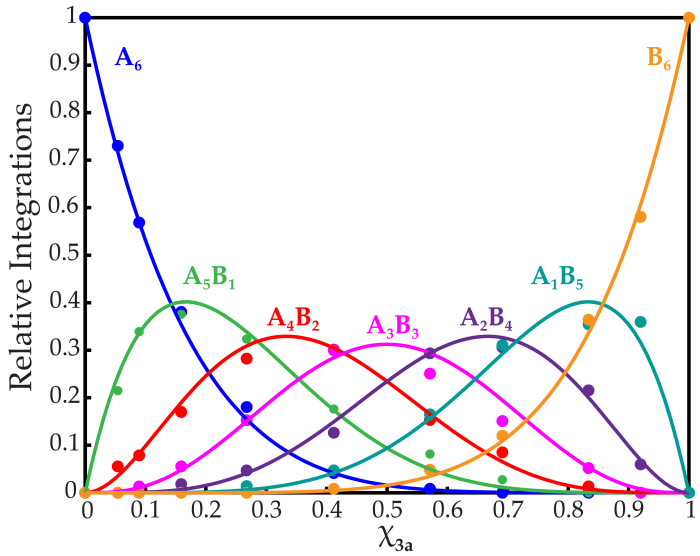


Figure 22. Job Plot of 0.10 M [^{6}Li]**1a** and [^{6}Li]**3a** mixtures in toluene at 35 °C showing the relative integrations versus measured mole fraction of **3a**. The Job plot indicates **1a** and **3a** are hexamers.

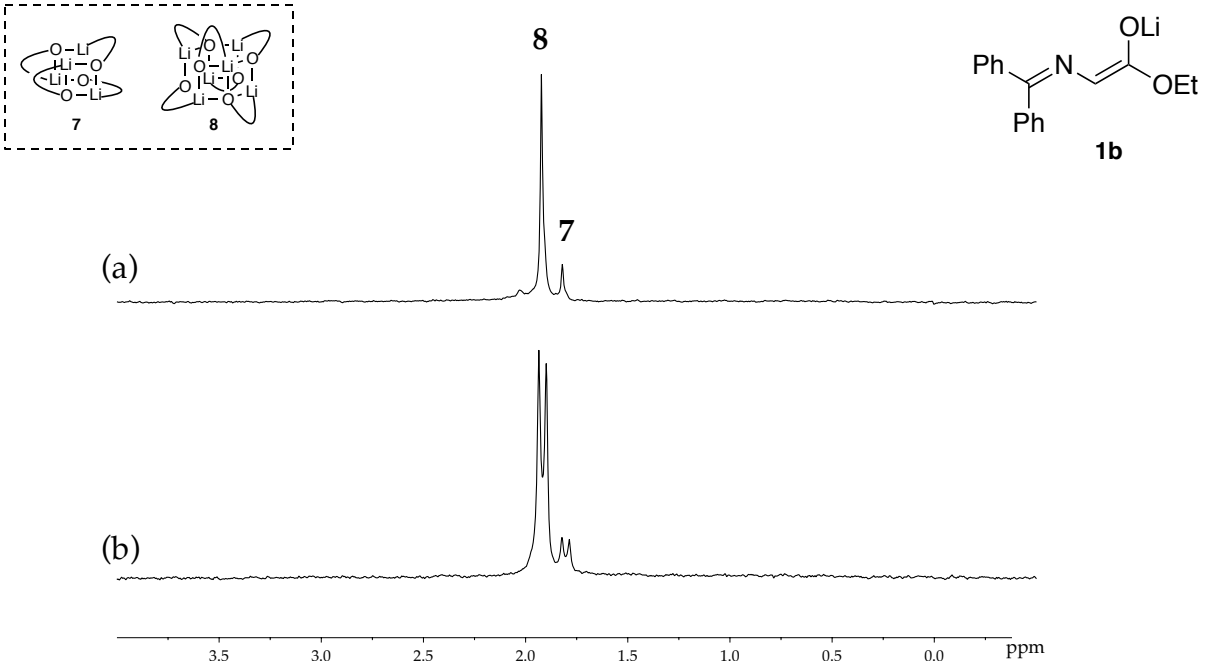


Figure 23. ^{6}Li NMR spectra of (a) [^{6}Li]**1b** at -70 °C and (b) [^{6}Li,^{15}N]**1b** at -75 °C showing the tetramer **7** and hexamer **8** with J = 3.1 Hz for both. The enolate concentration is 0.10 M in toluene.

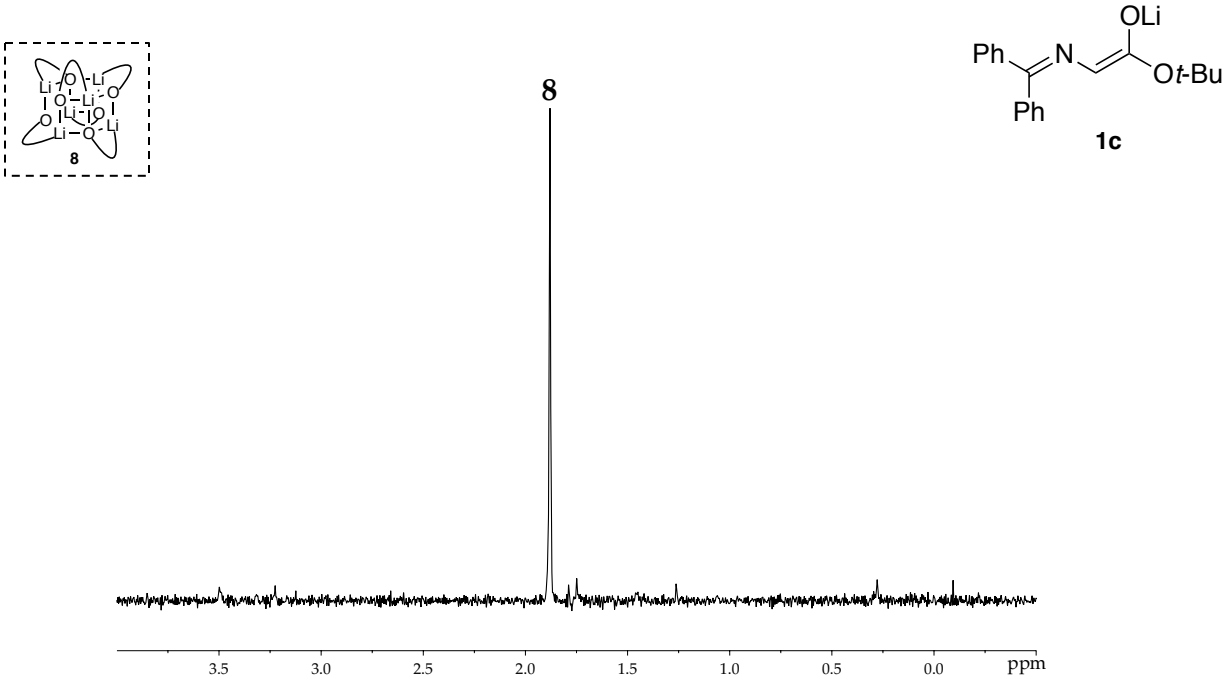


Figure 24. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**1c** in toluene at -75 °C assigned as the unsolvated hexamer **8** based on results from MCV and crystallography of analogous enolates.

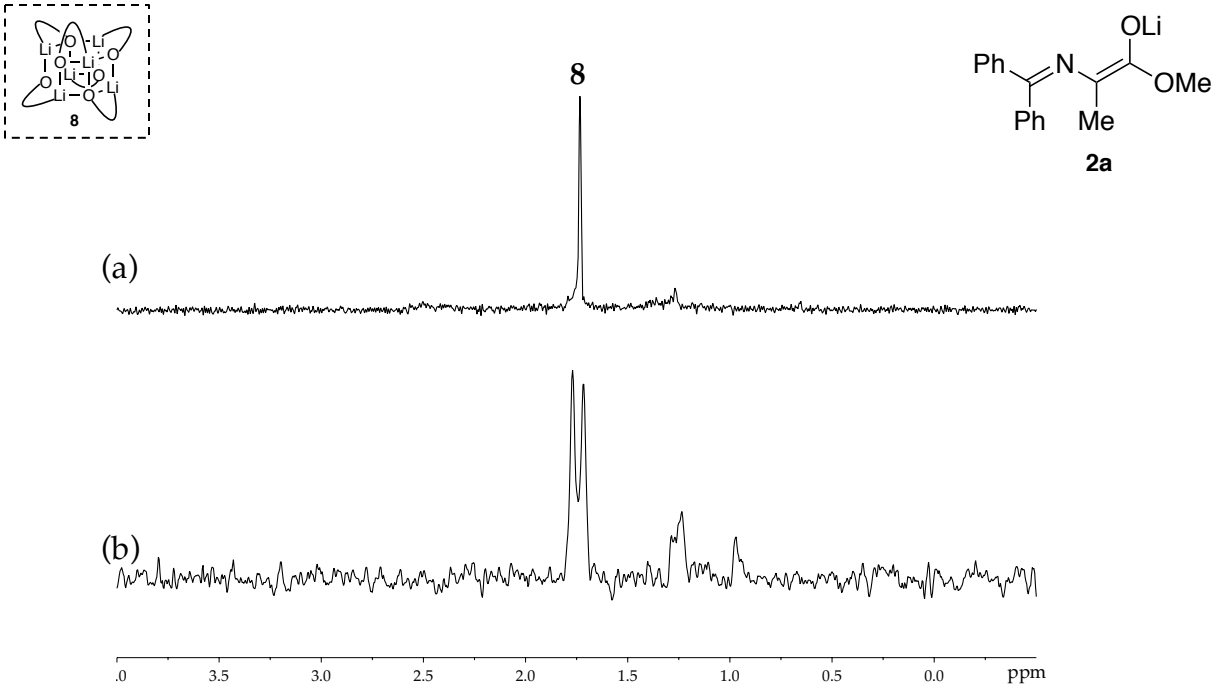


Figure 25. ^{6}Li NMR spectra of (a) 0.10 M [^{6}Li]**2a** and (b) 0.10 M [^{6}Li,^{15}N]**2a** in toluene at -75 °C. Enolate **2a** is assigned as unsolvated hexamer **8** based on the studies of analogous enolates. J = 4.0 Hz.

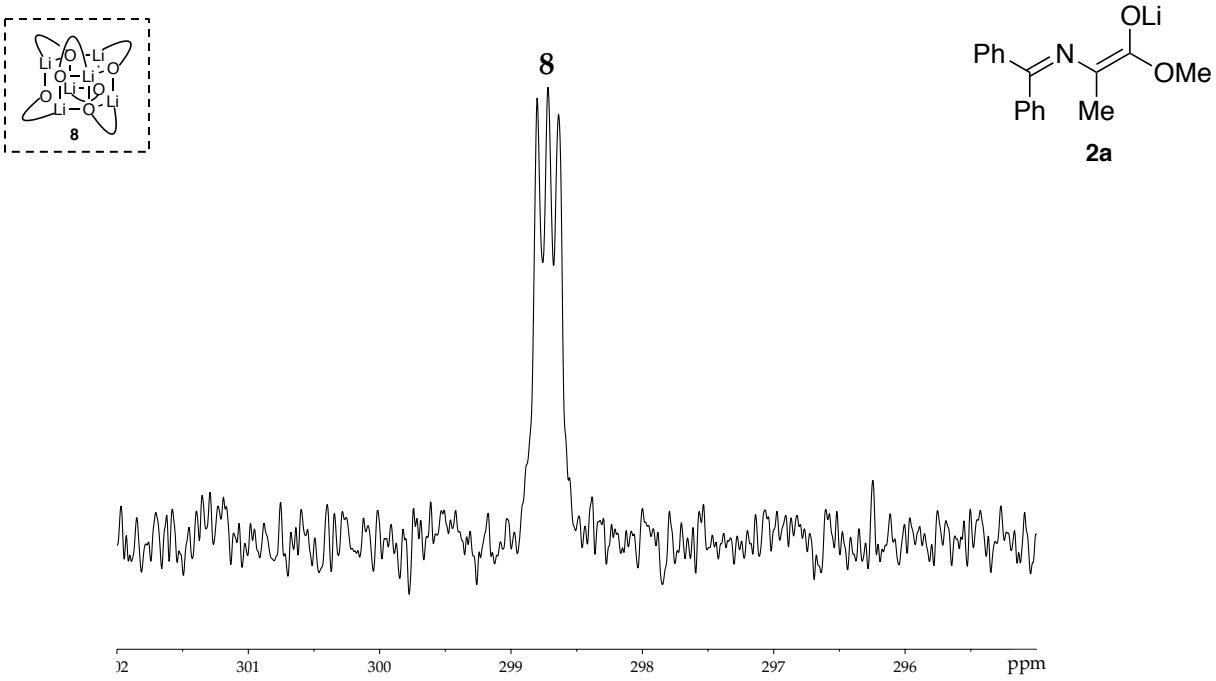
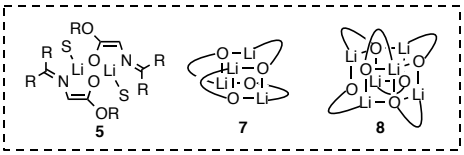
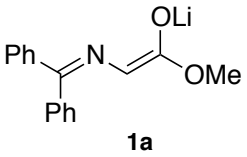


Figure 26. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**2a** in toluene at -55 °C. J = 4.1 Hz for the unsolvated hexamer **8**.

III. NMR Spectroscopic Studies with Tetrahydrofuran (THF)





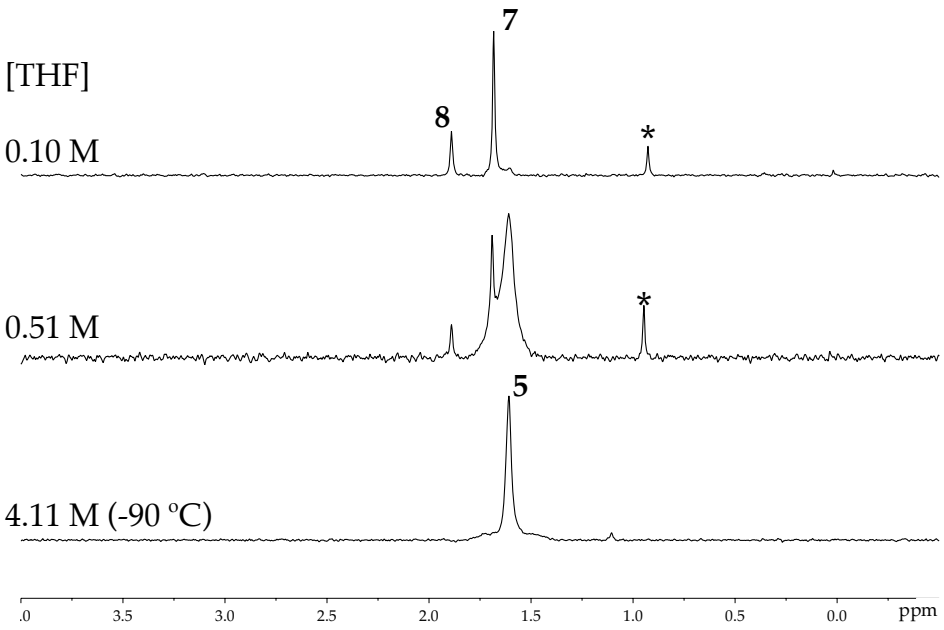


Figure 27. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** with various THF concentrations in toluene at -70 °C. The symmetric dimer **5** is the sole species at [THF] ≥ 1.03 M whereas the unsolvated tetramer **7** and the hexamer **8** are the major species at low THF concentrations. Asterisks indicate LiHMDS.

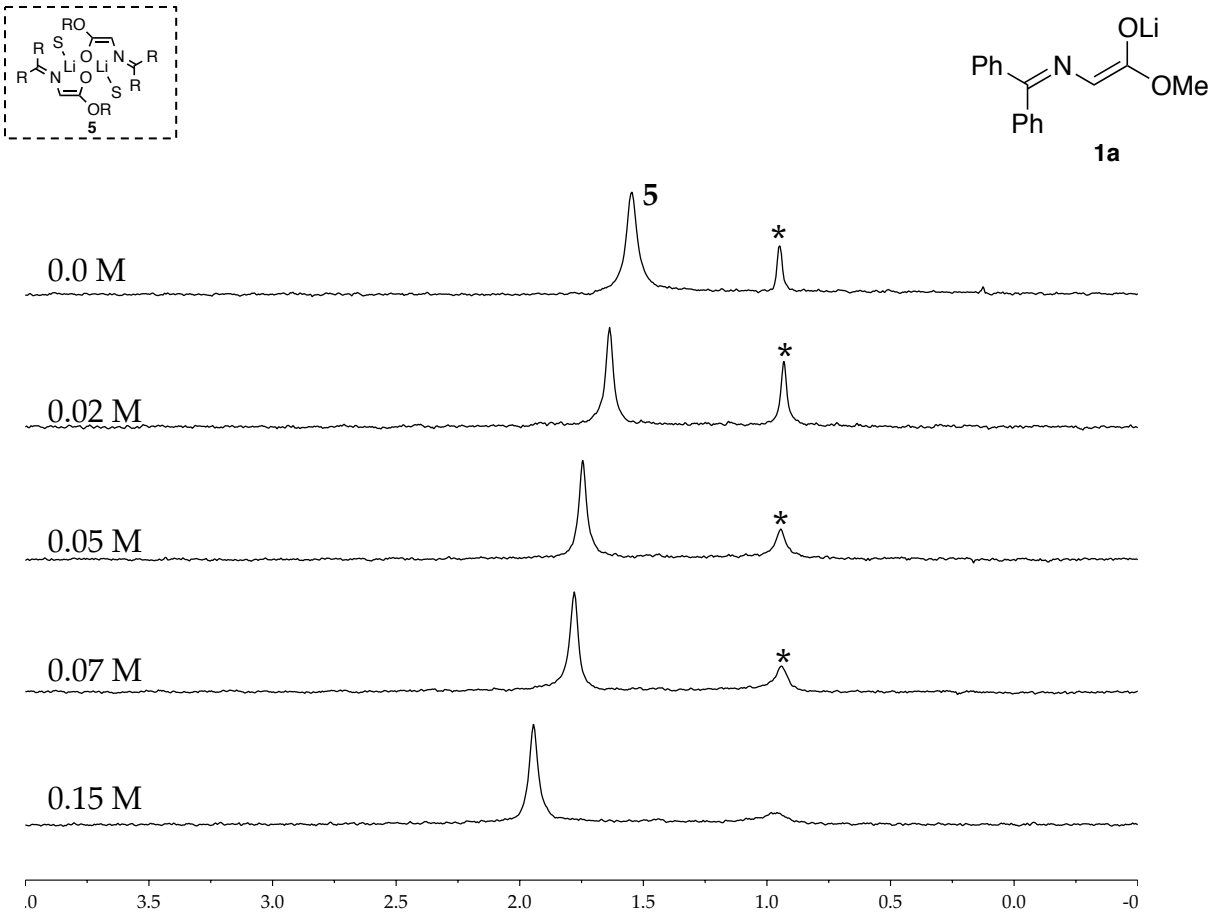


Figure 28. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** in 1.0 M THF in toluene with various concentrations of pyridine at -80 °C. The chemical shift change indicates the solvation of the dimer **5**. Asterisks (*) denote LiHMDS.

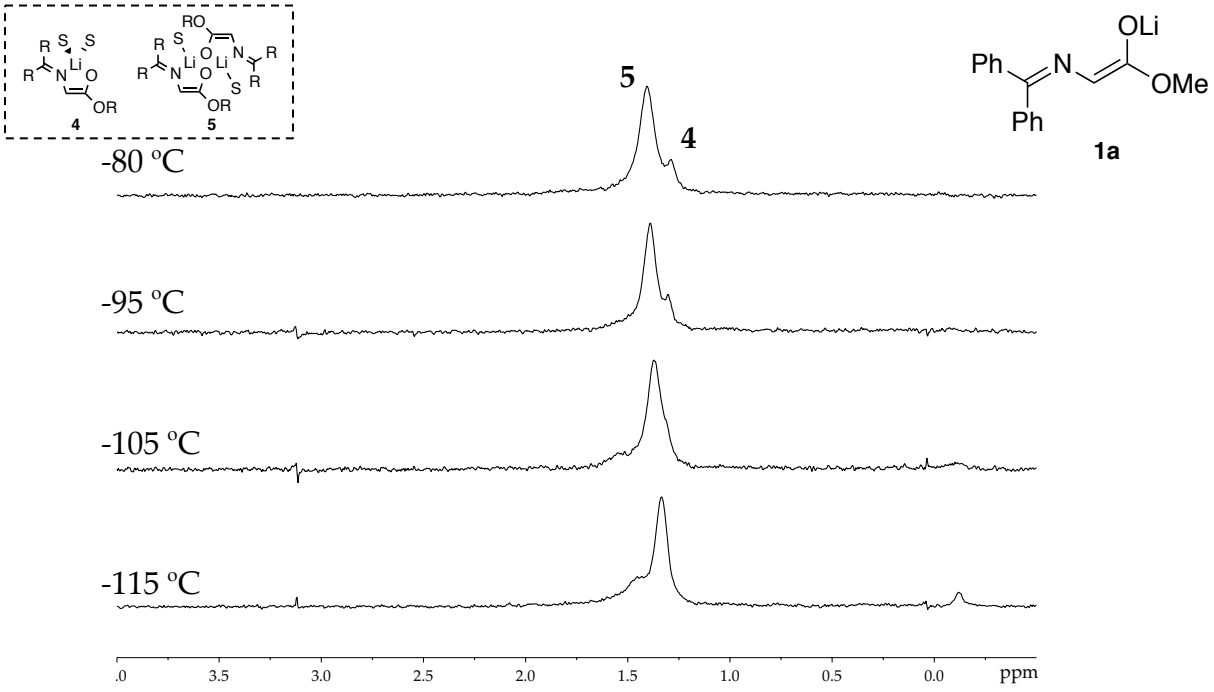


Figure 29. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**1a** with 8.0 M THF in toluene at various temperatures showing the symmetric dimer **5** and putative monomer **4**.

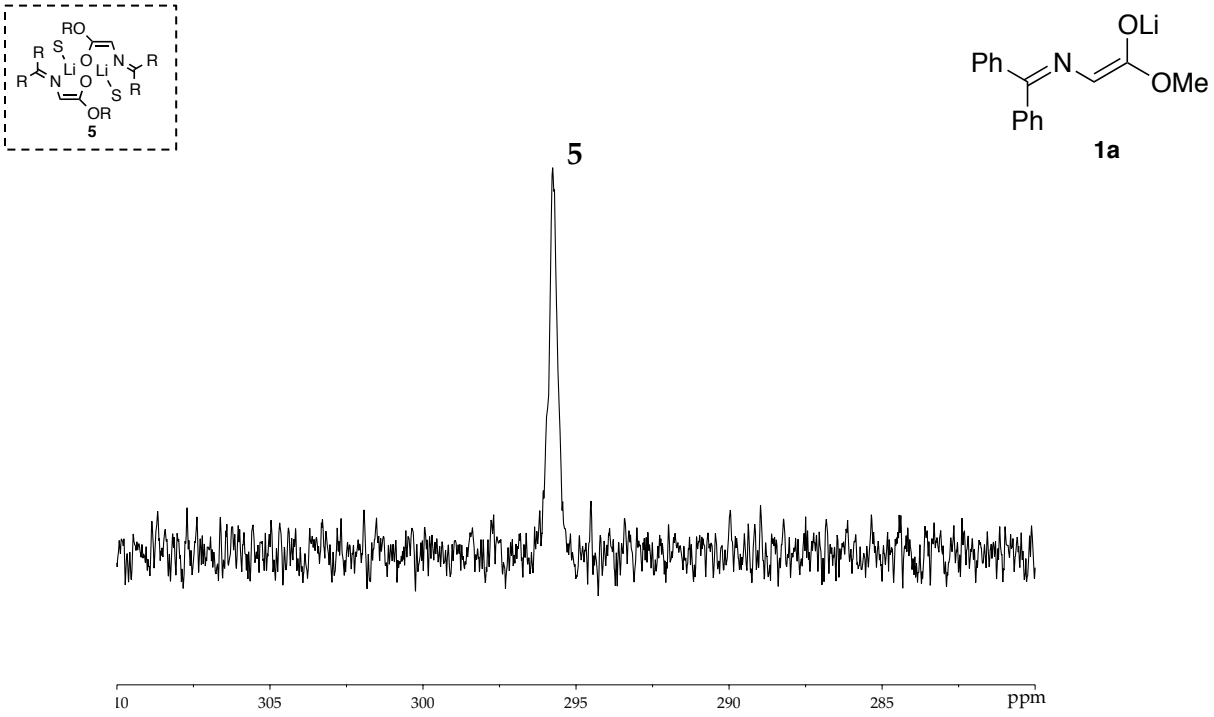


Figure 30. ^{15}N NMR spectrum of [^{6}Li,^{15}N]**1a** with 8.0 M THF in toluene at -60 °C showing the dimer **5**. The enolate concentration is 0.10 M.

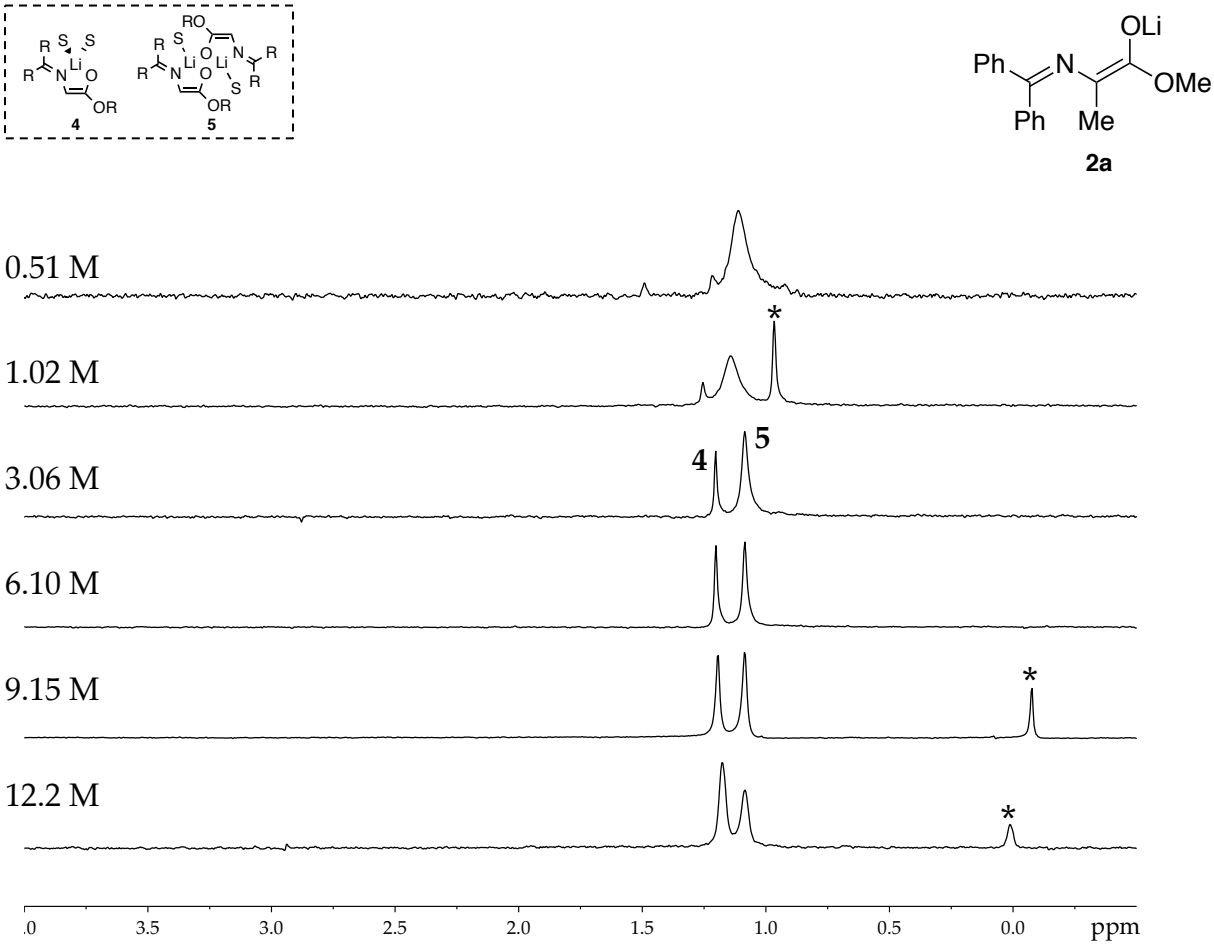


Figure 31. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**2a** with various THF concentrations in toluene at -90 °C showing the change in the ratio of symmetric dimer **5** and monomer **4**. Asterisks (*) indicate LiHMDS.

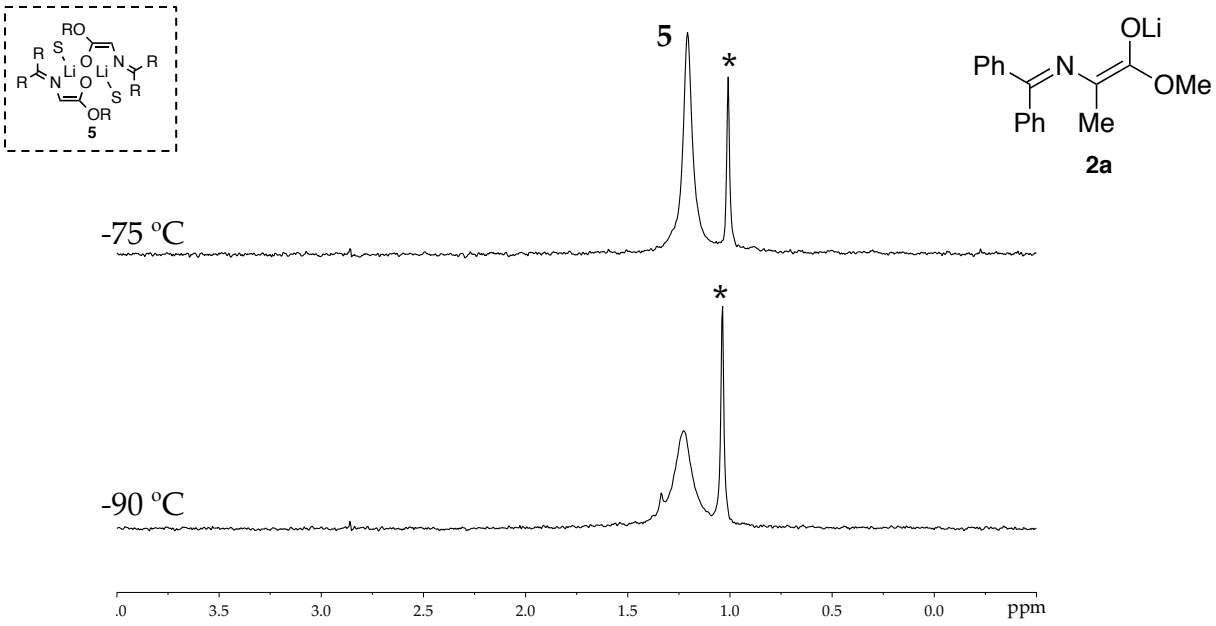


Figure 32. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**2a** with 0.51 M THF in toluene at various temperatures showing exclusively the symmetric dimer **5** at -75 °C. Asterisks (*) indicate LiHMDS.

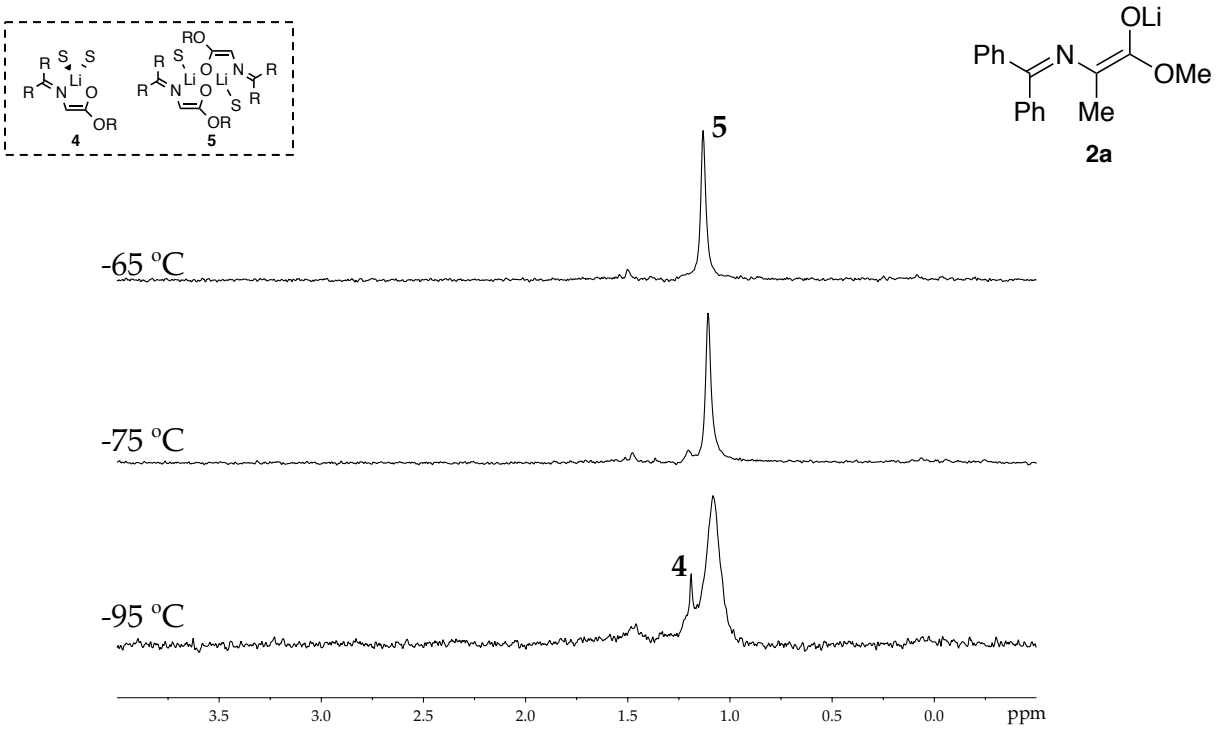


Figure 33. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**2a** with 1.02 M THF in toluene at various temperatures showing the dimer **5** and monomer **4** at lower temperatures.

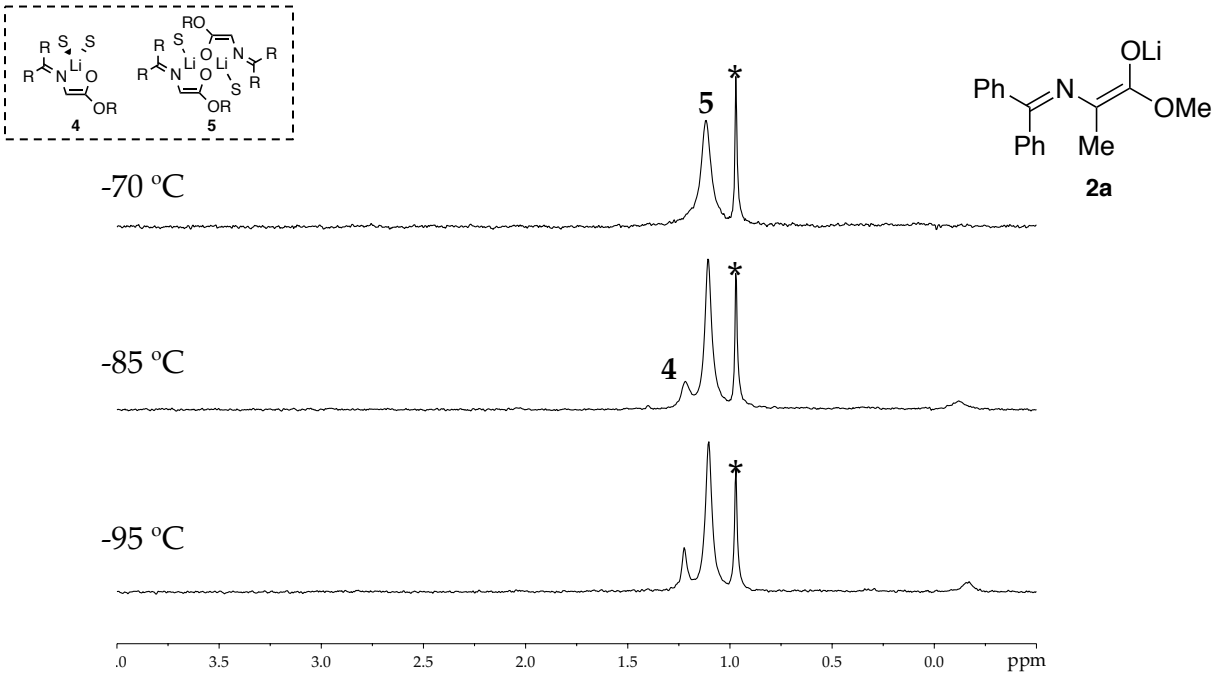


Figure 34. ^{6}Li NMR spectra of 0.20 M [^{6}Li]**2a** with 3.0 M THF in toluene at various temperatures showing the change in the distribution between the dimer **5** and the monomer **4**. Asterisks (*) indicate LiHMDS.

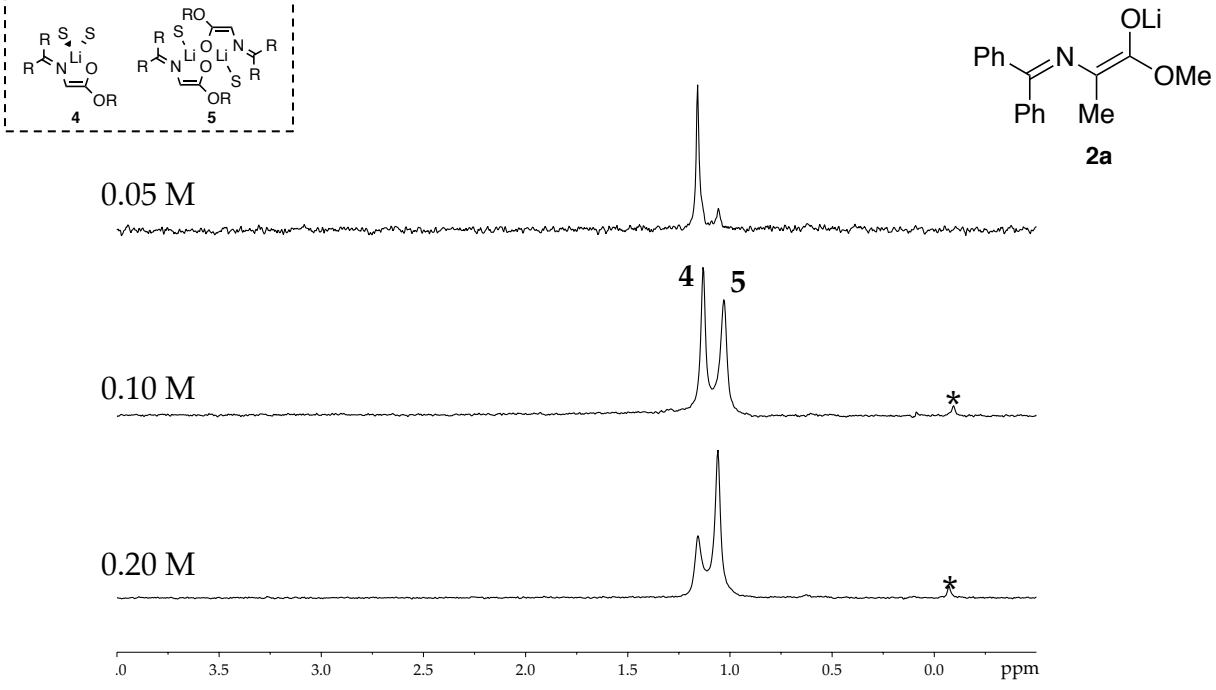


Figure 35. ^{6}Li NMR spectra of various [^{6}Li]**2a** concentrations in 10.0 M THF at -90 °C. At lower enolate concentration, the monomer **4** is the dominant species whereas the dimer **5** grows as the enolate concentration increases.

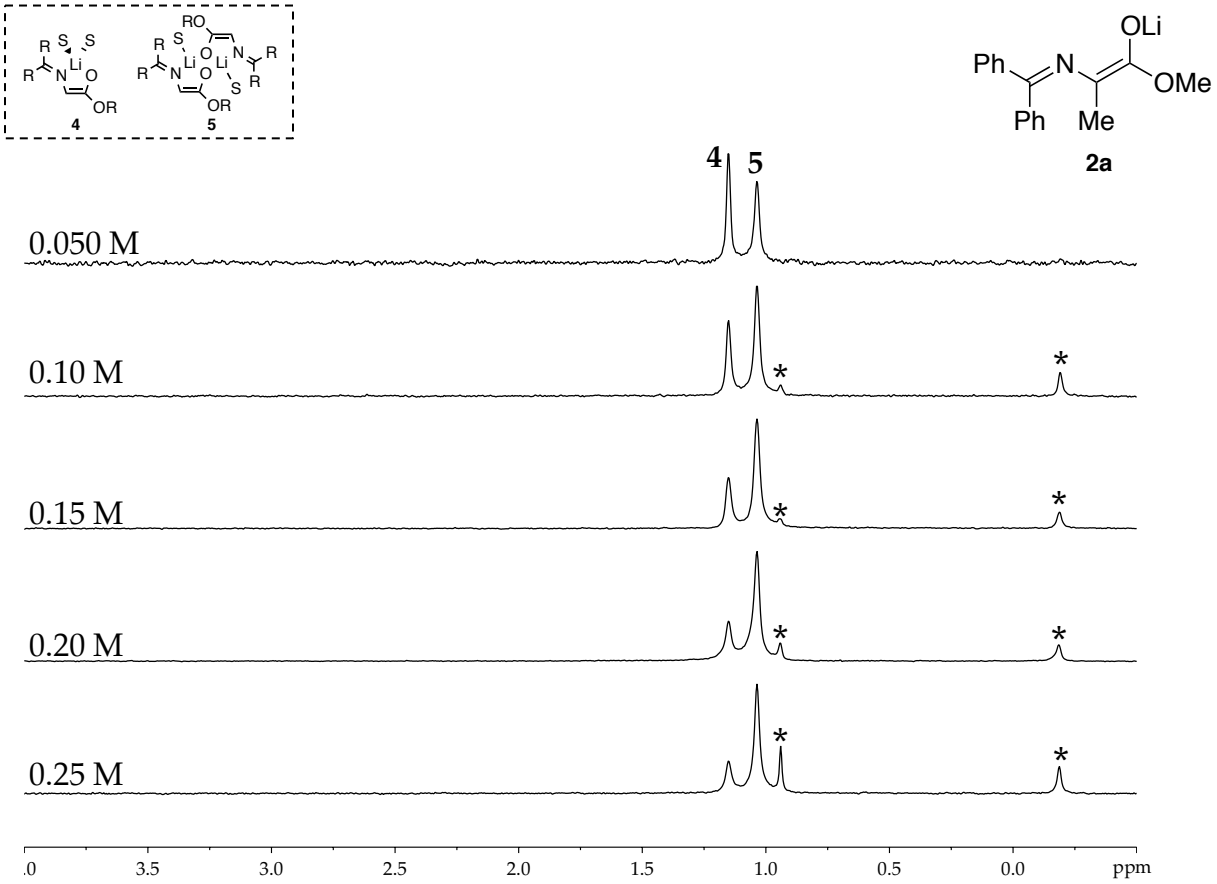
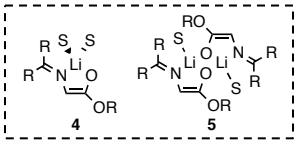
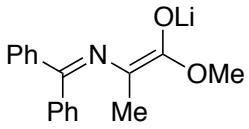


Figure 36. ^{6}Li NMR spectra of [^{6}Li]**2a** in 6.0 M THF at -90 °C showing the change in monomer **4**/dimer **5** distributions as the concentration of **2a** varies. Asterisks (*) denote LiHMDS.





2a

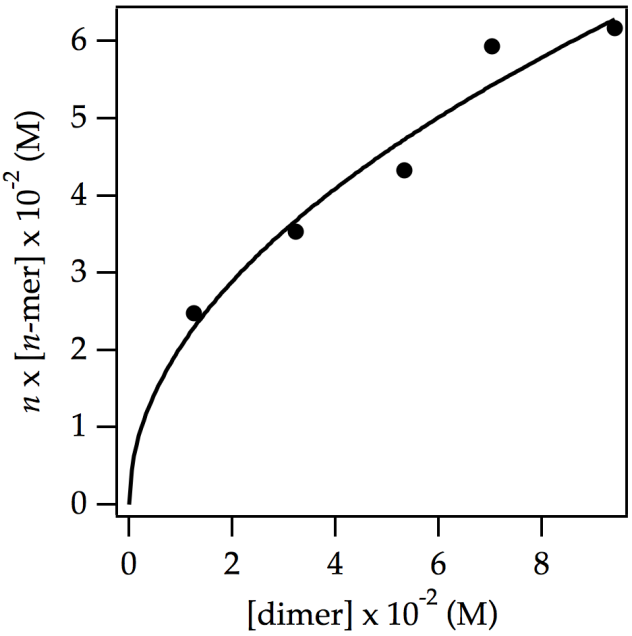


Figure 37. Plot of n x [n-mer] vs. [dimer] for **2a** in 6.0 M THF at -90 °C. n-mer corresponds to the ^{6}Li resonance at 1.15 ppm, labeled as **4** in Figure 36. The best fit gives $n = 1.0 \pm 0.2$, confirming the lower aggregate as a monomer. For related derivations, see Derivation 1 in page S35. The plot was fitted to $y = n(K_{eq}^{1/2} x^{n/2})$. [$n = 1.0 \pm 0.2$, $K_{eq} = (4.2 \pm 0.6) \times 10^{-2}$]

n x [n-mer] (M)	[dimer] (M)
0.0248	0.0126
0.0353	0.0323
0.0433	0.0533
0.0593	0.0704
0.0617	0.0942

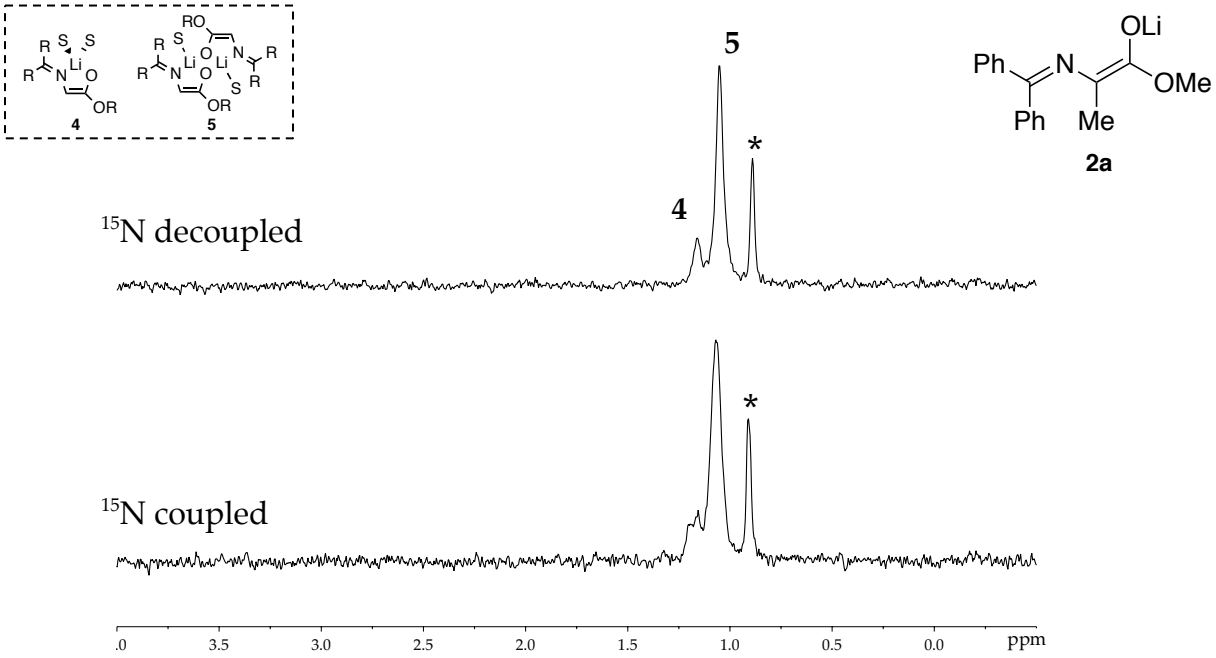


Figure 38. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**2a** with 2.0 M THF in toluene at -90 °C. The Li-N coupling was not observed due to fast exchange. Asterisks (*) indicate LiHMDS.

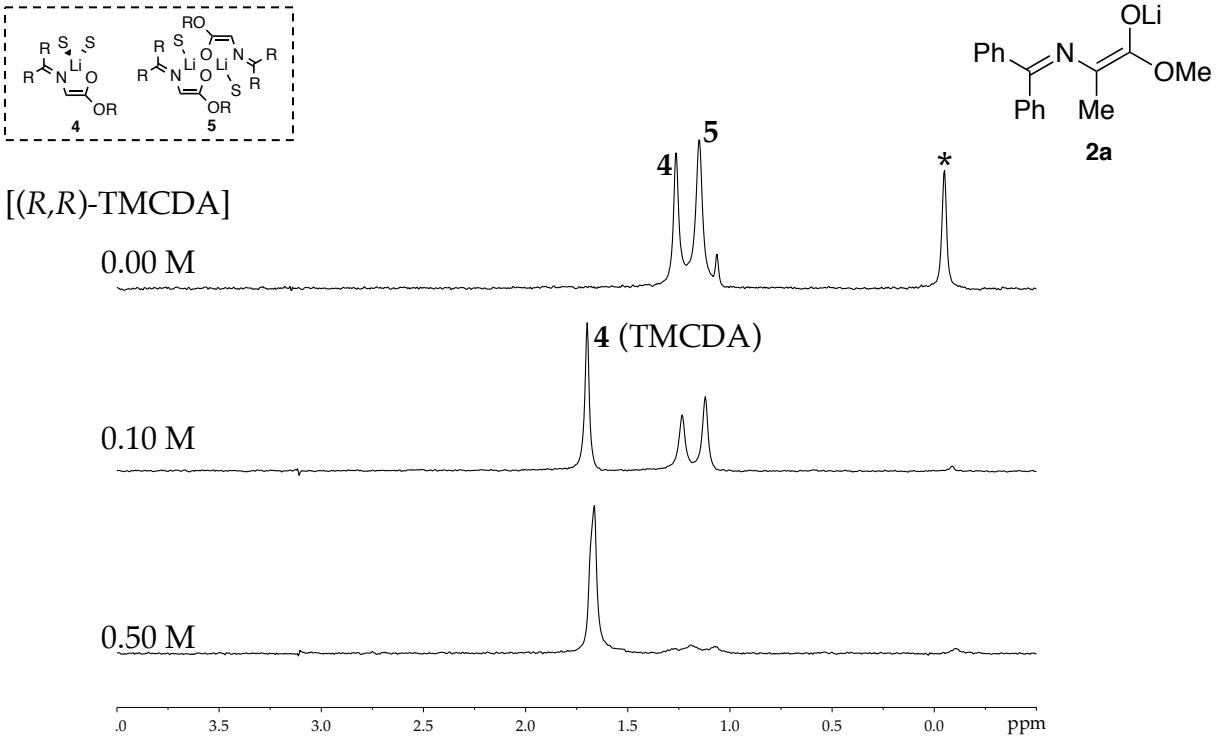


Figure 39. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**2a** with 7.0 M THF and various concentrations of (*R,R*)-TMCDA in toluene at -95 °C. Relatively low concentrations of (*R,R*)-TMCDA deplete both THF-solvated monomer and dimer.

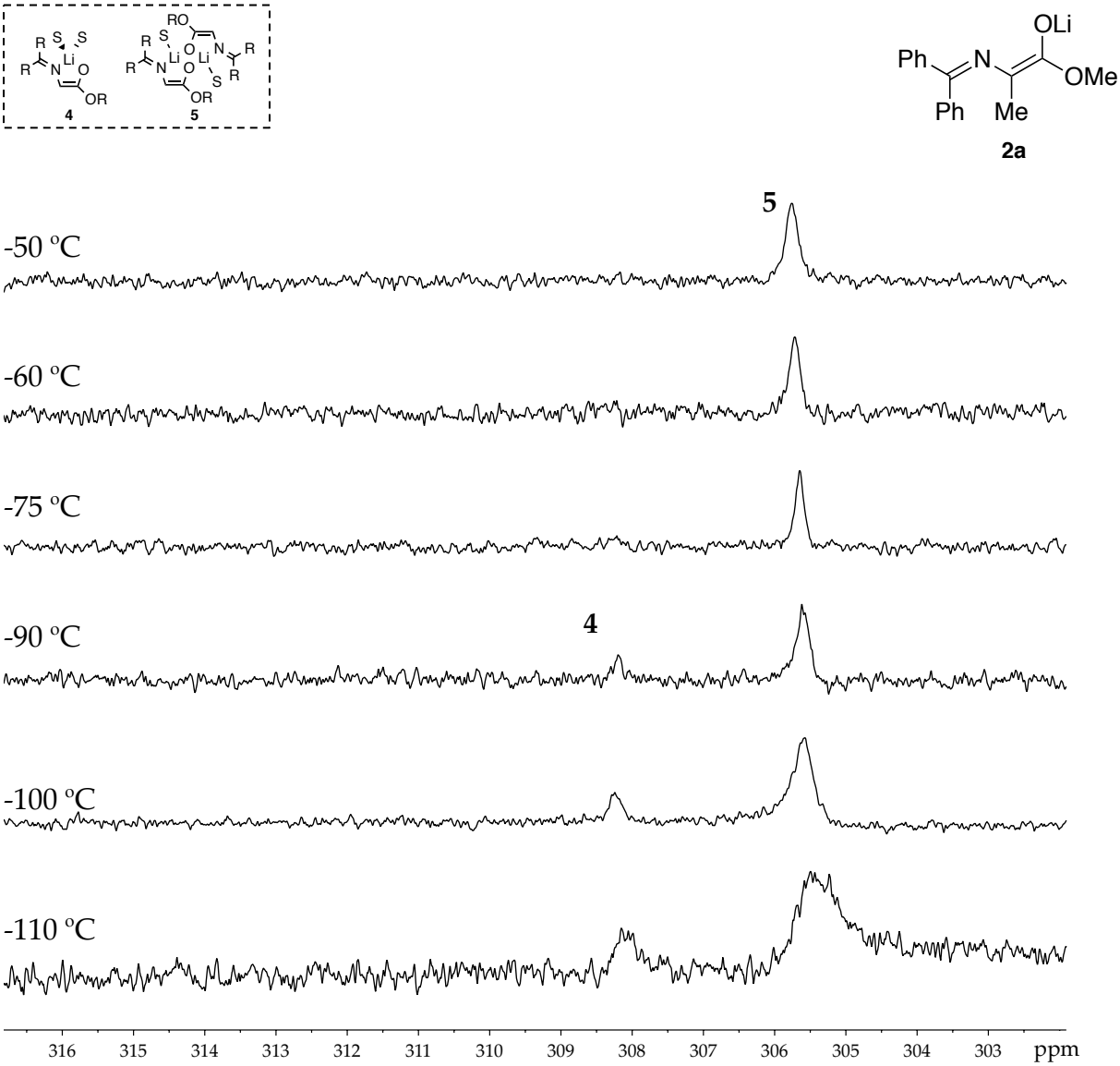


Figure 40. ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]**2a** with 2.0 M THF in toluene at various temperatures. The Li-N couplings for both monomer **4** and the dimer **5** were not observed due to fast exchange.

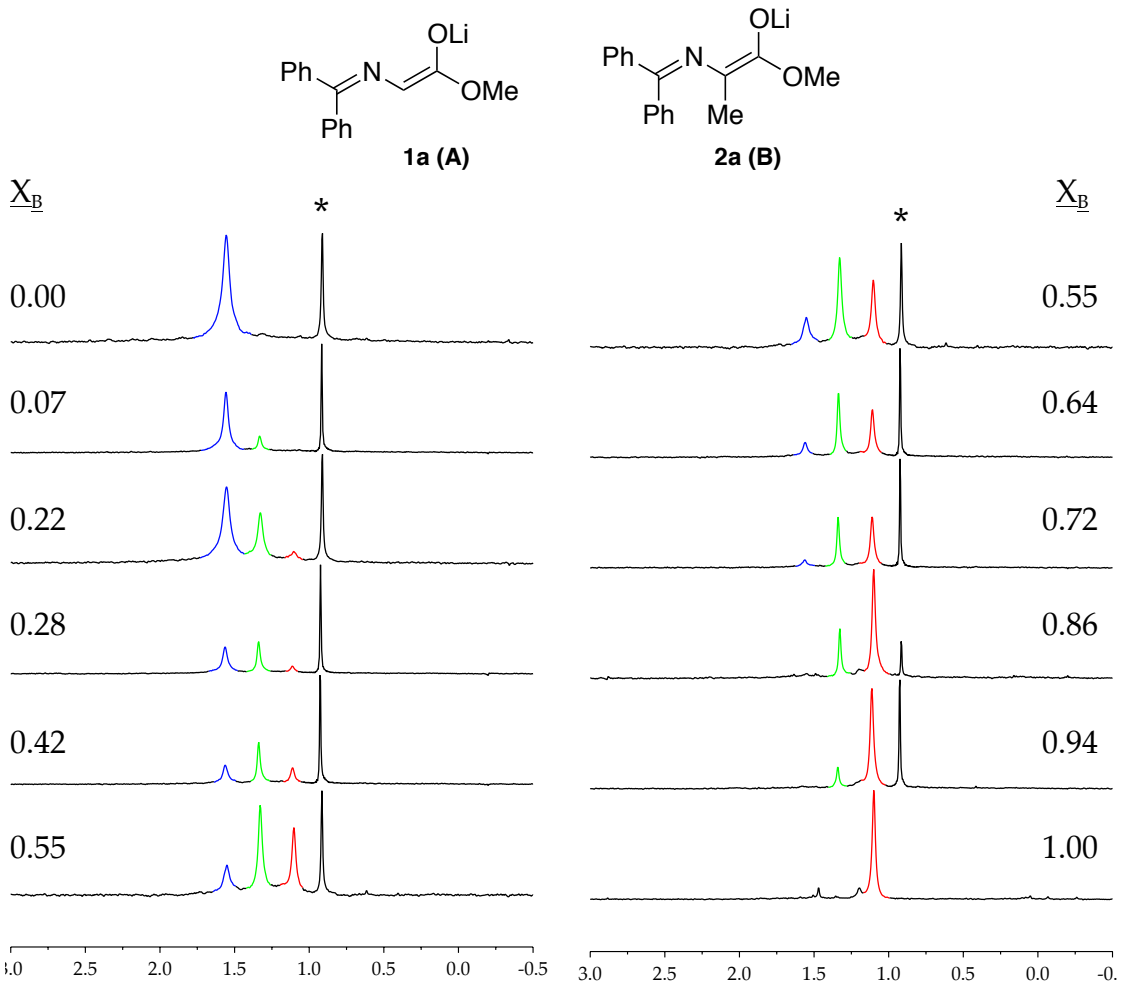


Figure 41. ^{6}Li NMR spectra of mixtures of 0.10 M [^{6}Li]**1a** and [^{6}Li]**2a** at various mole fractions in 1.0 M THF in toluene at -75 °C. X_B indicates the measured mole fractions of **2a** (**B**). The ensemble is consistent with dimer assignment.

Table 15. Resonance integrations for each aggregate in an ensemble of [^{6}Li]**1a** (**A**) and [^{6}Li]**2a** (**B**).

X_B	Resonance Integrations		
	A_2	**AB**	**B_2**
0.00	1.00	0.00	0.00
0.071	66095.313	10872.583	0.00
0.22	120097.981	57697.051	14098.401
0.28	28528.681	20570.368	4728.122
0.42	20129.145	25891.357	11470.371
0.55	39812.576	66746.25	57461.752
0.64	13672.054	34813.651	38352.769
0.72	7235.654	24833.328	38753.675
0.86	2671.214	23487.313	73589.239

0.94	0.00	11207.319	75908.079
1.00	0.00	0.00	1.00

Table 16. Relative resonance integrations for each aggregate in an ensemble of [^{6}Li]**1a** (**A**) and [^{6}Li]**2a** (**B**).

X_B	Resonance Integrations		
	A_2	**AB**	**B_2**
0.00	1.00	0.00	0.00
0.071	0.86	0.14	0.00
0.22	0.63	0.30	0.073
0.28	0.53	0.38	0.088
0.42	0.35	0.45	0.20
0.55	0.24	0.41	0.35
0.64	0.16	0.40	0.44
0.72	0.10	0.35	0.55
0.86	0.027	0.24	0.74
0.94	0.00	0.13	0.87
1.00	0.00	0.00	1.00

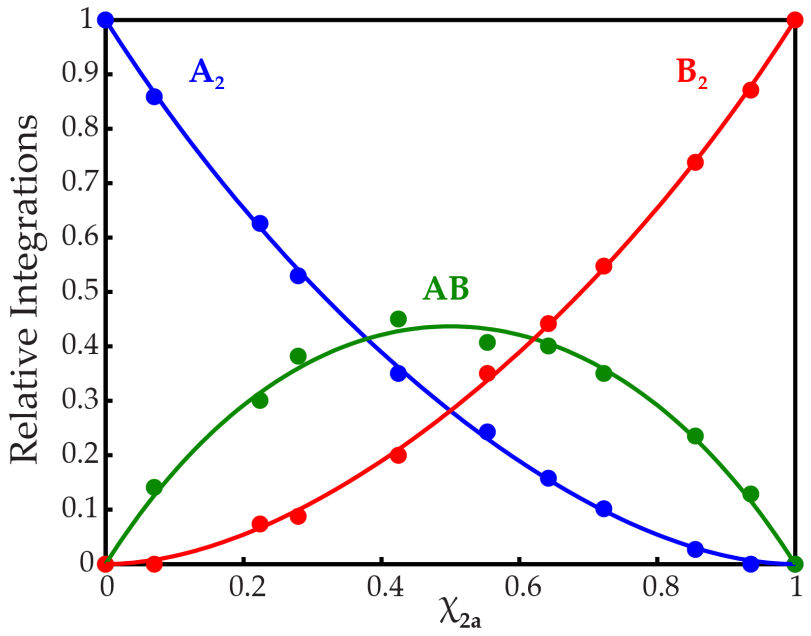


Figure 42. Job plot showing the relative integrations versus measured mole fraction of **2a** for the ensemble of [^{6}Li]**1a** and [^{6}Li]**2a** in 1.0 M THF in toluene at -75 °C. The Job plot indicates dimers for **1a** and **2a**.

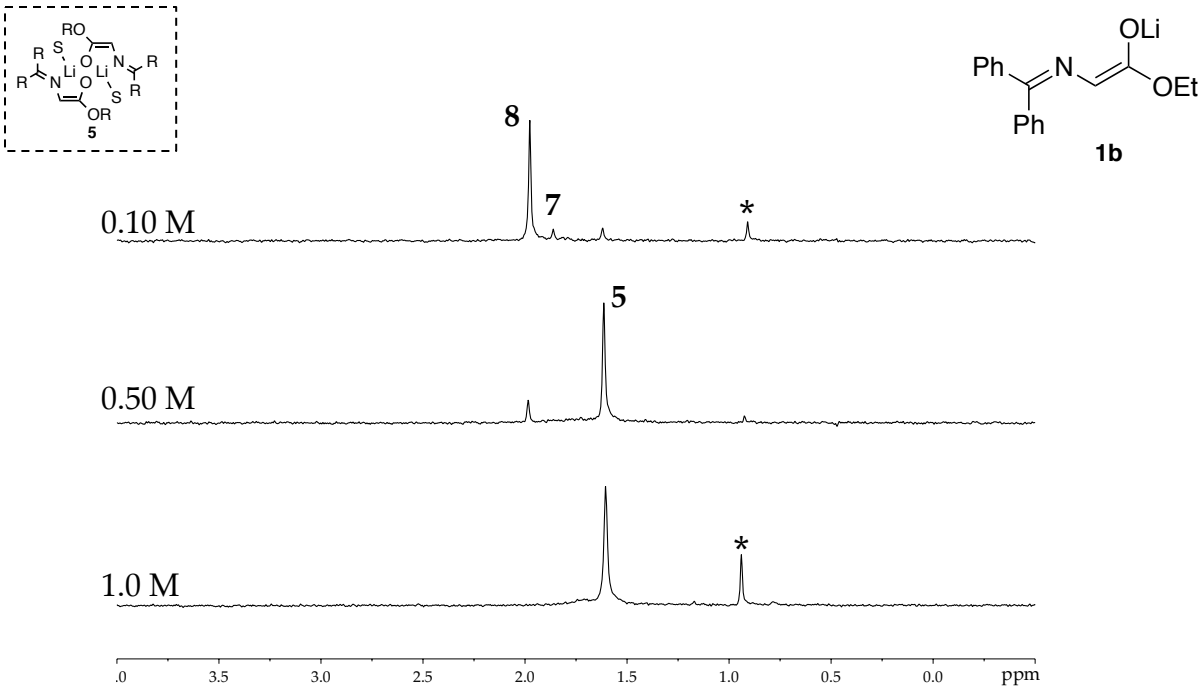


Figure 43. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1b** with various THF concentrations in toluene at -78 °C showing the unsolvated hexamer **8**, tetramer **7**, and symmetric dimer **5**. Asterisks (*) denote LiHMDS.

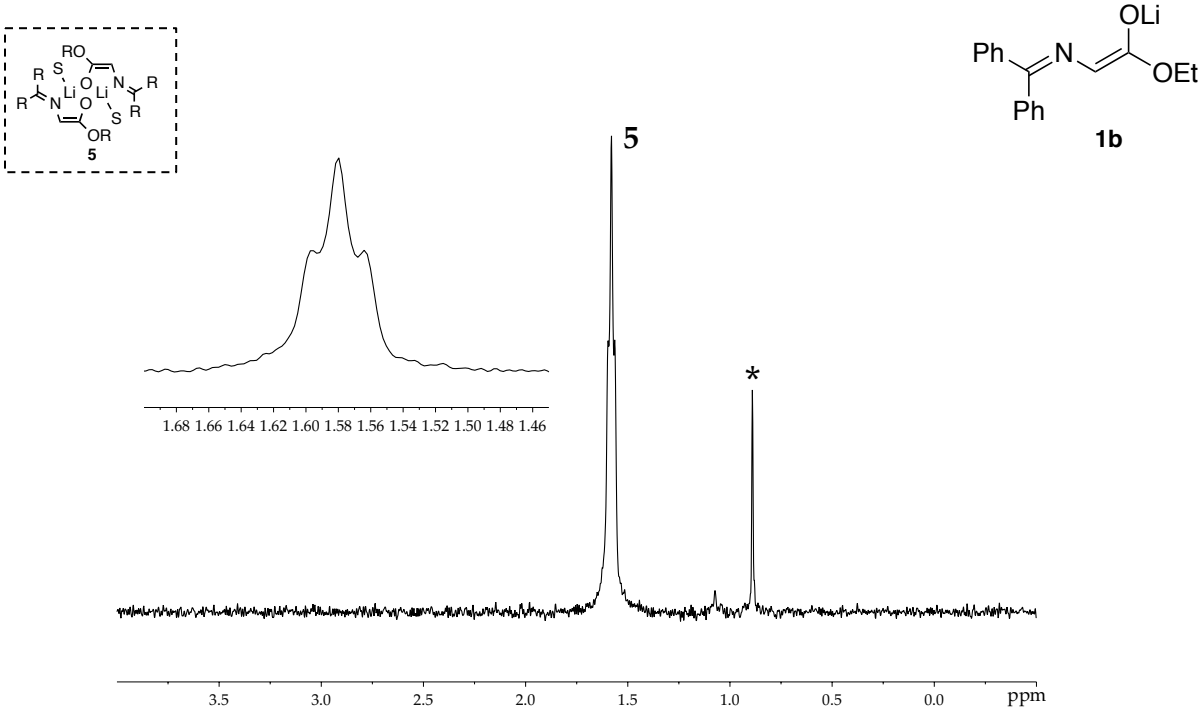


Figure 44. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]**1b** in 0.51 M THF in toluene at -95 °C showing the symmetric dimer **5** with J=1.5 Hz.

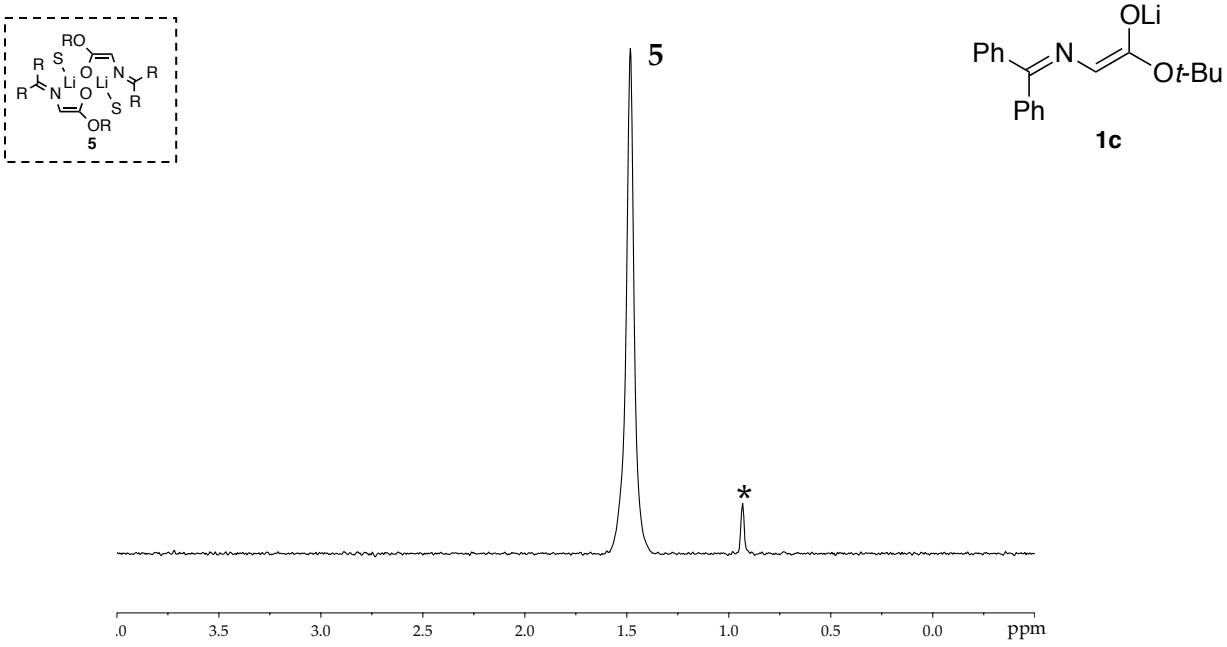


Figure 45. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**1c** with 2.0 M THF in toluene at -75 °C. The dimer **5** was assigned based on the structural studies of analogous enolates. Asterisk (*) denotes LiHMDS.

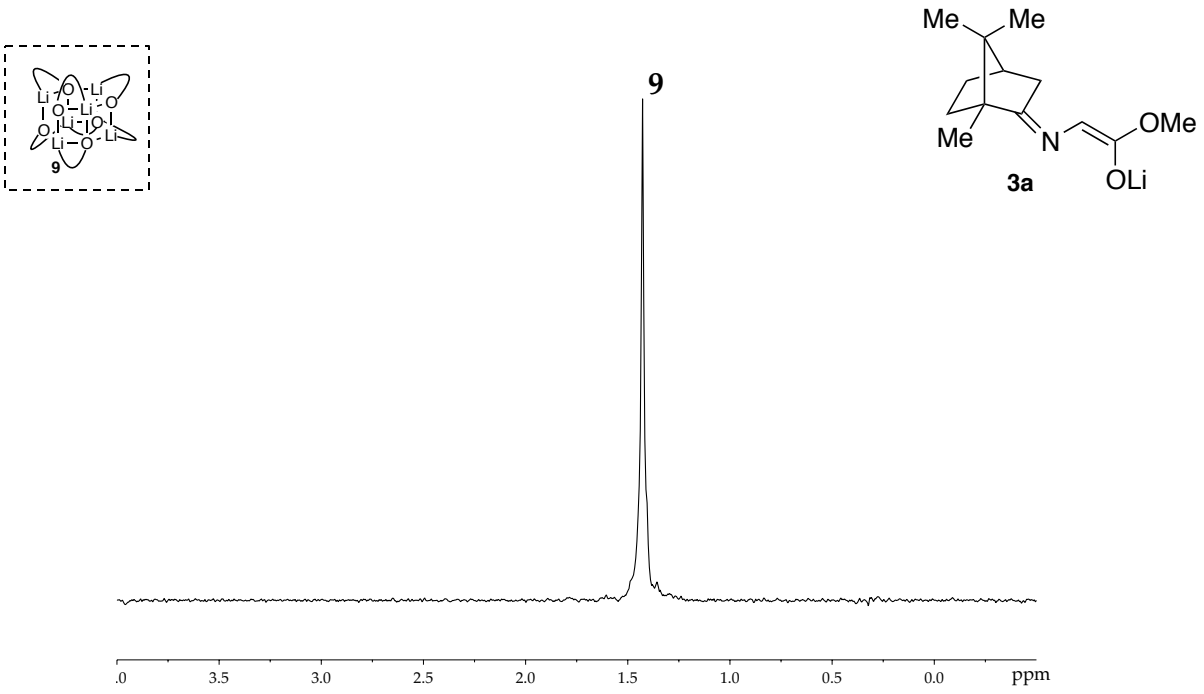


Figure 46. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**3a** with 0.51 M THF in toluene at -70 °C showing the unsolvated hexamer **9**.

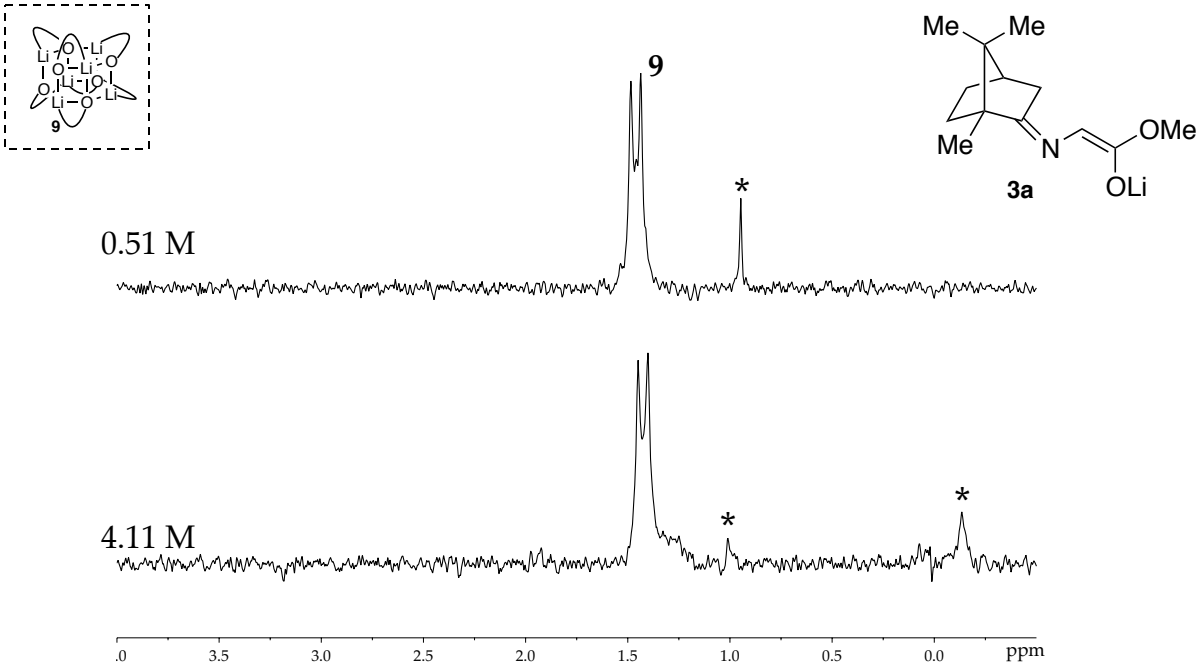


Figure 47. ^{6}Li NMR spectra of [^{6}Li,^{15}N]**3a** with various THF concentrations in toluene. Samples are 0.10 M enolate and -70 °C showing strong preference of unsolvated hexamer **9**. J = 3.5 Hz. Asterisks (*) denote LiHMDS dimer and monomer.

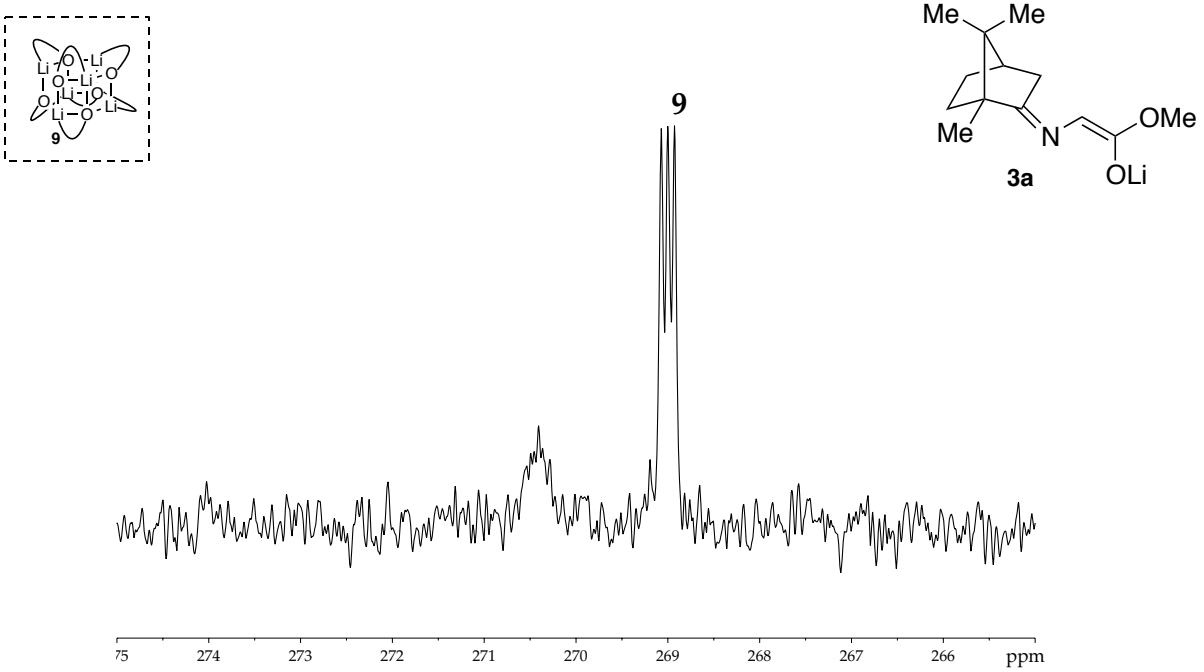


Figure 48. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3a** with 4.11 M THF in toluene at -45 °C. The chemical shift and the coupling constant (J = 3.6 Hz) match those of unsolvated hexamer **9**.

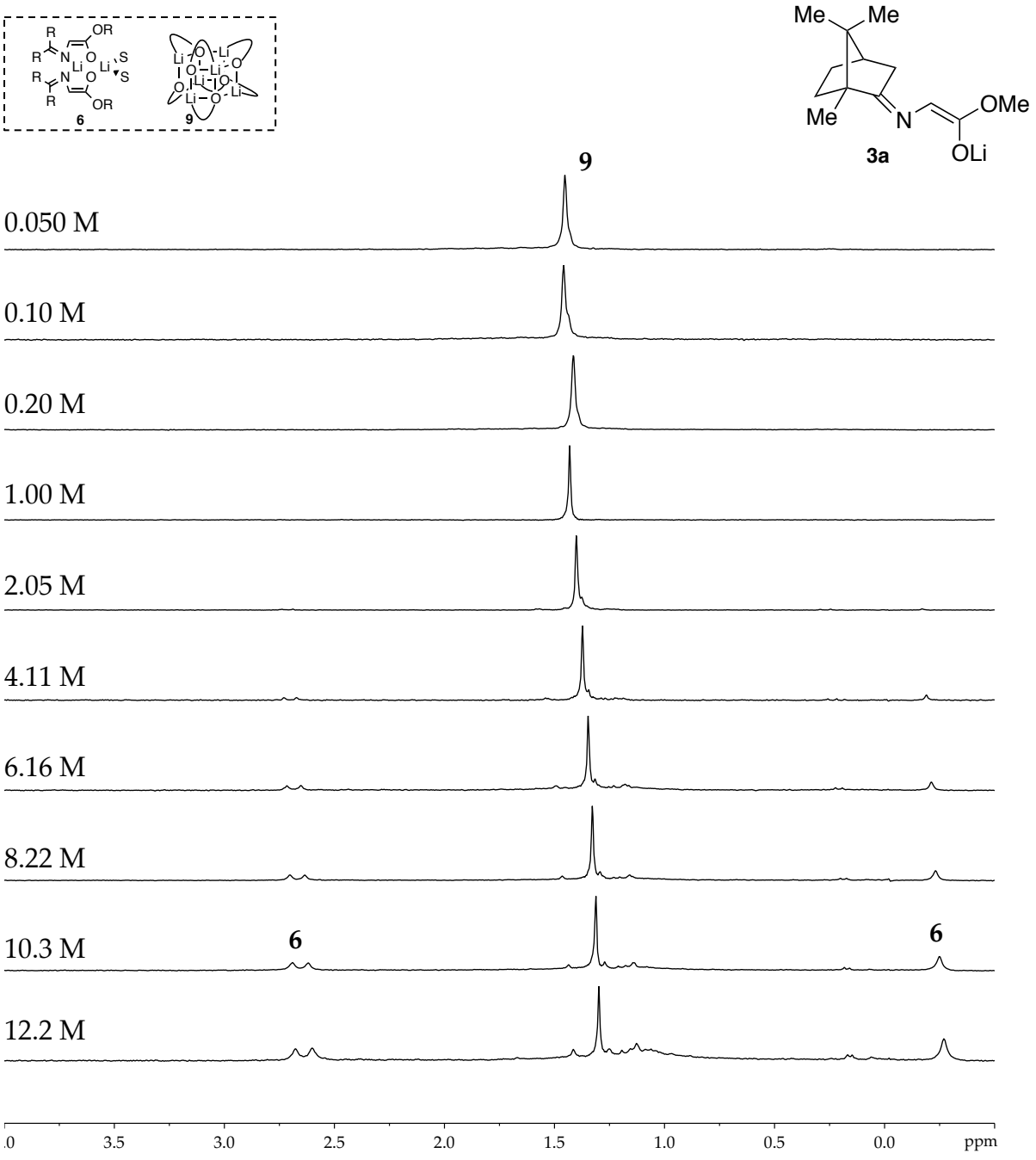


Figure 49. ^{6}Li NMR spectra of 0.20 M [^{6}Li]**3a** with various concentrations of THF in toluene at -78 °C. The resonances characteristic of unsymmetric dimer **6** appear in addition to the unsolvated hexamer **9** at very high concentration of THF.

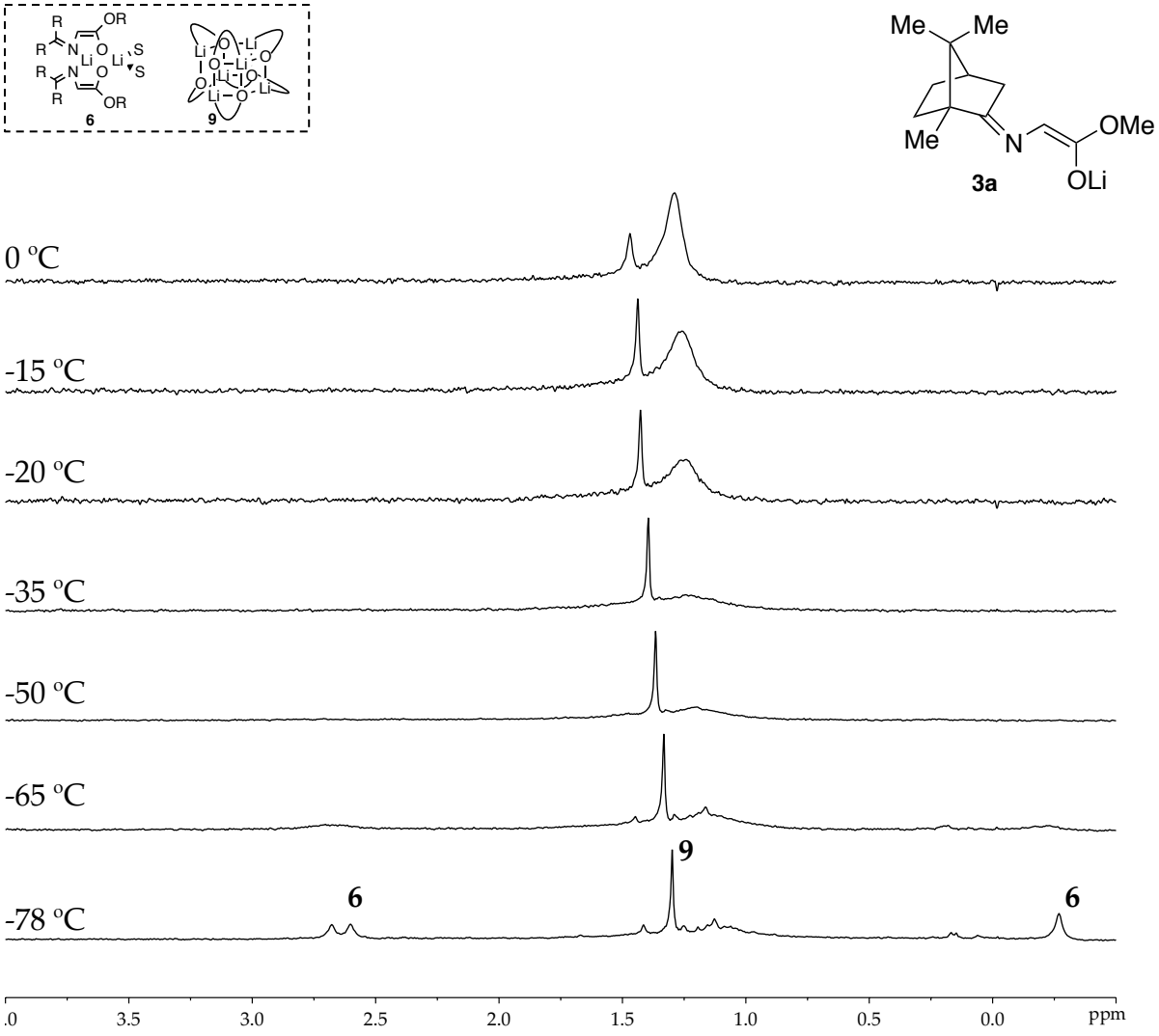


Figure 50. ^{6}Li NMR spectra of 0.20 M [^{6}Li]**3a** in neat THF at various temperatures showing the unsolvated hexamer **9** and unsymmetric dimer **6** that coalescence at higher temperatures.

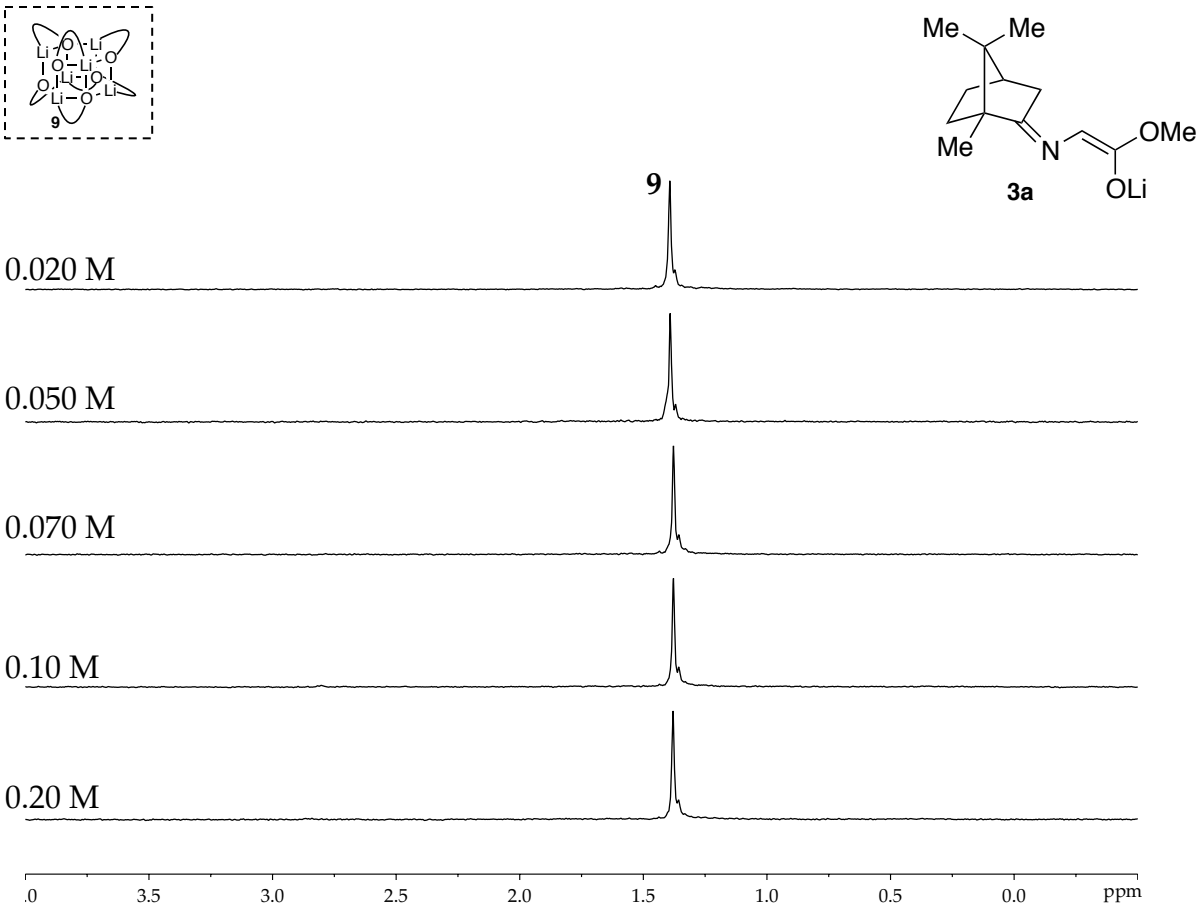


Figure 51. ^{6}Li NMR spectra of 0.10 M[^{6}Li]**3a** in 1.0 M THF with various pyridine concentrations at -75 °C. Undisturbed chemical shift signifies the lack of solvation.

IV. NMR Spectroscopic Studies with *N,N,N′,N′*-tetramethylethylenediamine (TMEDA) in Toluene

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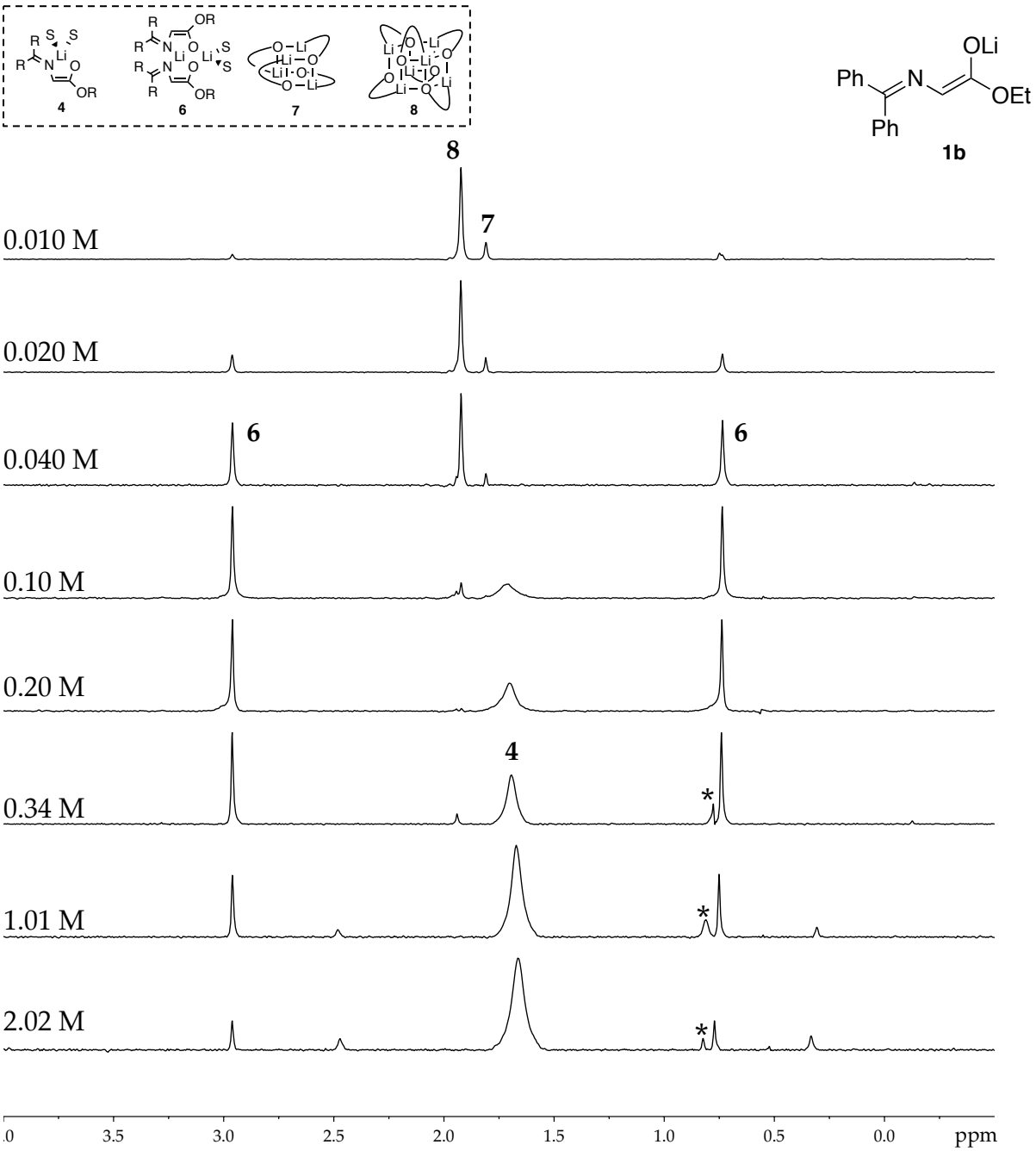
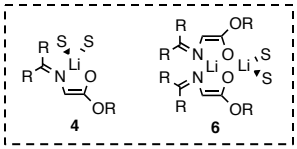
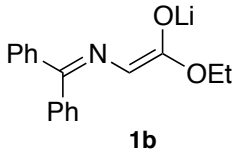


Figure 52. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1b** at -75 °C with various TMEDA concentrations in toluene showing the unsolvated hexamer **8**, tetramer **7**, unsymmetric dimer **6**, and monomer **4**. Asterisks (*) are LiHMDS. The tetramer may be more susceptible to deaggregation than the hexamer.





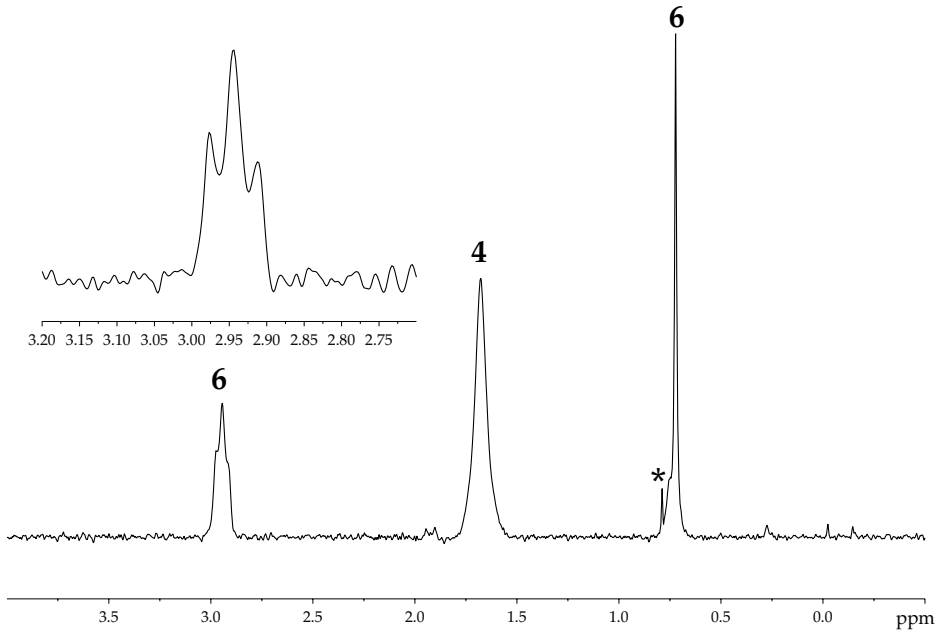
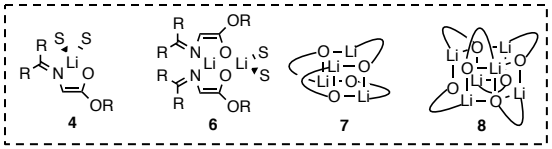
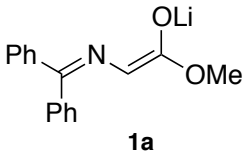


Figure 53. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**1b** in 0.34 M TMEDA in toluene at -75 ^{o}C. Window functions applied to the inset (J = 2.9 Hz). The splitting was not observed for monomer **4** due to broadening. Asterisk (*) denotes LiHMDS.





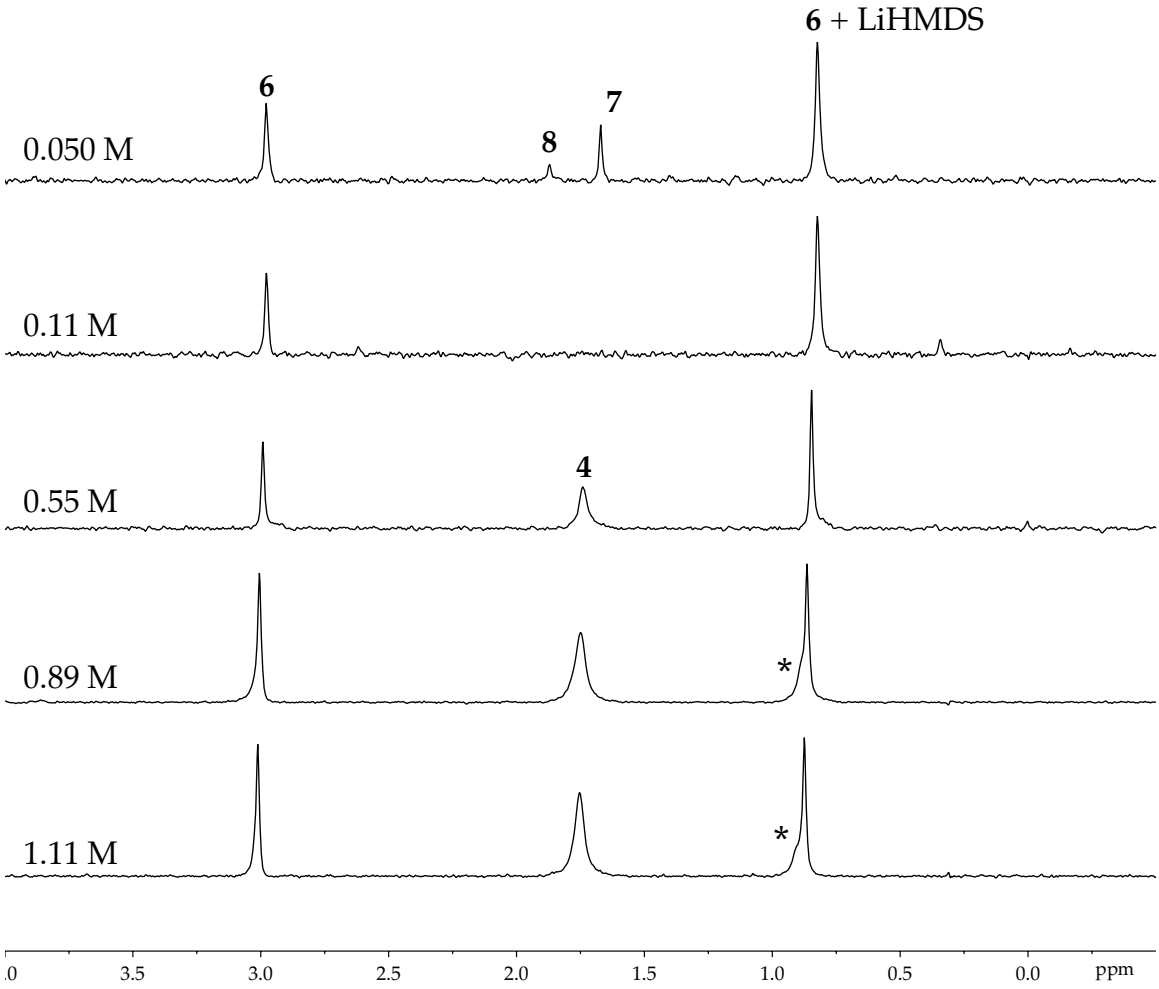


Figure 54. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** with various TMEDA concentrations in toluene at -70 °C. The integrations of the two ^{6}Li resonances for the unsymmetric dimer **6** do not agree with each other due to an overlap of the upfield resonance, the excess base, and possibly an unassigned oligomer. Asterisks (*) denote LiHMDS.

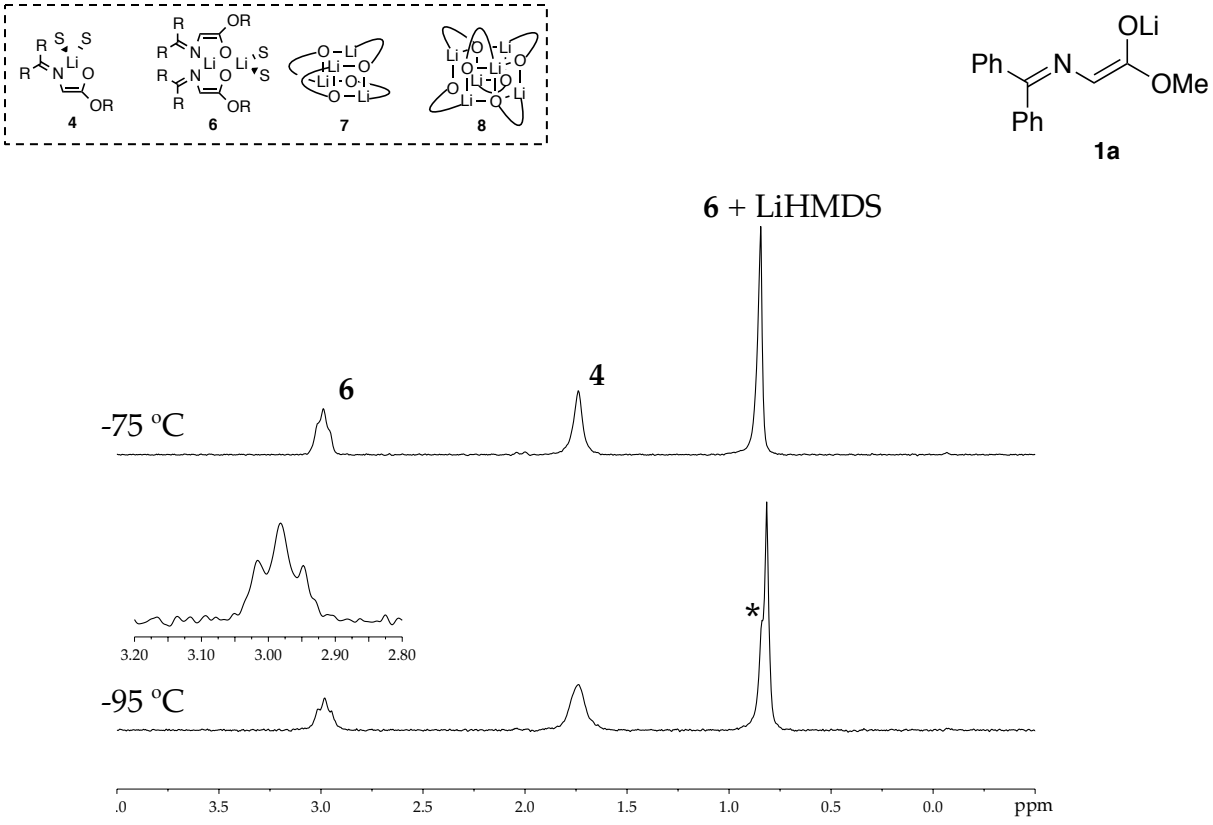
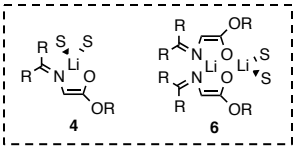
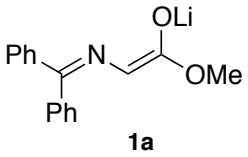


Figure 55. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**1a** with 0.55 M TMEDA in toluene showing monomer **4** and unsymmetric dimer **6** (J = 3.0 Hz; inset) partially obscured by LiHMDS. Asterisk (*) denotes LiHMDS.





1a

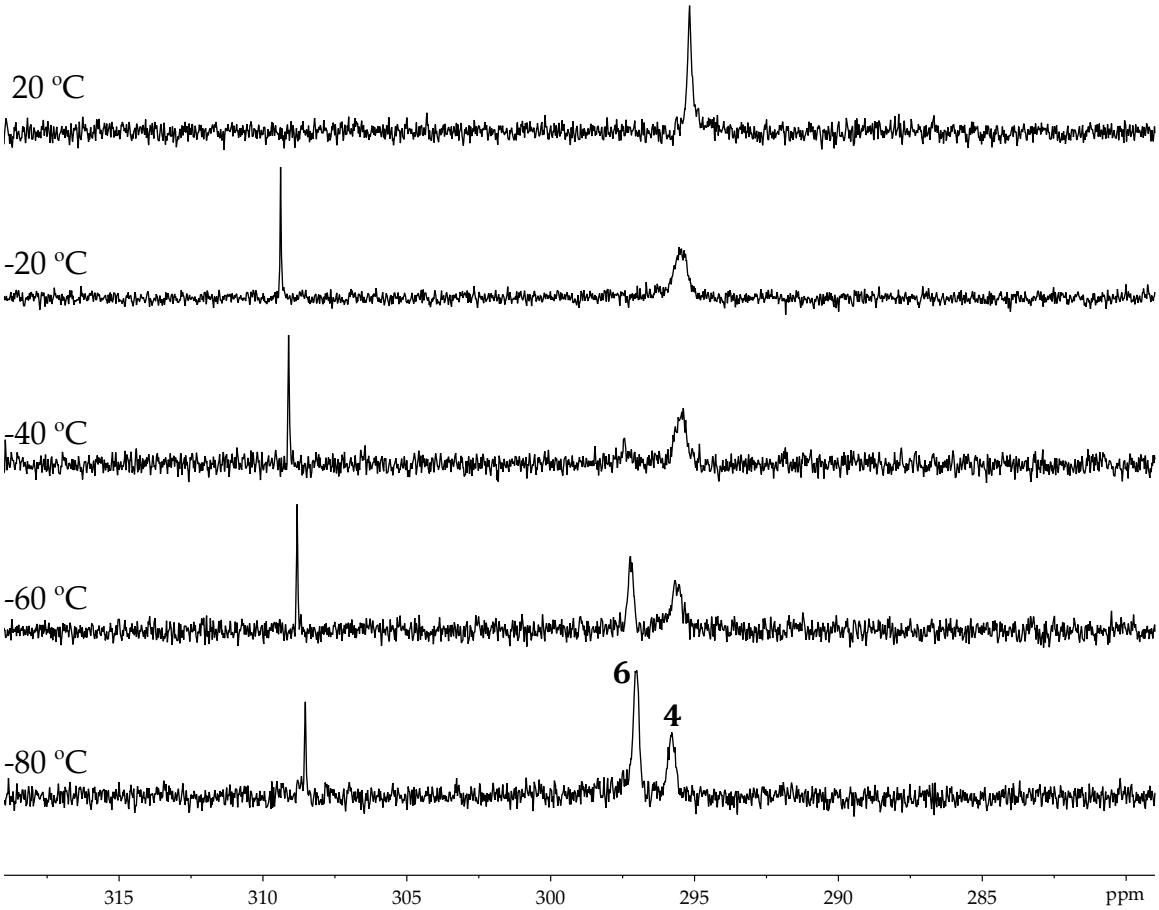


Figure 56. ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]**1a** in 0.55 M TMEDA in toluene at various temperatures. The splitting was not visible for either monomer **4** or unsymmetric dimer **6** due to broadening. The sharp downfield resonance is the unreacted imine **10a**.

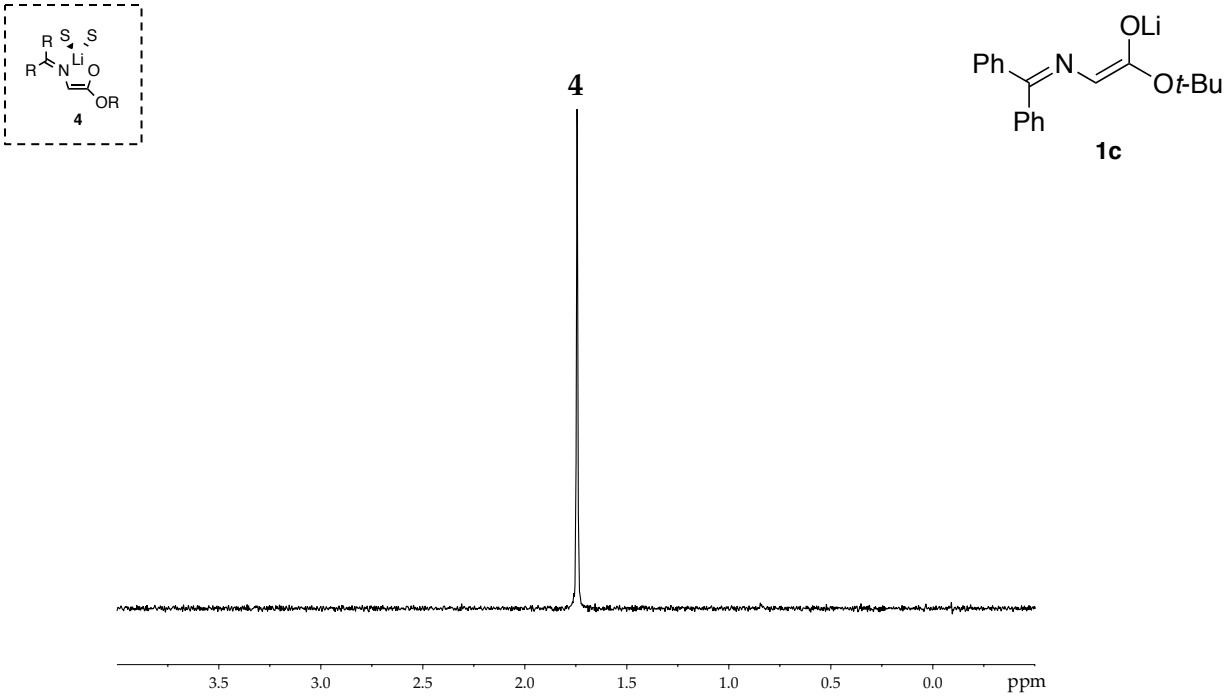


Figure 57. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**1c** in 0.55 M TMEDA in toluene at -75 ^{o}C. The aggregate is assigned as monomer **4** based on the X-ray crystallographic result and structural studies of the analogous enolates.

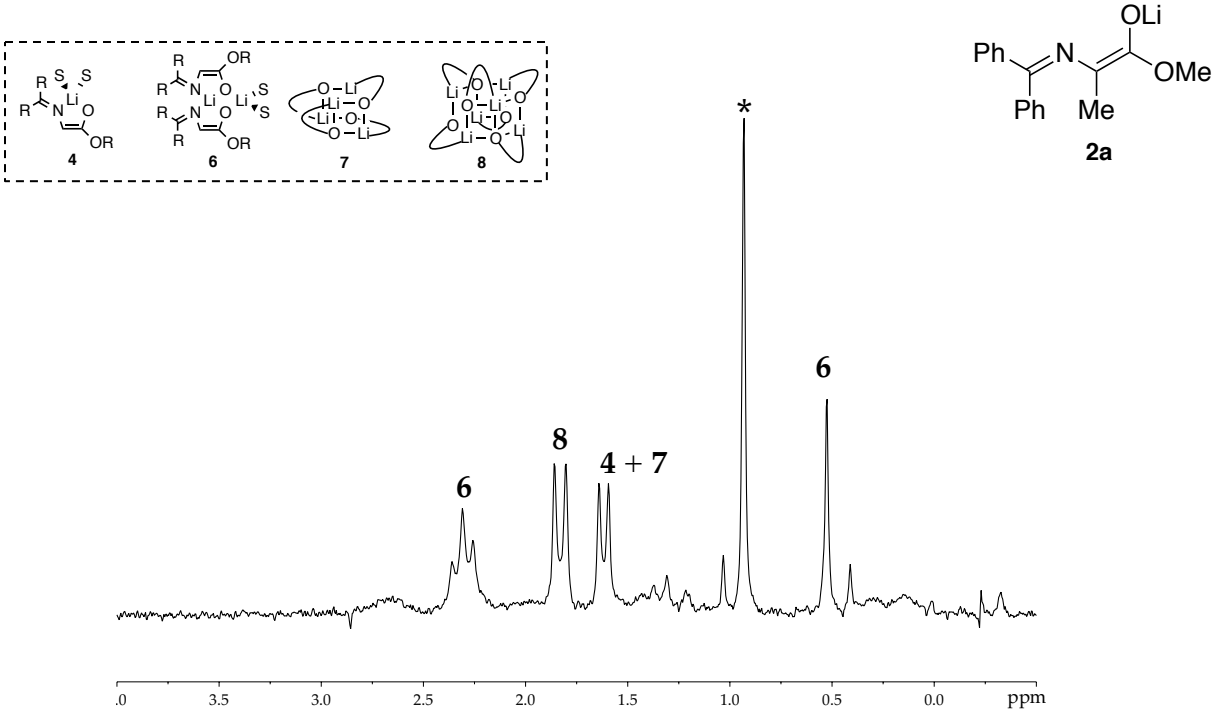


Figure 58. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]**2a** in 0.030 M TMEDA/toluene at -75 °C. **4**, $J_{\text{Li-N}}$ = 3.3 Hz; **6**, $J_{\text{Li-N}}$ = 3.8 Hz, and **8**, $J_{\text{Li-N}}$ = 4.0 Hz.

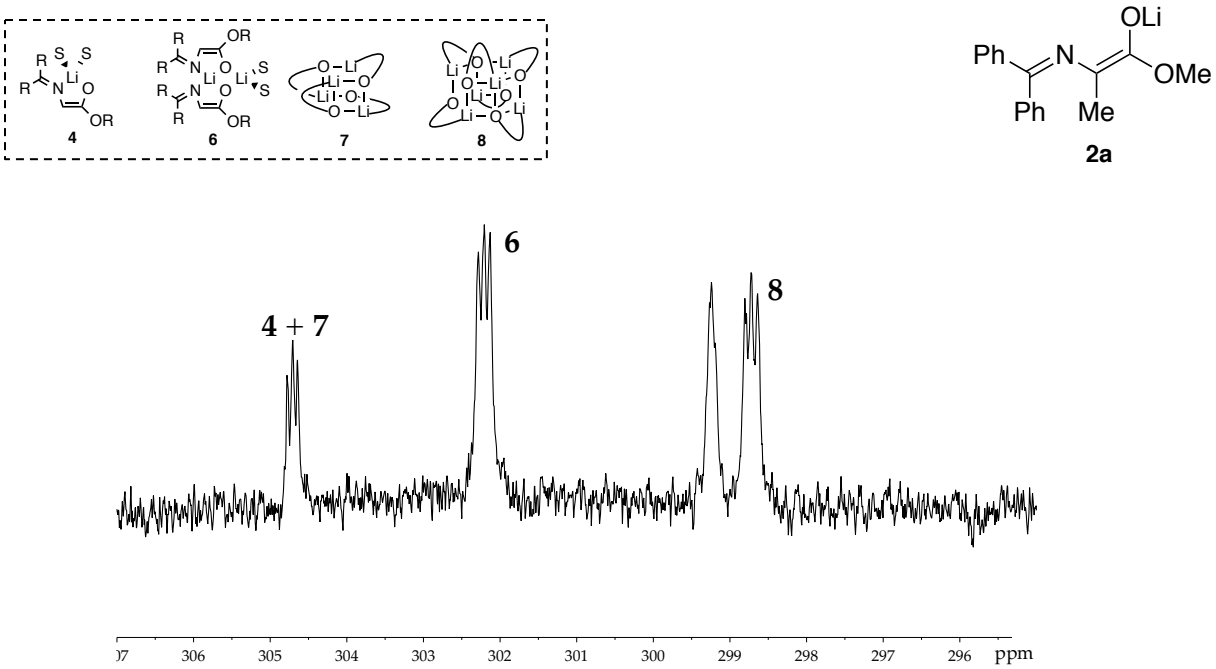


Figure 59. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**2a** in 0.030 M TMEDA/toluene at -55 °C showing monomer **4**, dimer **6**, and hexamer **8**. The singlet is believed to be unreacted substrate **11a**.

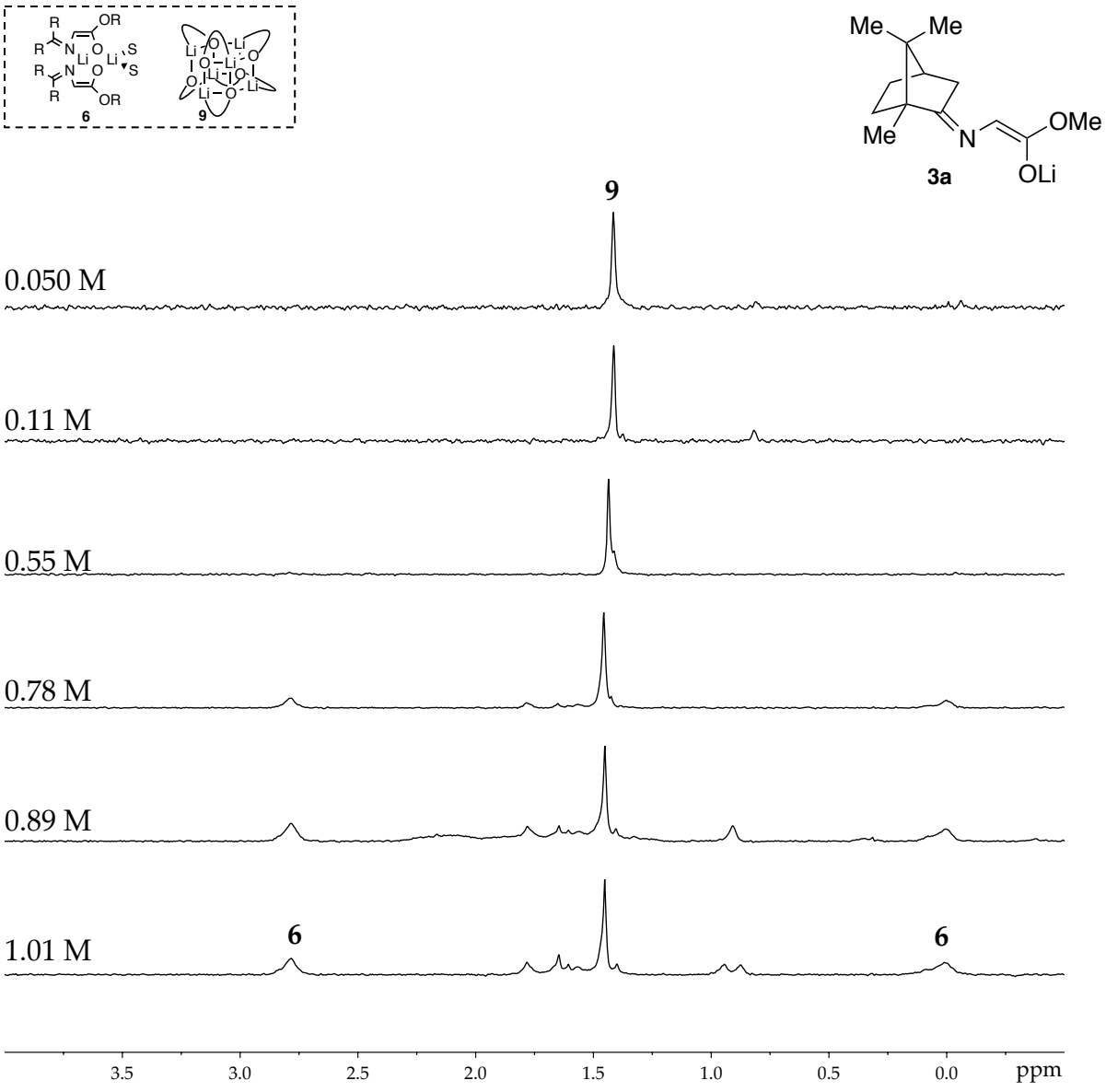


Figure 60. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3a** with various TMEDA concentrations in toluene at -70 °C. The unsolvated hexamer **9** is predominant throughout the series with only traces of unsymmetric dimer **6**.

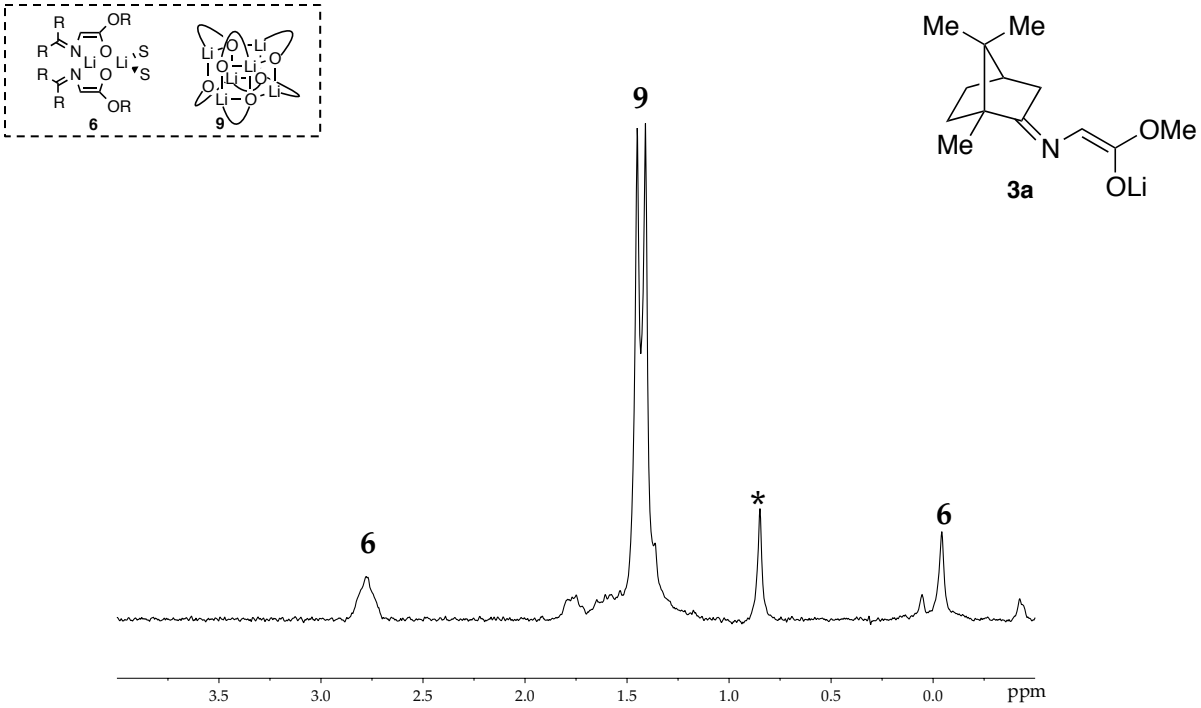


Figure 61. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3a** in 0.55 M TMEDA/toluene at -75 °C. The coupling constant for the hexamer **9** is 3.5 Hz. The coupling constant of the unsymmetric dimer **6** could not be determined owing to broad resonance. Asterisk (*) denotes LiHMDS.

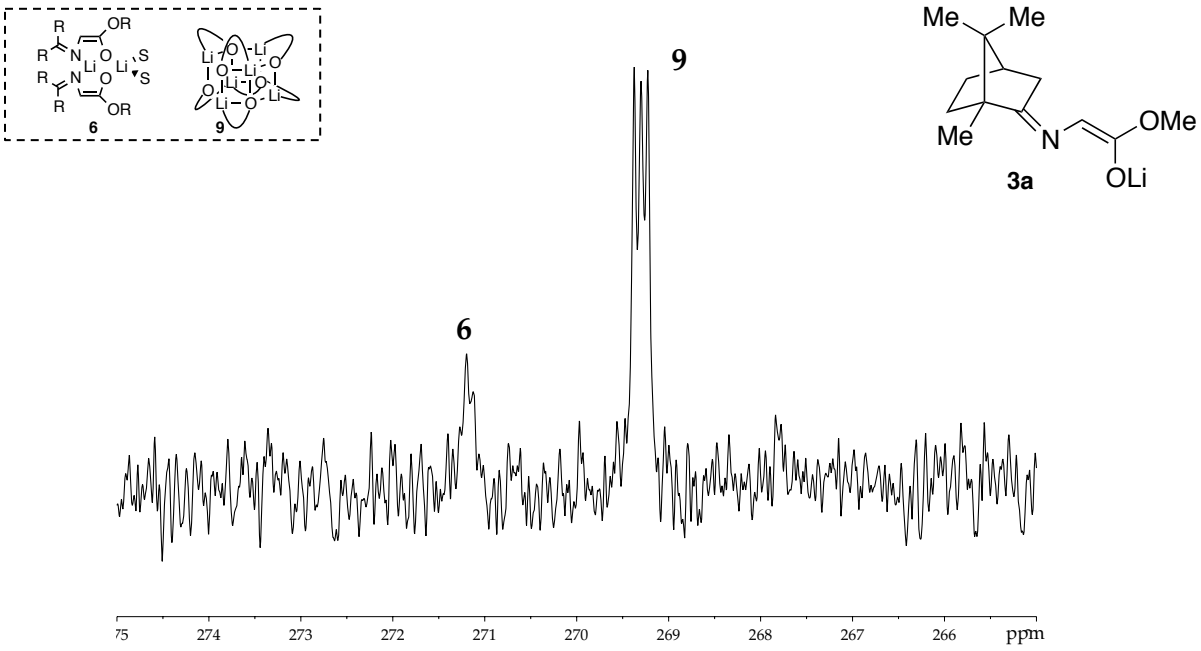


Figure 62. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3a** in 0.55 M TMEDA in toluene at -45 °C showing the hexamer **9** with J = 3.8 Hz and unsymmetric dimer **6**.

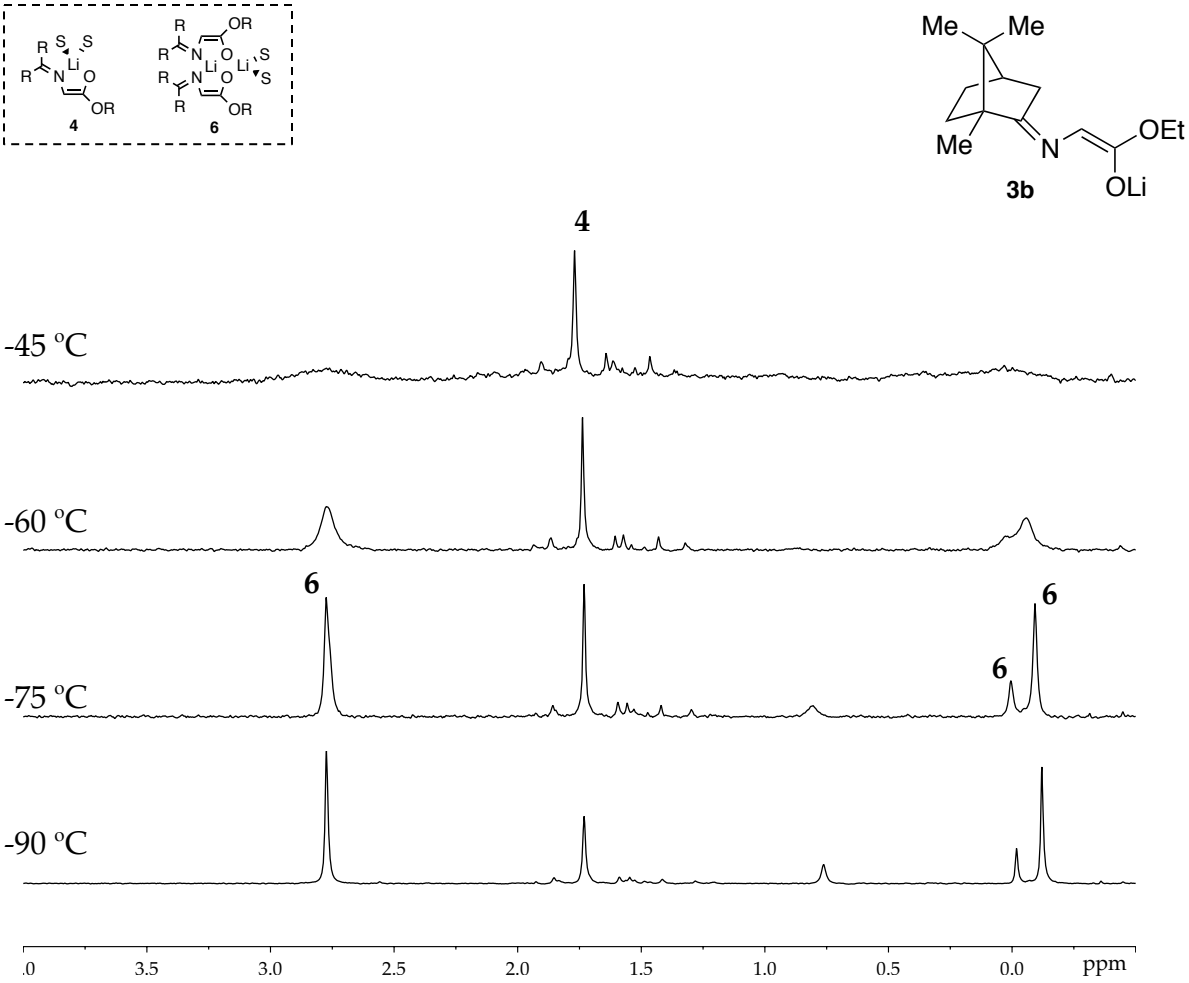


Figure 63. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3b** at various temperatures with 0.55 M TMEDA in toluene showing the monomer **4** and unsymmetric dimer **6**. The two upfield resonances of **6** are assigned to diastereomers not resolved in the downfield resonance.

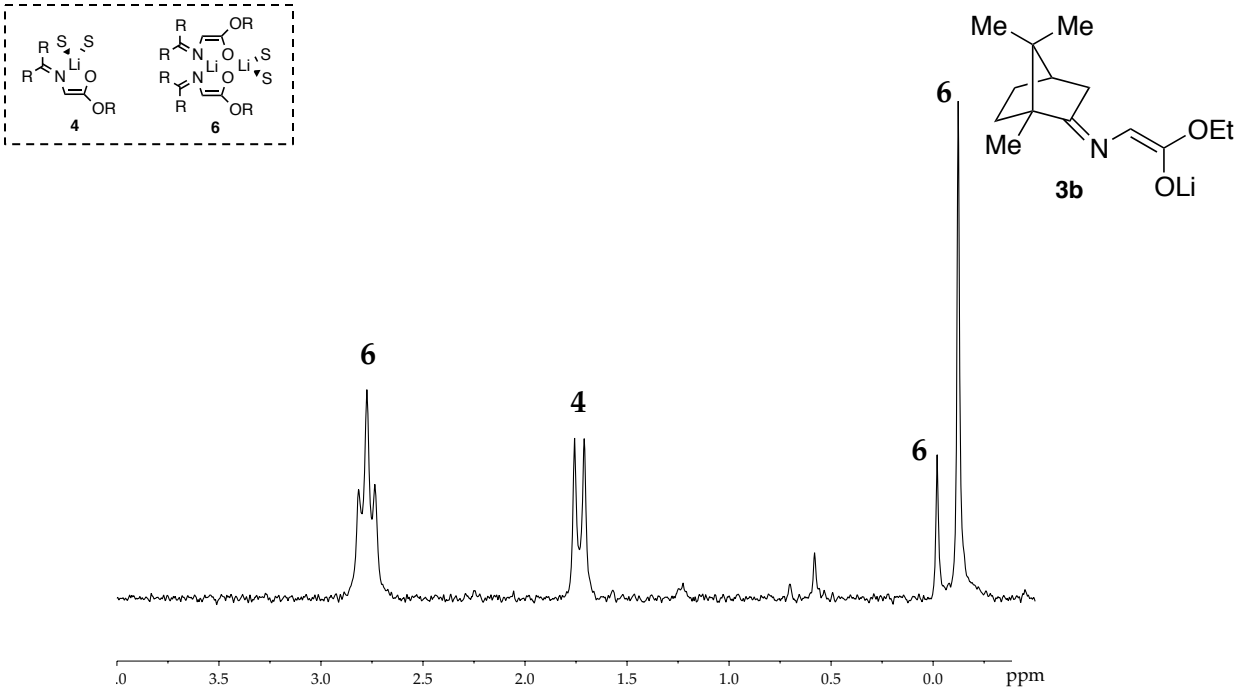


Figure 64. ^{6}Li NMR spectrum of [^{6}Li,^{15}N]**3b** at -95 °C. The enolate concentration is 0.10 M with 0.55 M TMEDA in toluene showing the monomer **4** with J = 4.1 Hz and the unsymmetric dimer **6** with J = 3.6 Hz.

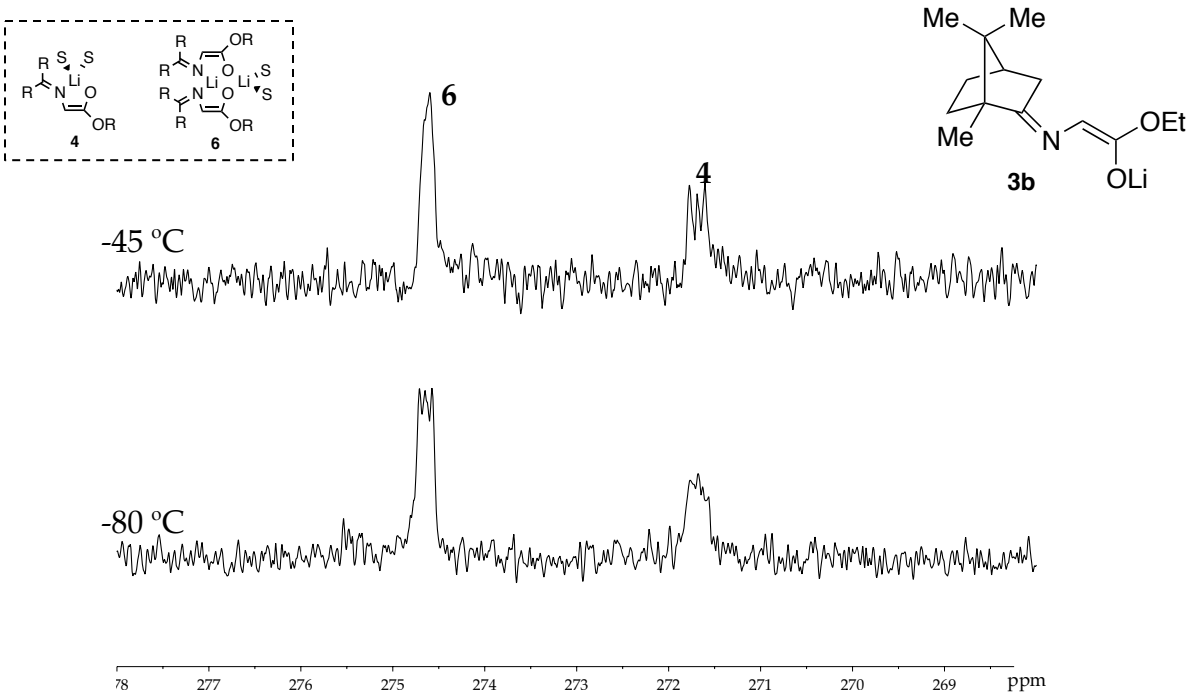


Figure 65. ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]**3b** with 0.55 M TMEDA in toluene at various temperatures with monomer **4** with J = 4.3 Hz and dimer **6** with J = 3.5 Hz.

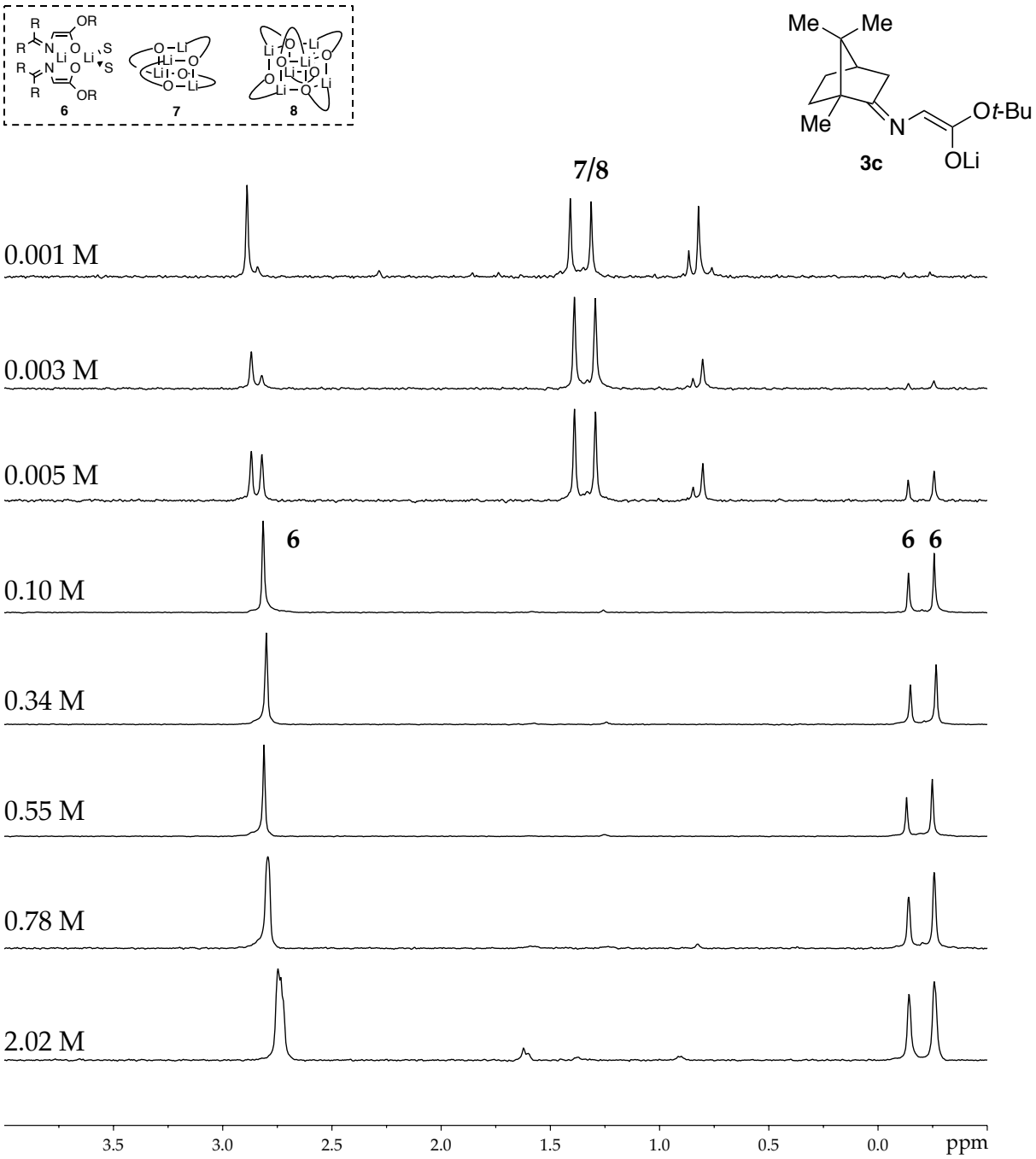


Figure 66. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3c** at -75 °C with various TMEDA concentrations in toluene. The doubling of the ^{6}Li resonances for the may be indicative of S_6-hexamer **8** or S_4-tetramer **7**. The upfield resonance of **6** resolved into two peaks corresponding to diastereomers, whereas the downfield resonance remained unresolved.

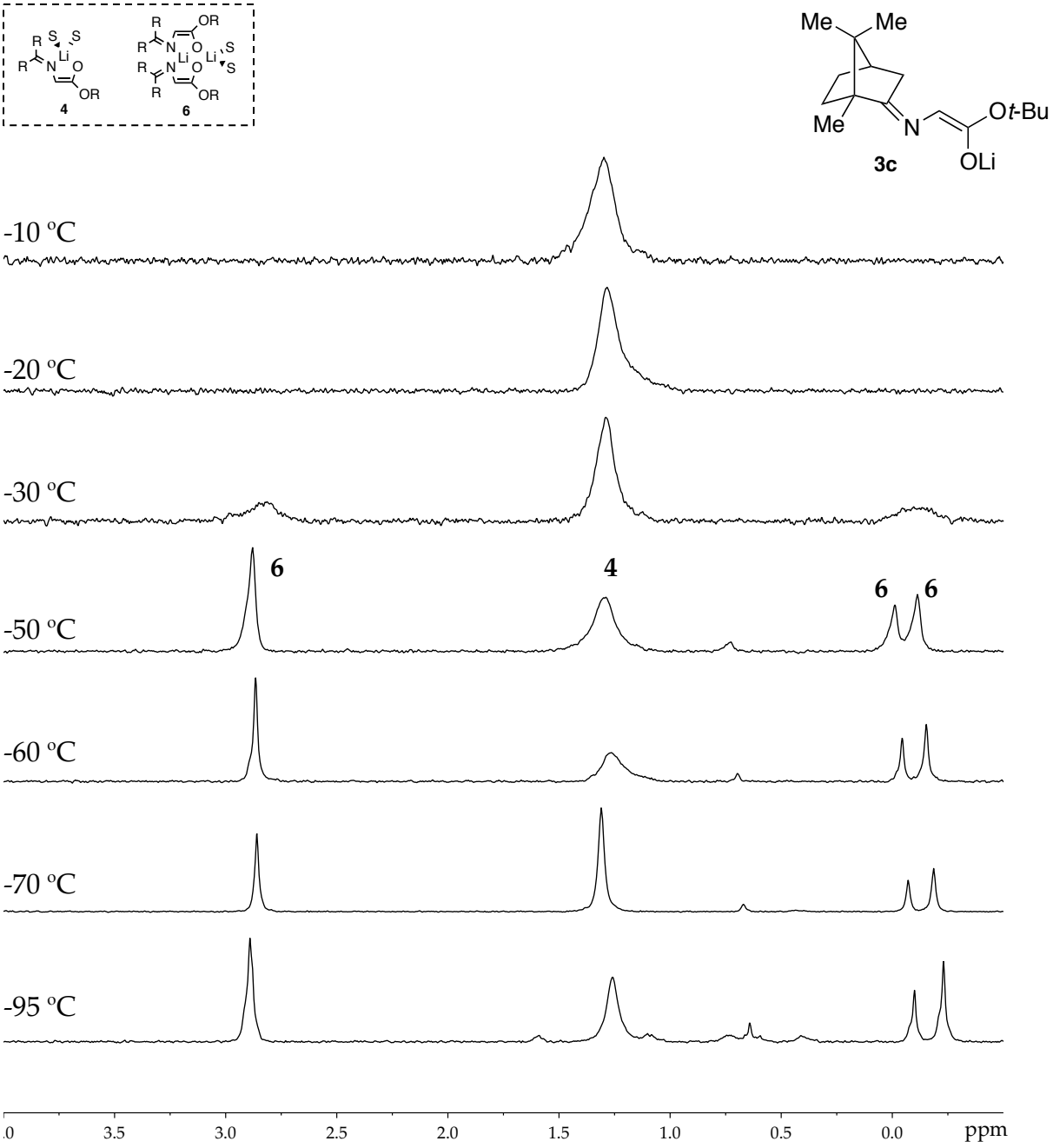


Figure 67. ^{6}Li NMR spectra of [^{6}Li]**3c** at various temperatures. The enolate concentration is 0.10 M in 0.55 M TMEDA in toluene showing the unsymmetric dimer **6** and monomer **4**.

V. NMR Spectroscopic Studies with *trans-N,N,N′,N′*-tetramethylcyclohexanediamine (TMCDA) in Toluene

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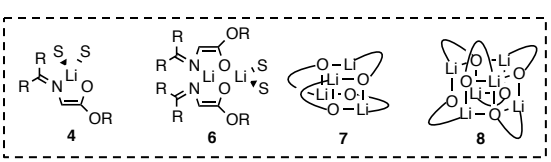
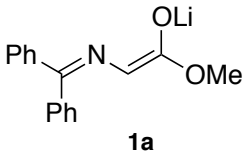




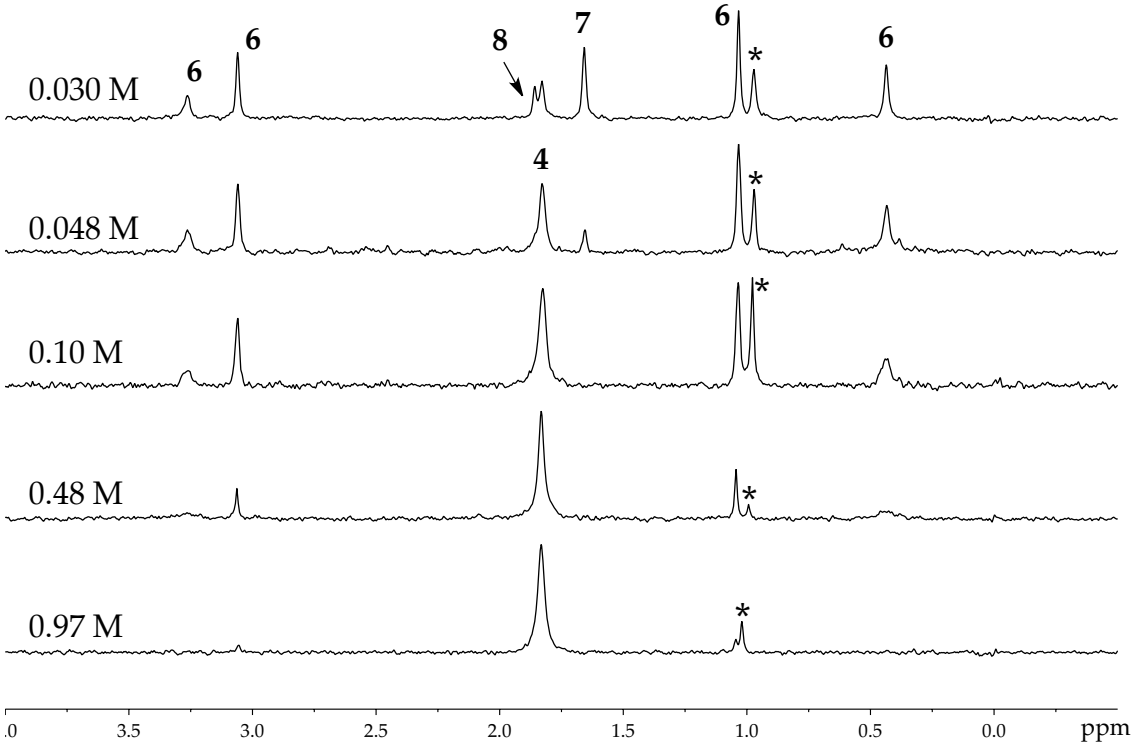


Figure 68. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**1a** with various (*R,R*)-TMCDA concentrations in toluene at -70 °C showing monomer **4**, two disastereomers of unsymmetric dimer **6**, tetramer **7**, and hexamer **8**.

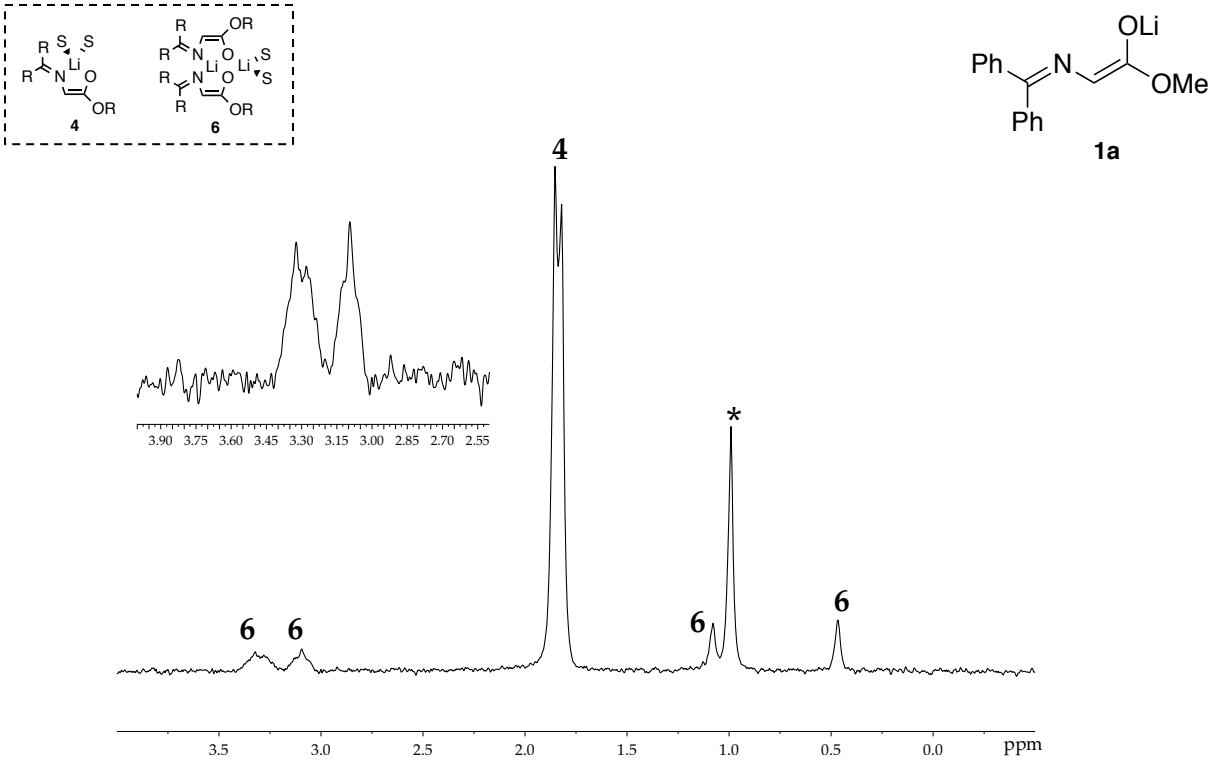


Figure 69. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]**1a** with 0.48 M (*R,R*)-TMCDA in toluene at -95 °C. The coupling constant of monomer **4** is 2.7 Hz. The unsymmetric dimers **6** did not show measurable coupling constants. LiHMDS is flagged with an asterisk.

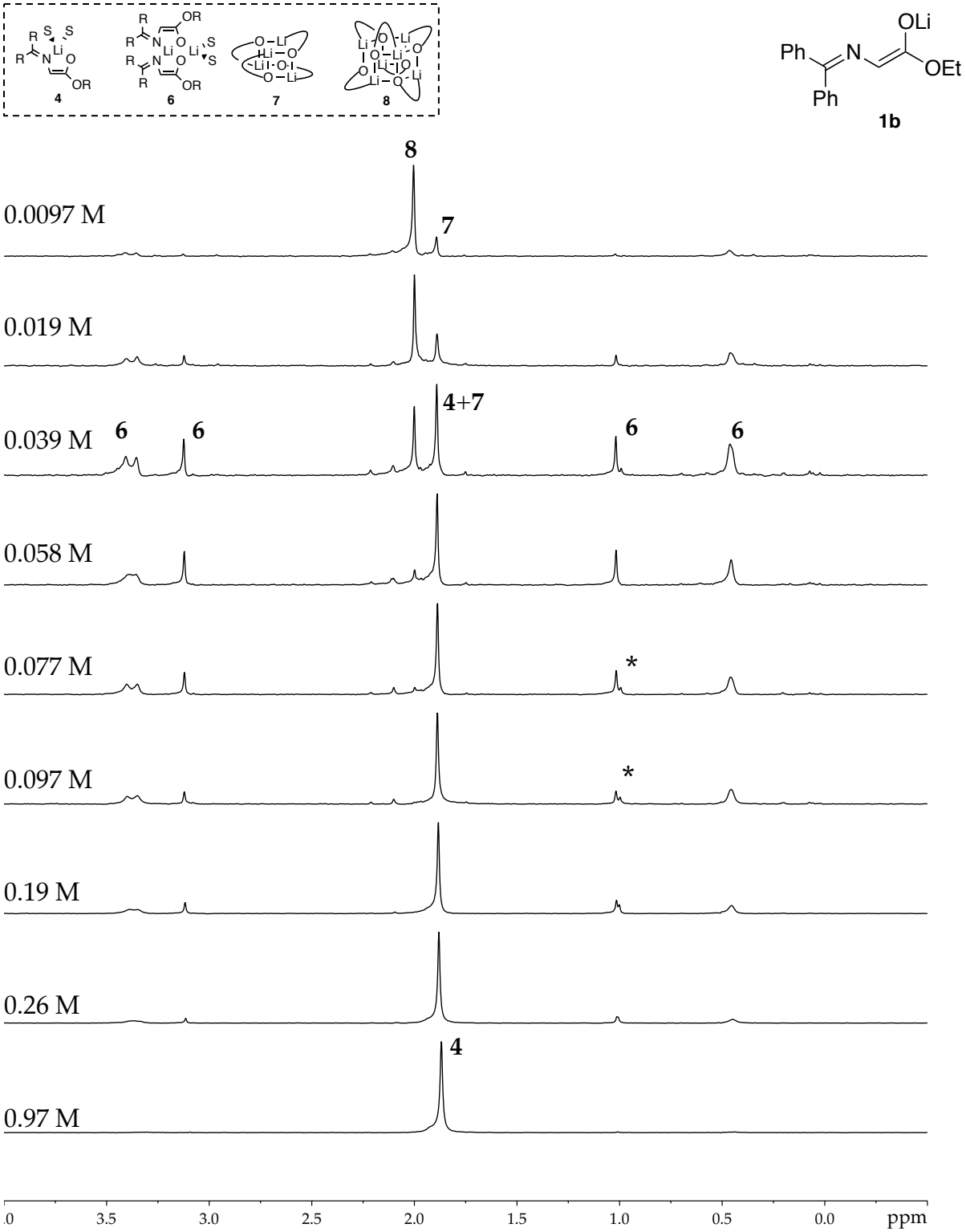


Figure 70. ^{6}Li NMR spectra of [^{6}Li]**1b** with various (*R,R*)-TMCDA concentrations in toluene. All samples are 0.10 M enolate at -75 °C showing monomer **4**, unsymmetric dimer **6**, tetramer **7**, and hexamer **8**.

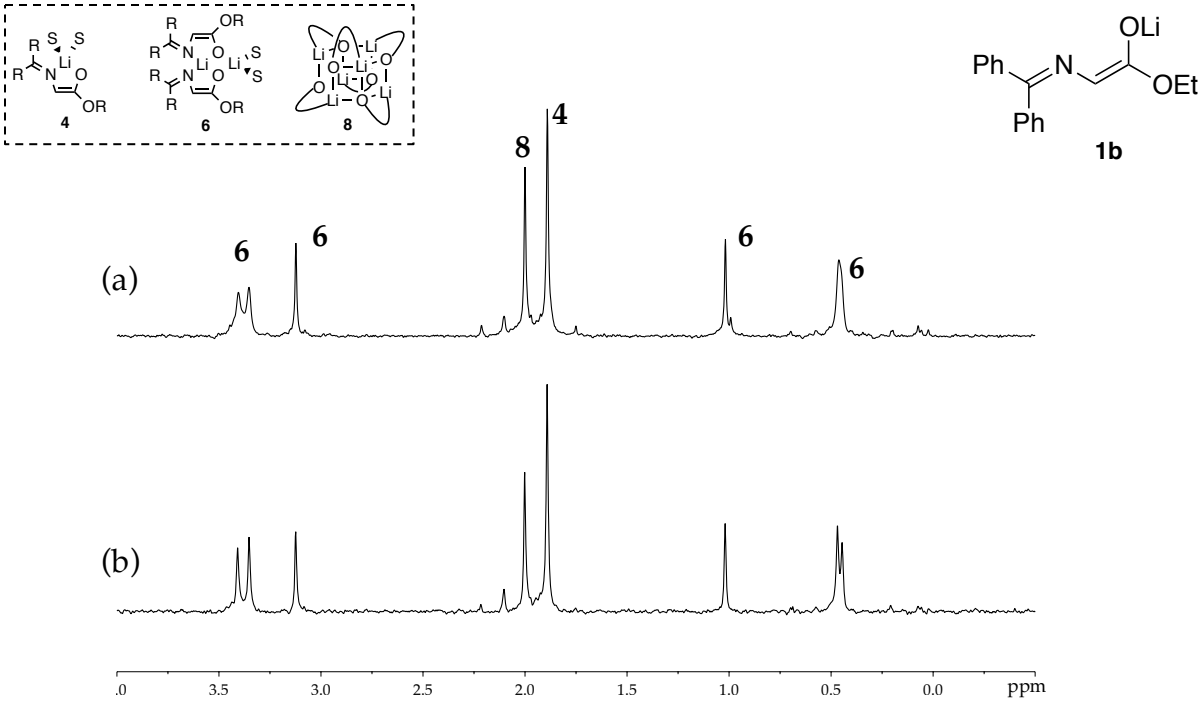


Figure 71. ^{6}Li NMR spectra of 0.10 M[^{6}Li]**1b** with (a) 0.040 M (*R,R*)-TMCDA in toluene and (b) 0.040 M (*S,S*)-TMCDA in toluene at -75 °C showing monomer **4**, unsymmetric dimer **6**, and hexamer **8**.

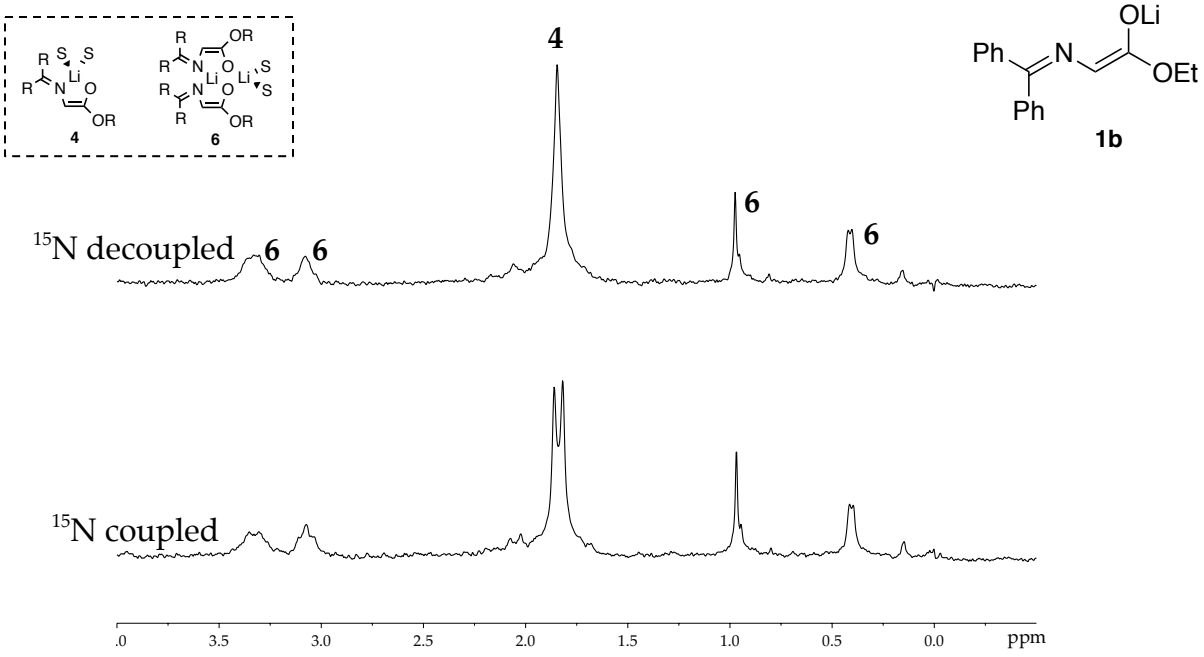


Figure 72. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**1b** with 0.077 M (*R,R*)-TMCDA in toluene at -75 °C. Only the monomer **4** presents measurable coupling constant of 2.8 Hz.

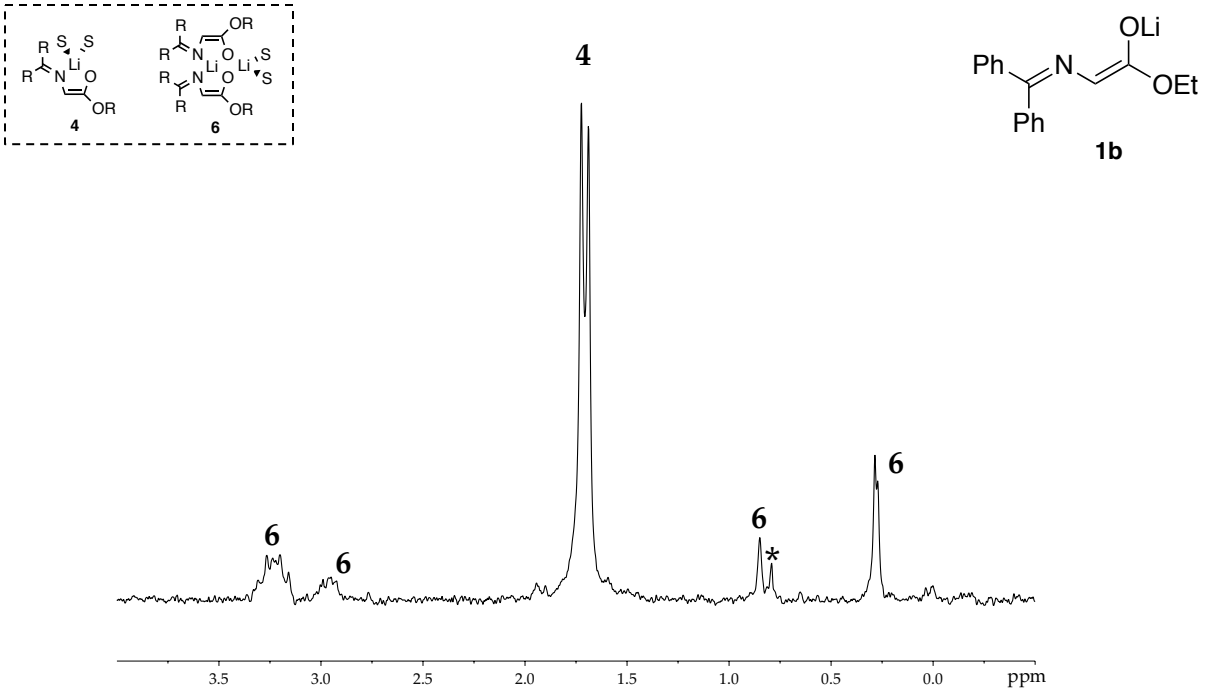


Figure 73. ^{6}Li NMR spectrum of 0.10 M [^{6}Li,^{15}N]**1b** with 0.077 M (*R,R*)-TMCDA in toluene at -95 °C. It is apparent the most downfield peak of **6** is an overlap of multiple resonances.

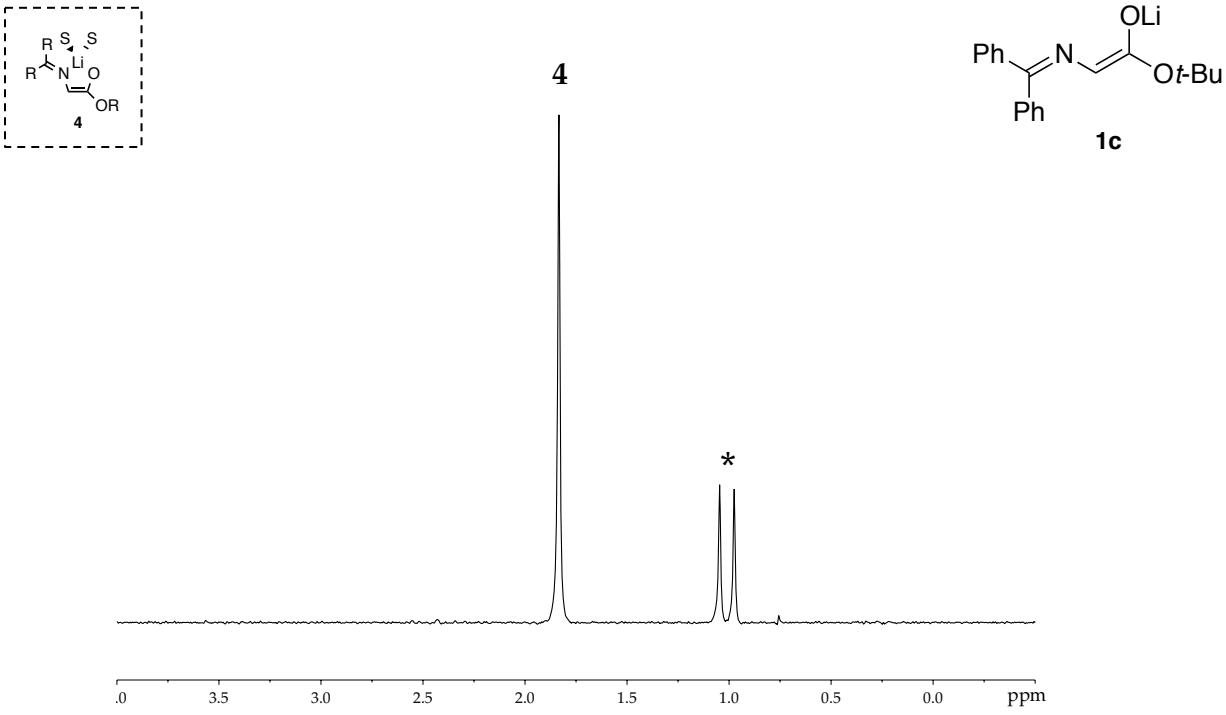


Figure 74. ^{6}Li NMR spectrum of 0.10 M [^{6}Li]**1c** with 0.48 M (*R,R*)-TMCDA in toluene at -75 °C. The resonance is assigned as monomer **4** is based on the studies of analogous enolates. [^{6}Li,^{15}N]LiHMDS was used to generate the enolate **1c**.

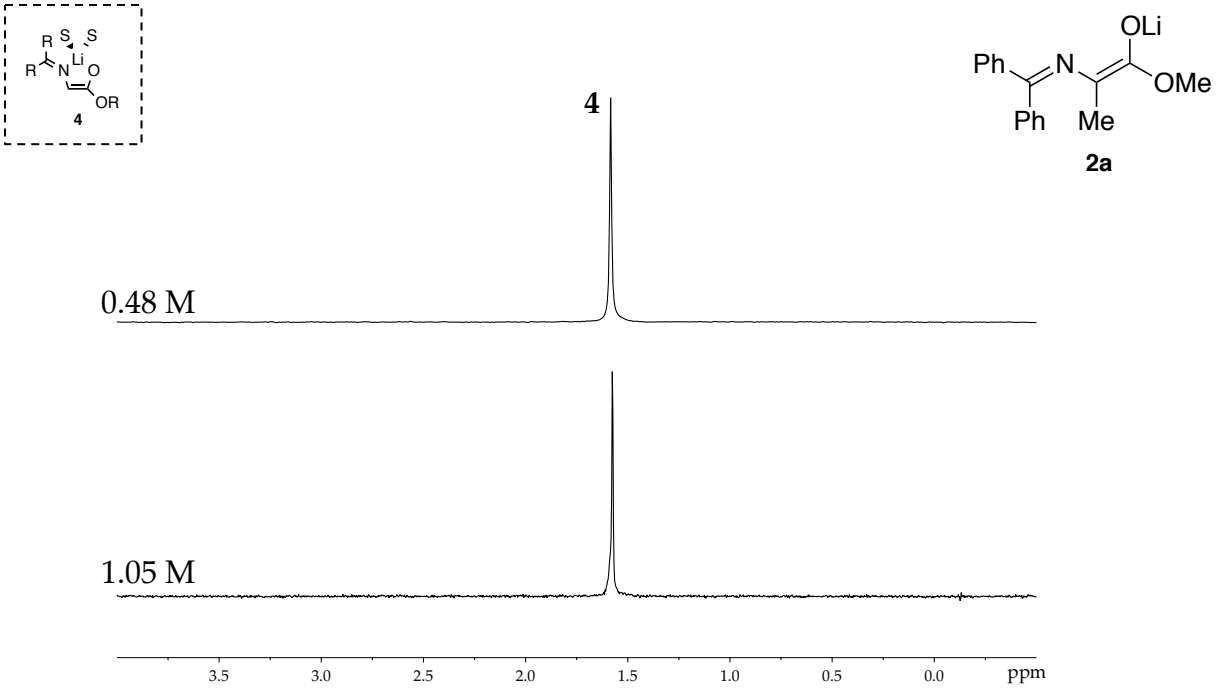


Figure 75. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**2a** with various (*R,R*)-TMCDA concentrations in toluene at -70 °C showing the putative monomer **4**.

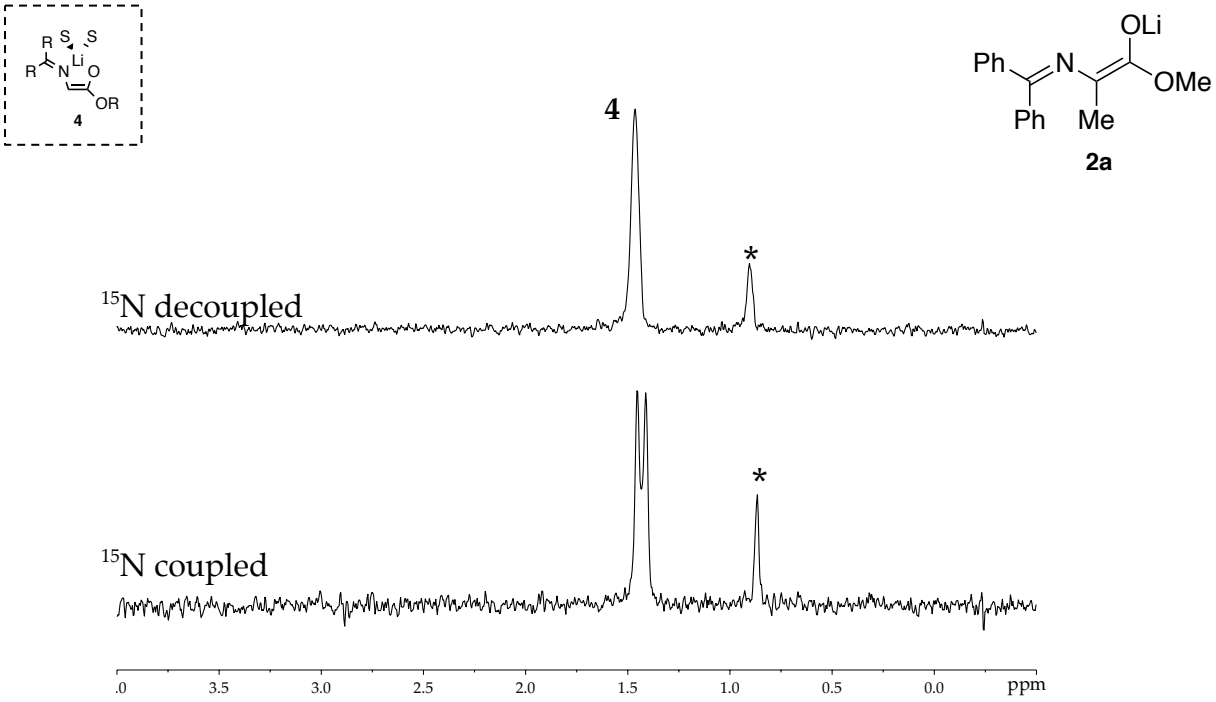


Figure 76. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**2a** with 0.70 M (*R,R*)-TMCDA in toluene at -75 °C showing the monomer **4** with J = 3.0 Hz. Asterisks (*) denote LiHMDS.

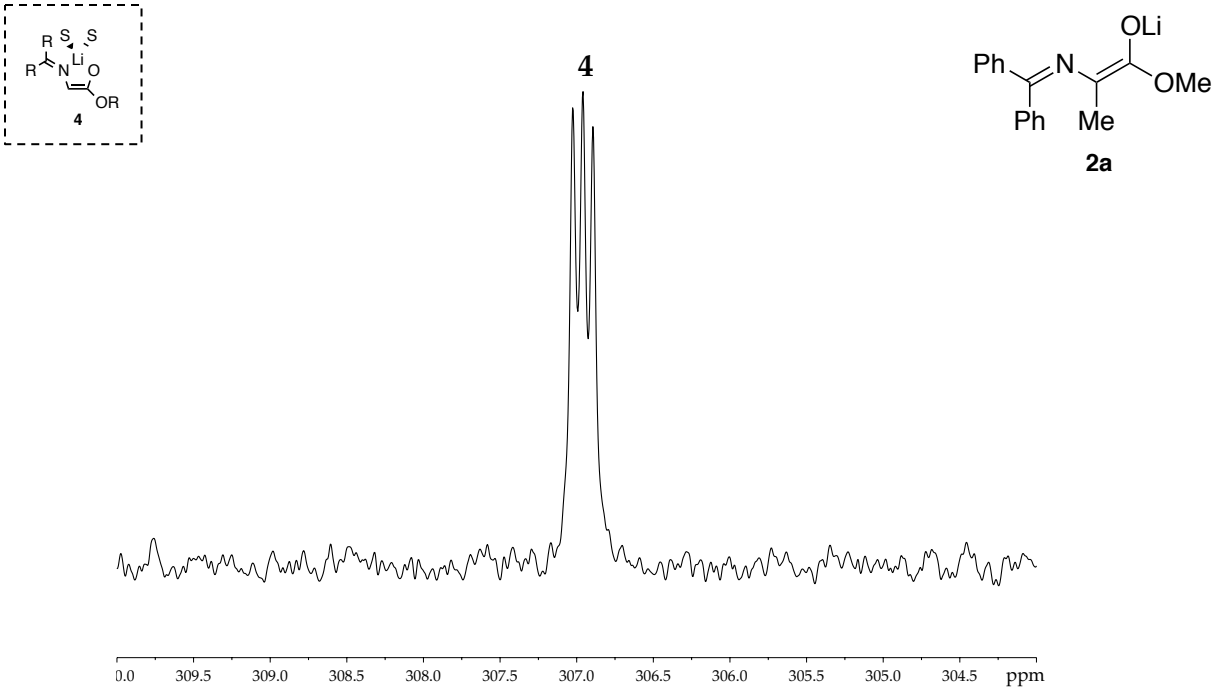


Figure 77. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**2a** with 0.70 M (*R,R*)-TMCDA in toluene at -50 °C showing the monomer **4** with J = 3.3 Hz.

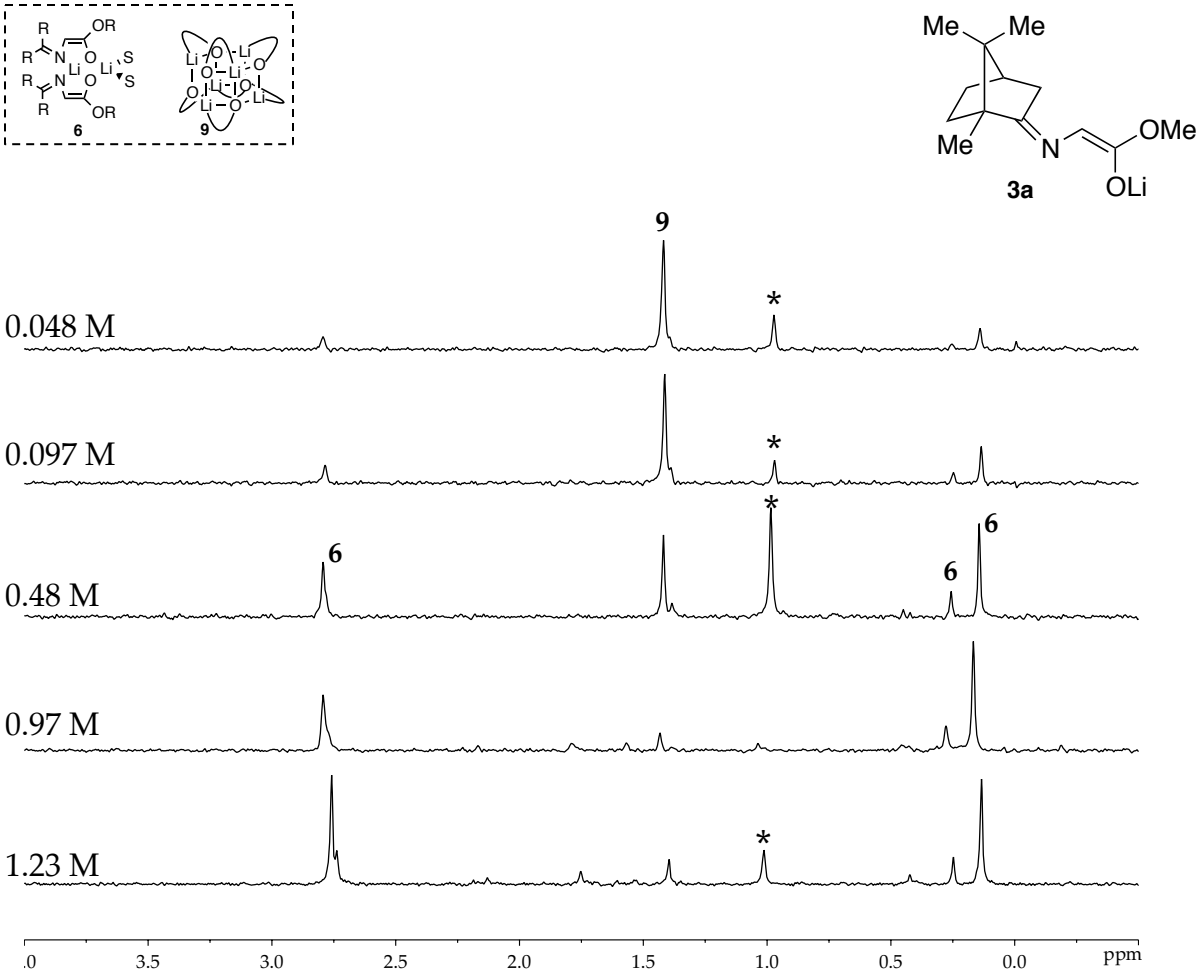


Figure 78. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3a** with various (*R,R*)-TMCDA concentrations in toluene at -70 °C showing the unsymmetric dimer **6** and hexamer **9**. Asterisk corresponds to LiHMDS.

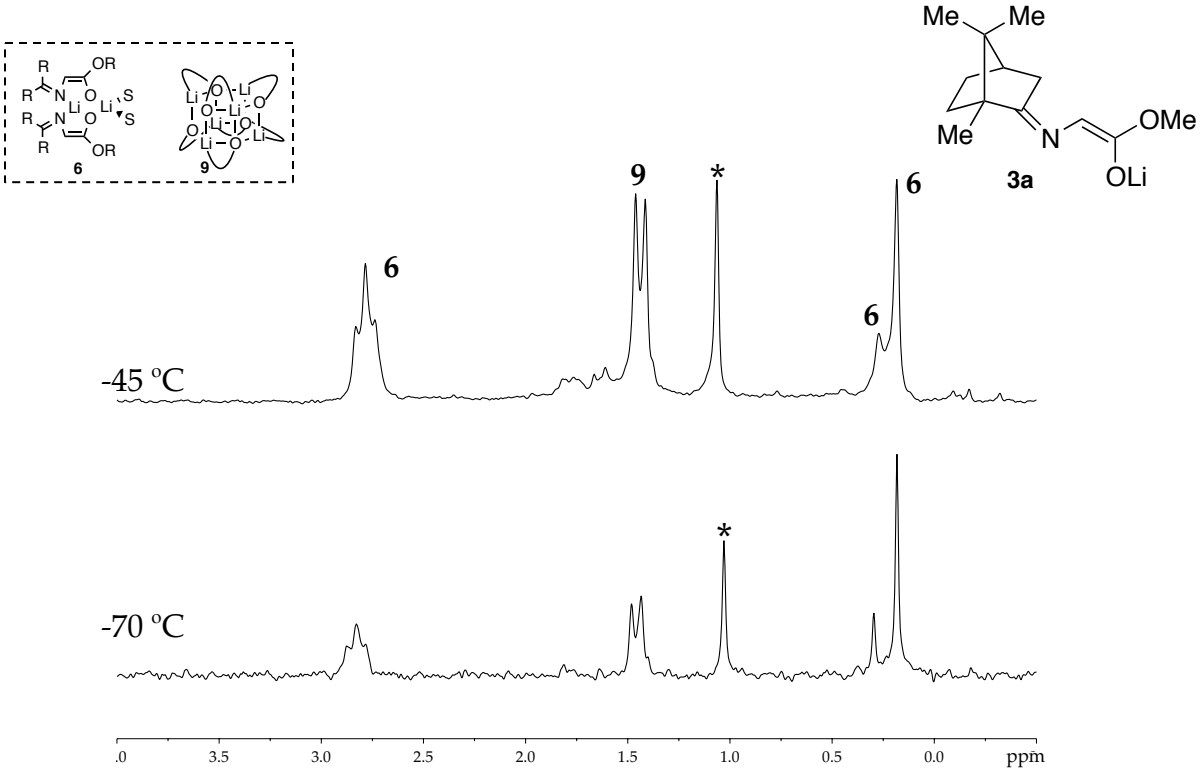


Figure 79. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**3a** with 0.48 M (*R,R*)-TMCDA in toluene at various temperatures with the unsymmetric dimer **6** with J = 3.2 Hz and hexamer **9** with J = 3.6 Hz.

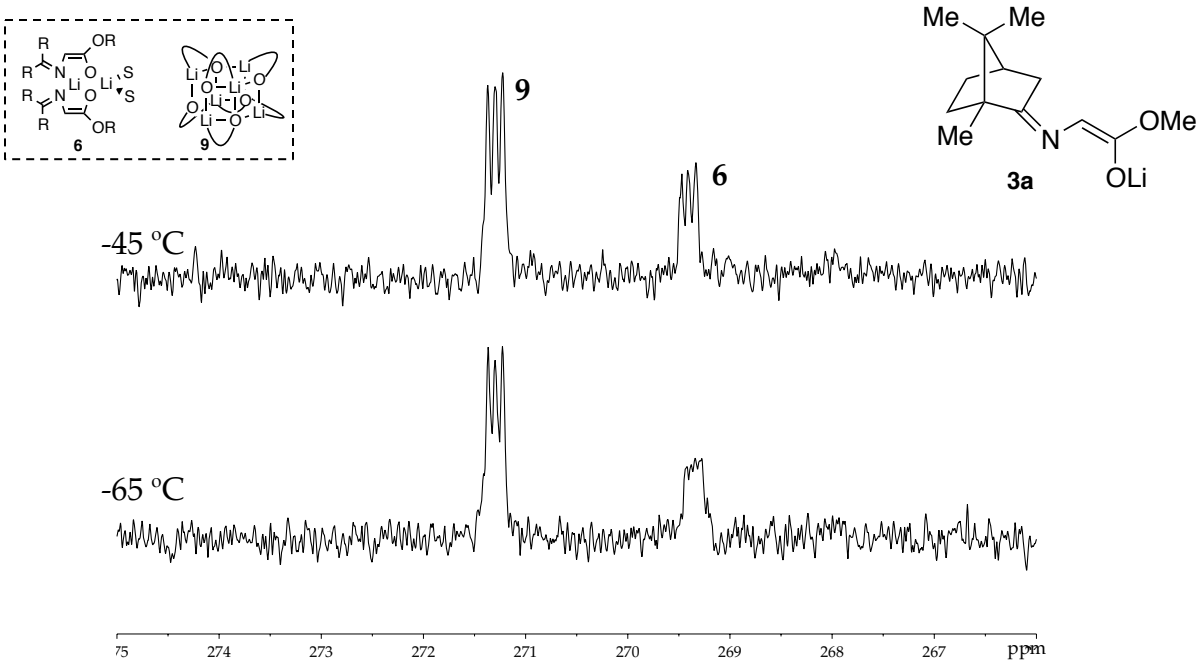


Figure 80. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3a** in 0.48 M (*R,R*)-TMCDA in toluene at various temperatures showing the unsymmetric dimer **6** wth J = 3.4 Hz and hexamer **9** with J = 3.7 Hz.

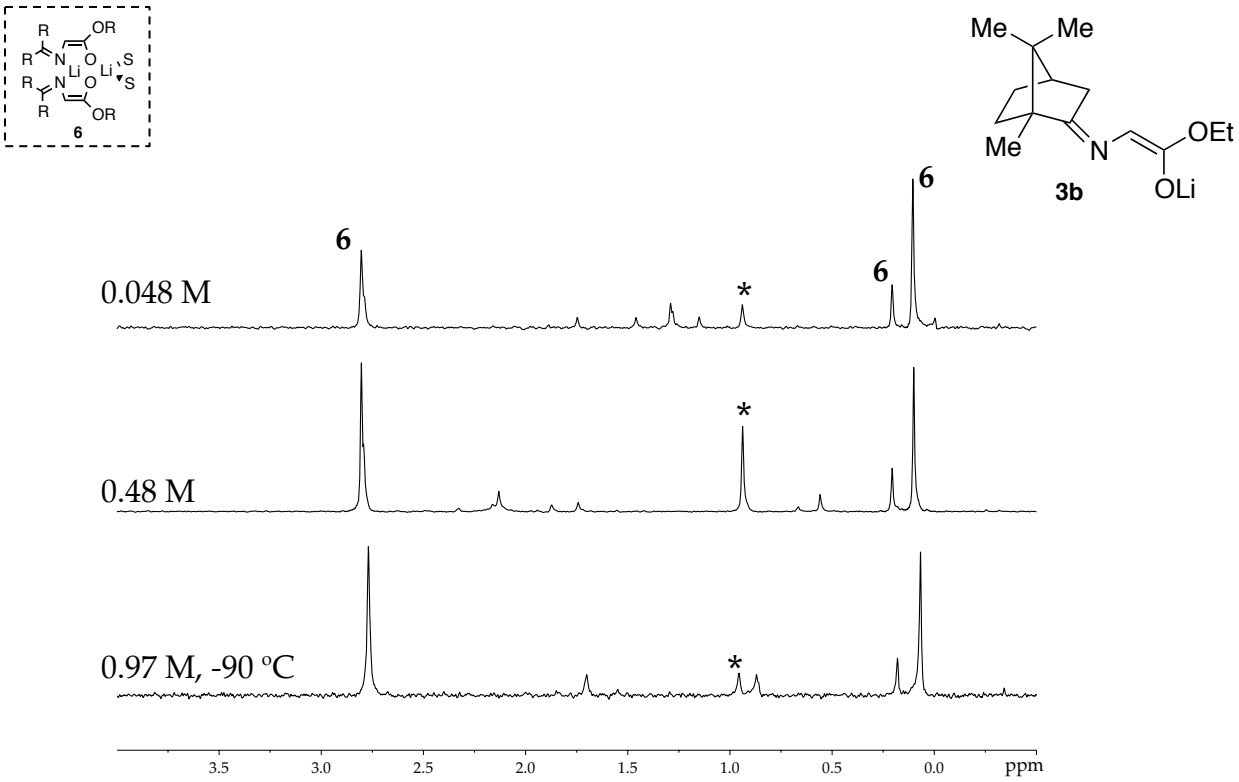


Figure 81. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3b** with various (*R,R*)-TMCDA concentrations in toluene at -75 °C unless otherwise noted. The unsymmetric dimers **6** are the major species throughout the series. Asterisks (*) denote LiHMDS.

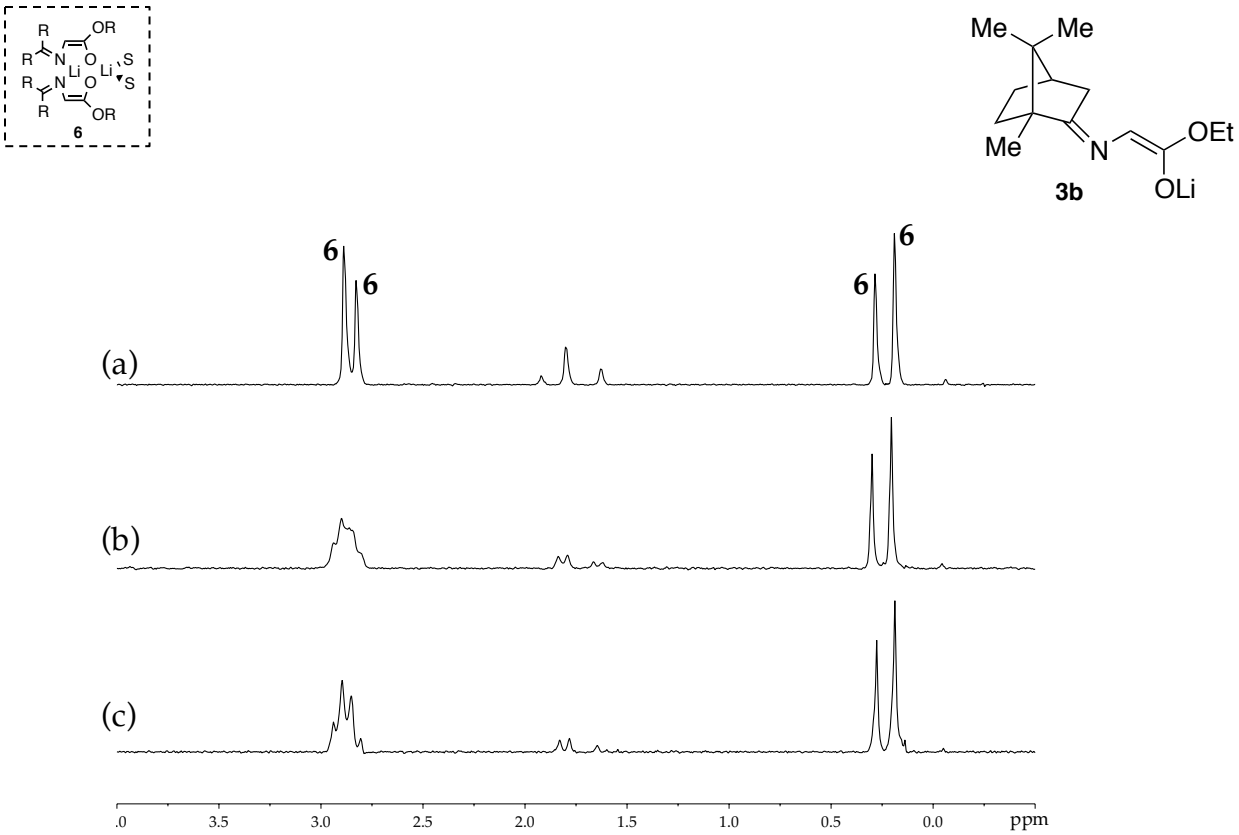


Figure 82. ^{6}Li NMR spectra of (a) [^{6}Li]**3b** at -75 °C; (b) [^{6}Li,^{15}N]**3b** at -75 °C; and (c) [^{6}Li,^{15}N]**2b** at -95 °C. Samples are 0.10 M enolate in 0.48 M (*S,S*)-TMCDA/toluene. The unsymmetric dimers **6** appear as two pairs, signifying two diastereomers. (*S,S*)-TMCDA promotes better resolution than (*R,R*)-TMCDA (see above Figure 81).

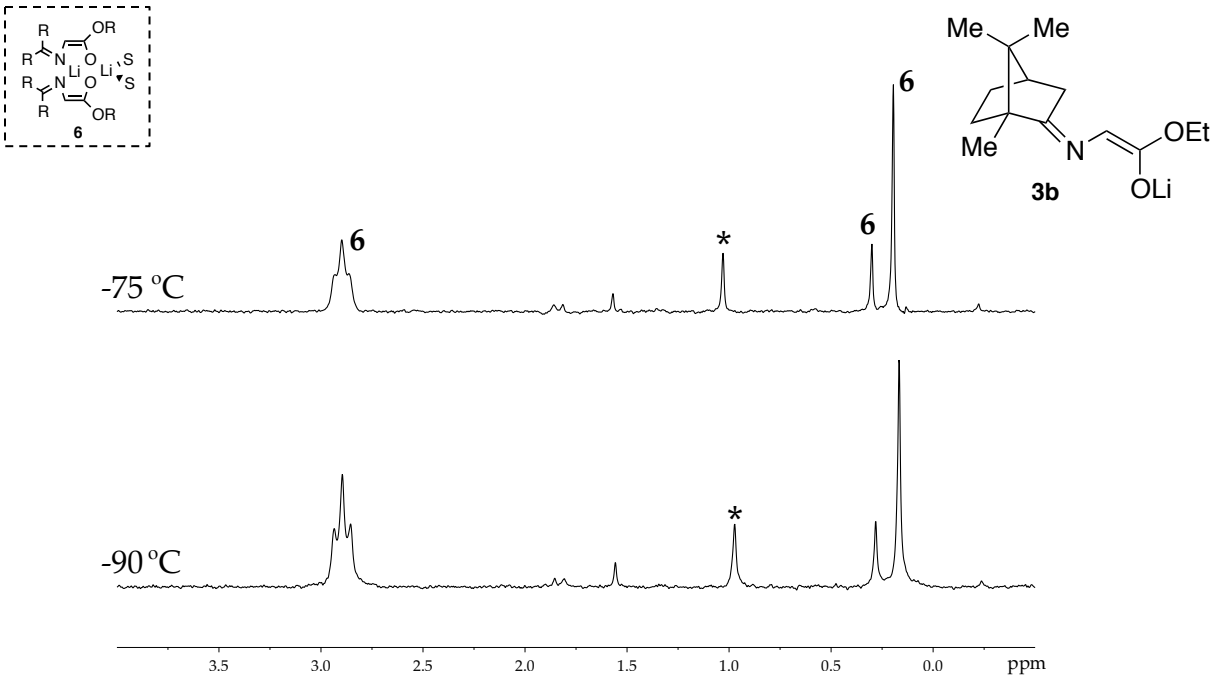


Figure 83. ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]**3b** in 0.48 M (*R,R*)-TMCDA in toluene at various temperatures. J = 3.5 Hz for the unsymmetric dimer **6**. Integrations suggest overlap of two resonances in the downfield peaks. Asterisks (*) denote LiHMDS.

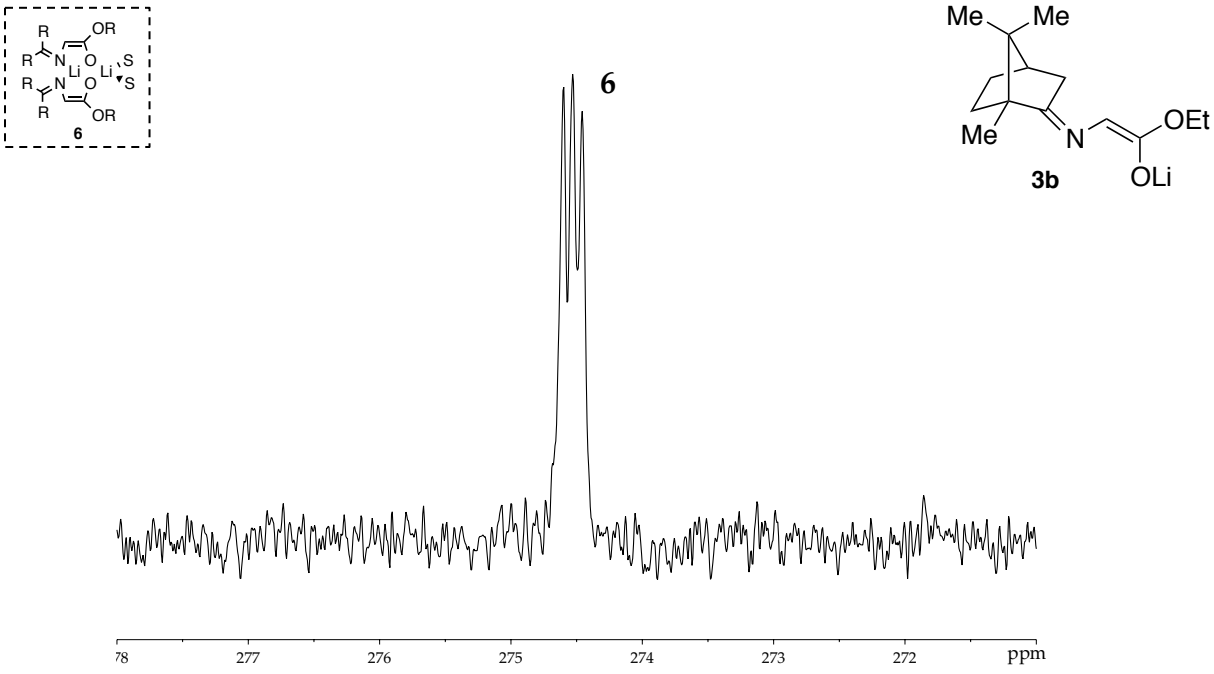


Figure 84. ^{15}N NMR spectrum of 0.10 M [^{6}Li,^{15}N]**3b** in 0.48 M (*R,R*)-TMCDA in toluene at -65 °C showing the unsymmetric dimer **6** with J = 3.6 Hz.

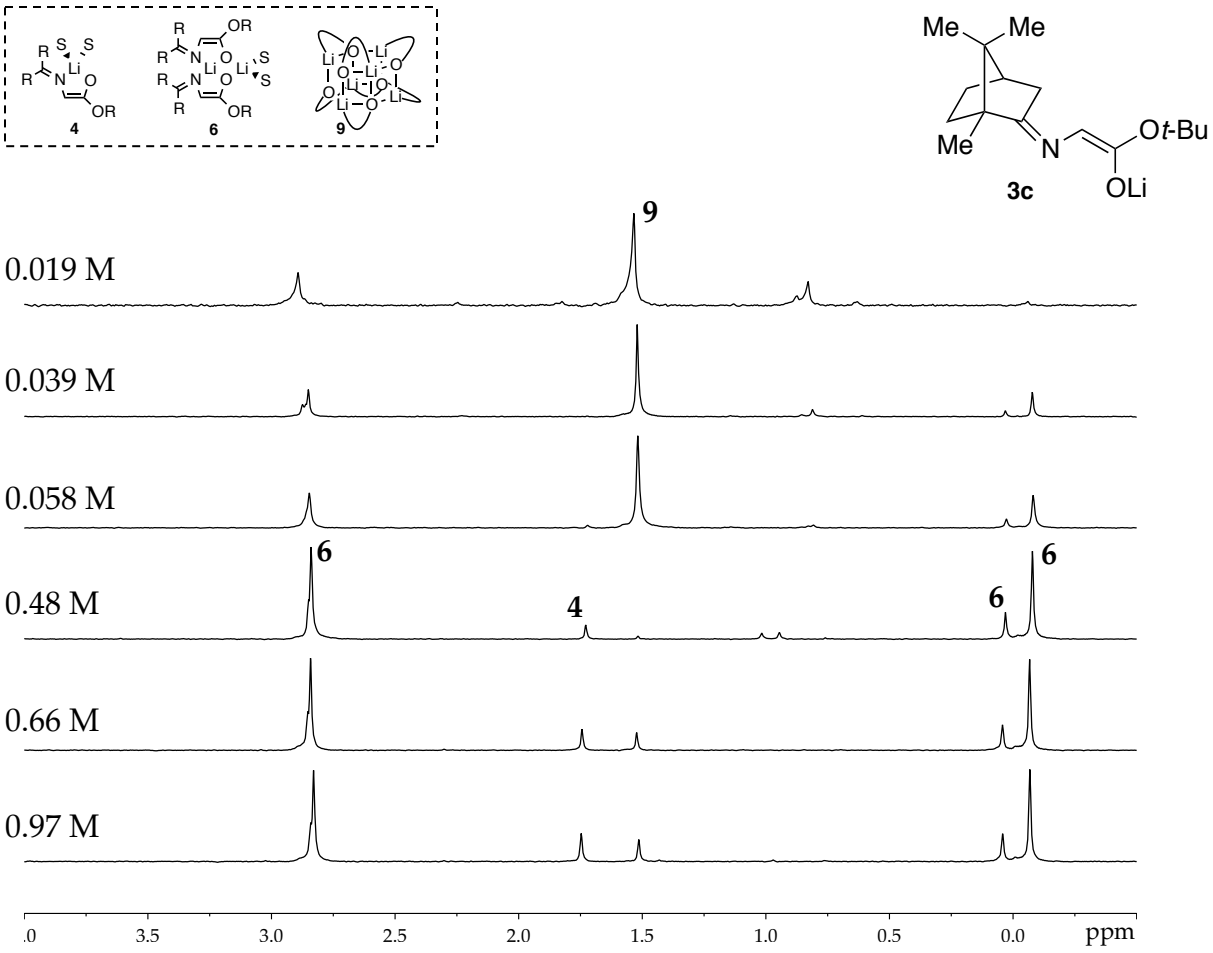


Figure 85. [6]Li NMR spectra of [6Li]**3c** with various (*R,R*)-TMCDA concentrations in toluene. Samples are 0.10 M enolate at -75 °C showing the putative hexamer **9** at low TMCDA, monomer **4** and unsymmetric dimer **6** with excess TMCDA.

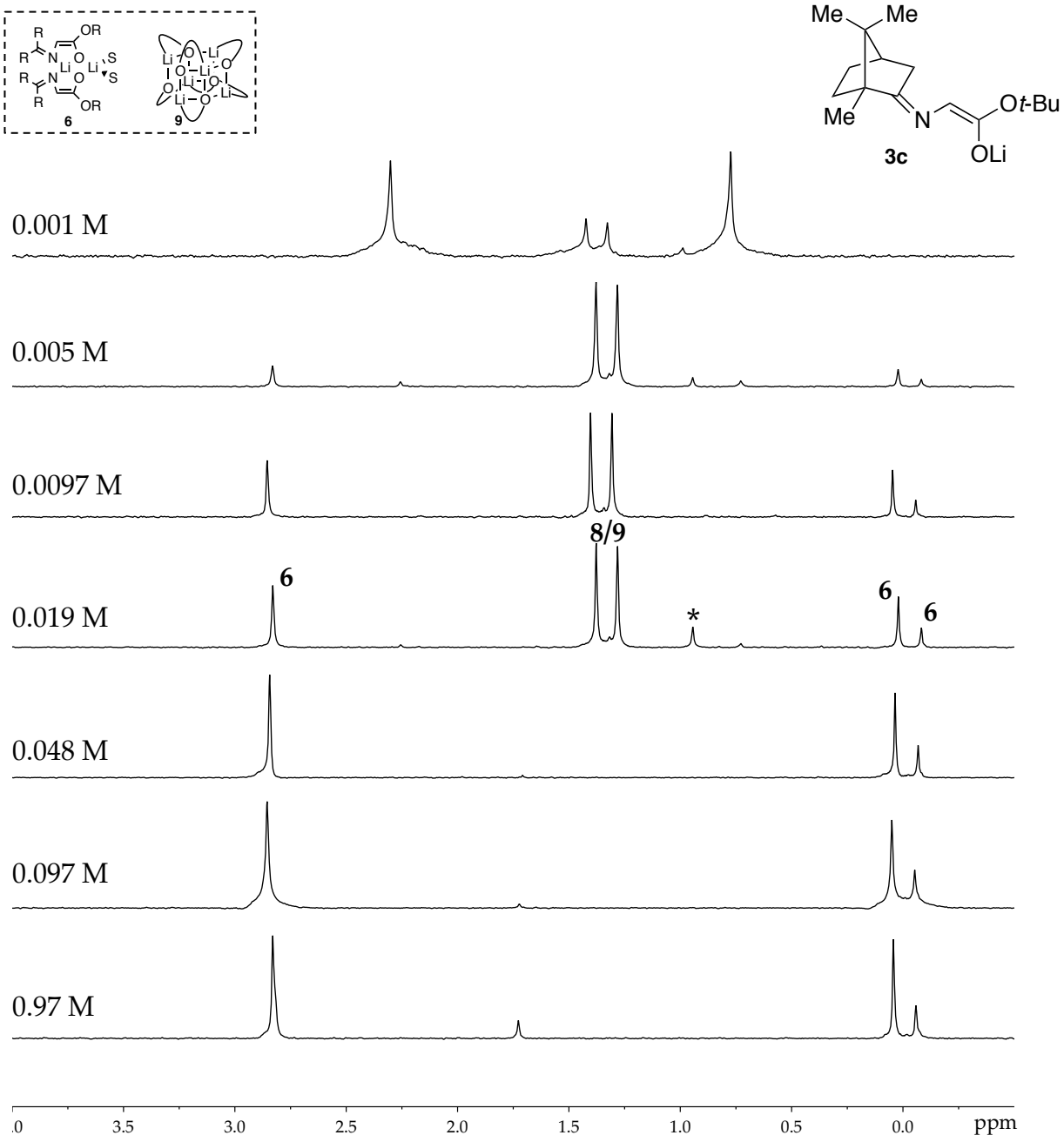
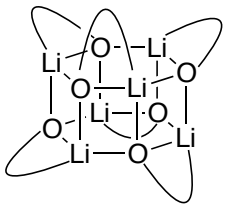
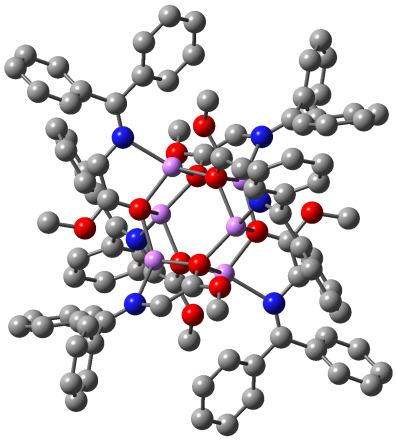


Figure 86. ^{6}Li NMR spectra of 0.10 M [^{6}Li]**3c** with various concentrations of (*S,S*)-TMCDA in toluene at -75 °C showing the unsymmetric dimer **6** and hexamer **8** or **9**.

VI. Computational Studies

Table 17. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated S_6 hexamer **8** for **1a** with free energies and coordinates.





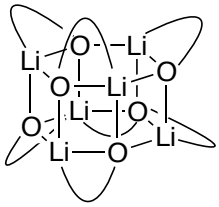
G = -4984.317843
G_{MP2} = -4968.631287

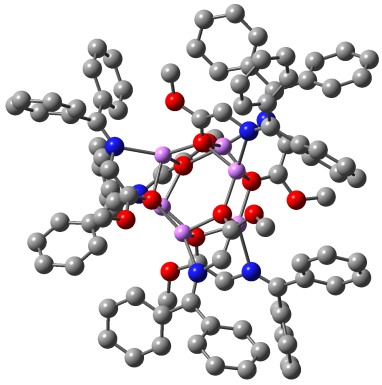
Atom	X	Y	Z	Atom	X	Y	Z
N	2.02900	-2.99300	-2.13900	C	-0.73000	2.69300	-2.02500
C	2.84100	-1.97800	-2.59900	O	-2.03800	2.84400	-2.37200
H	3.57500	-2.16500	-3.37300	C	-2.40900	3.81800	-3.34500
C	2.72200	-0.72800	-2.02000	H	-3.49600	3.76900	-3.40800
O	1.86900	-0.41300	-1.09600	H	-2.10000	4.82200	-3.03000
Li	0.61100	-1.93600	-0.90800	H	-1.96500	3.58900	-4.32100
Li	1.38300	1.49600	-0.91100	N	-3.60800	-0.27200	-2.15300
Li	-1.99800	0.44200	-0.91200	C	-3.12200	-1.47800	-2.61100
Li	-1.38300	-1.49600	0.91000	C	-4.68500	0.28800	-2.63400
Li	1.99800	-0.44200	0.91200	H	-3.64000	-2.02500	-3.38900
Li	-0.61100	1.93600	0.90800	C	-1.97700	-1.98800	-2.02700
O	-1.28800	-1.40300	-1.09900	O	-1.44700	-3.19000	-2.38600
O	1.28800	1.40400	1.09900	C	-2.09600	-3.98800	-3.37300
O	-0.56700	1.80100	-1.10000	H	-1.50100	-4.89800	-3.45100
O	-1.86900	0.41300	1.09600	H	-3.11800	-4.23900	-3.06300
O	0.56700	-1.80100	1.10000	H	-2.12400	-3.47300	-4.34100
O	3.51100	0.32200	-2.37500	N	-1.57300	-3.23600	2.15900
C	4.52900	0.14600	-3.35800	C	-0.28500	-3.42300	2.61400
H	5.02900	1.11200	-3.43700	C	-2.59800	-3.88200	2.64700
H	5.24800	-0.61900	-3.04500	H	-0.07200	-4.14500	3.39300
H	4.09800	-0.13300	-4.32700	C	0.73000	-2.69200	2.02500
C	2.07300	-4.20700	-2.61700	O	2.03800	-2.84400	2.37200
N	1.57300	3.23700	-2.15900	C	2.40800	-3.81800	3.34500
C	0.28500	3.42400	-2.61400	H	3.49500	-3.76900	3.40900
C	2.59800	3.88200	-2.64700	H	1.96400	-3.58900	4.32200
H	0.07100	4.14600	-3.39200	H	2.10000	-4.82200	3.03100

N	3.60800	0.27200	2.15200	C	0.28900	7.28900	0.75400
C	4.68500	-0.28800	2.63400	H	0.23800	8.26000	2.68000
C	1.97700	1.98800	2.02700	H	0.13400	6.08200	-1.03200
O	1.44700	3.19000	2.38600	H	0.88800	8.06400	0.28400
C	2.09700	3.98800	3.37300	C	-2.92900	4.59600	3.78500
H	1.50200	4.89800	3.45100	C	-2.73600	4.01200	5.04900
H	2.12500	3.47400	4.34100	C	-3.93400	5.56600	3.64400
H	3.11800	4.23800	3.06300	C	-3.52800	4.38300	6.13500
N	-2.02800	2.99300	2.13900	H	-1.95700	3.26500	5.17400
C	-2.84000	1.97800	2.59900	C	-4.73400	5.93000	4.72800
C	-2.07200	4.20800	2.61700	H	-4.08500	6.03500	2.67500
H	-3.57500	2.16600	3.37300	C	-4.53300	5.34100	5.97700
C	-2.72100	0.72800	2.01900	H	-3.35900	3.92600	7.10700
O	-3.51200	-0.32200	2.37500	H	-5.51200	6.67800	4.59700
C	-4.52900	-0.14600	3.35800	H	-5.15200	5.62800	6.82300
H	-5.02900	-1.11200	3.43700	C	5.44000	0.26000	3.80800
H	-4.09800	0.13300	4.32700	C	4.82900	0.38400	5.06600
H	-5.24800	0.62000	3.04500	C	6.78400	0.64700	3.67700
C	2.49700	4.80500	-3.82500	C	5.53800	0.88300	6.15900
C	2.82700	6.16400	-3.70000	H	3.79100	0.08200	5.18400
C	2.08600	4.32900	-5.08100	C	7.49100	1.15500	4.76700
C	2.73500	7.02500	-4.79400	H	7.27400	0.54400	2.71200
H	3.16000	6.54300	-2.73800	C	6.87100	1.27400	6.01200
C	2.00300	5.18800	-6.17800	H	5.05000	0.96300	7.12700
H	1.83400	3.27800	-5.19400	H	8.52800	1.45600	4.64400
C	2.32300	6.54000	-6.03700	H	7.42200	1.66500	6.86300
H	2.98800	8.07600	-4.67600	C	5.21400	-1.51100	1.98800
H	1.69100	4.80000	-7.14400	C	5.97900	-2.44500	2.71500
H	2.25600	7.20900	-6.89100	C	4.97500	-1.77200	0.62700
C	3.92500	3.73200	-2.00700	C	6.45700	-3.60700	2.11000
C	4.04200	3.39300	-0.64600	H	6.19100	-2.26200	3.76400
C	5.11100	3.93500	-2.74100	C	5.45000	-2.93400	0.02300
C	5.29100	3.23700	-0.05000	H	4.43200	-1.04000	0.04000
H	3.14300	3.27900	-0.05200	C	6.19100	-3.86000	0.76200
C	6.36100	3.78100	-2.14200	H	7.03800	-4.31600	2.69400
H	5.05000	4.21000	-3.78900	H	5.24500	-3.10800	-1.02900
C	6.45800	3.42700	-0.79500	H	6.56700	-4.76400	0.29000
H	5.34700	2.97300	1.00300	C	1.26900	-5.27200	-1.97400
H	7.26100	3.93800	-2.73100	C	0.85100	-6.40500	-2.69900
H	7.43200	3.31100	-0.32700	C	0.90600	-5.18700	-0.61700
C	-1.26800	5.27200	1.97400	C	0.07900	-7.39800	-2.09700
C	-0.85100	6.40500	2.69900	H	1.12800	-6.50300	-3.74400
C	-0.90500	5.18700	0.61700	C	0.13200	-6.17800	-0.01700
C	-0.07800	7.39800	2.09700	H	1.25800	-4.34700	-0.02900
H	-1.12800	6.50300	3.74500	C	-0.28900	-7.28800	-0.75400
C	0.13200	6.17800	0.01700	H	-0.23700	-8.25900	-2.68000
H	-1.25700	4.34700	0.02900	H	-0.13300	-6.08200	1.03200

H	-0.88800	-8.06400	-0.28400	H	-3.79200	-0.08300	-5.18400
C	2.92900	-4.59600	-3.78500	C	-6.87100	-1.27600	-6.01100
C	2.73700	-4.01200	-5.04800	H	-8.52800	-1.45800	-4.64200
C	3.93500	-5.56600	-3.64400	H	-5.05100	-0.96500	-7.12700
C	3.52900	-4.38300	-6.13500	H	-7.42300	-1.66800	-6.86200
H	1.95800	-3.26500	-5.17400	C	-3.92500	-3.73100	2.00700
C	4.73400	-5.93100	-4.72700	C	-5.11100	-3.93500	2.74000
H	4.08500	-6.03600	-2.67500	C	-4.04200	-3.39300	0.64600
C	4.53400	-5.34100	-5.97700	C	-6.36100	-3.78000	2.14100
H	3.36000	-3.92600	-7.10700	H	-5.05000	-4.21000	3.78900
H	5.51200	-6.67800	-4.59600	C	-5.29100	-3.23700	0.04900
H	5.15300	-5.62900	-6.82300	H	-3.14300	-3.27800	0.05200
C	-5.21400	1.51100	-1.98900	C	-6.45800	-3.42700	0.79400
C	-4.97500	1.77200	-0.62700	H	-7.26100	-3.93700	2.73100
C	-5.97900	2.44400	-2.71500	H	-5.34700	-2.97300	-1.00300
C	-5.45000	2.93400	-0.02400	H	-7.43300	-3.31100	0.32600
H	-4.43200	1.04000	-0.04000	C	-2.49800	-4.80400	3.82500
C	-6.45700	3.60600	-2.11000	C	-2.08600	-4.32900	5.08100
H	-6.19200	2.26000	-3.76400	C	-2.82700	-6.16300	3.70000
C	-6.19200	3.86000	-0.76300	C	-2.00400	-5.18700	6.17800
H	-5.24500	3.10900	1.02900	H	-1.83500	-3.27700	5.19300
H	-7.03900	4.31500	-2.69400	C	-2.73500	-7.02500	4.79400
H	-6.56700	4.76400	-0.29100	H	-3.16000	-6.54200	2.73800
C	-5.44100	-0.26100	-3.80700	C	-2.32400	-6.53900	6.03700
C	-6.78400	-0.64800	-3.67600	H	-1.69200	-4.79800	7.14400
C	-4.83000	-0.38500	-5.06600	H	-2.98800	-8.07500	4.67700
C	-7.49100	-1.15700	-4.76600	H	-2.25700	-7.20800	6.89100
H	-7.27400	-0.54500	-2.71100	C	3.12200	1.47800	2.61100
C	-5.53900	-0.88400	-6.15900	H	3.64000	2.02500	3.38900

Table 18. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated D_{3d} hexamer **9** for **1a** with free energies and coordinates. MP2 corrections were not made.





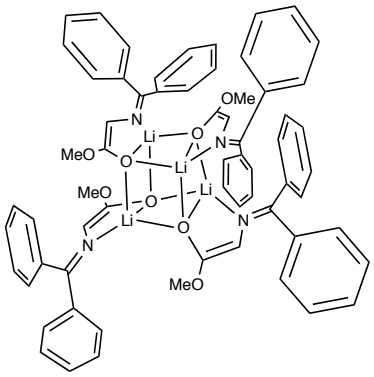
G = -4984.307169

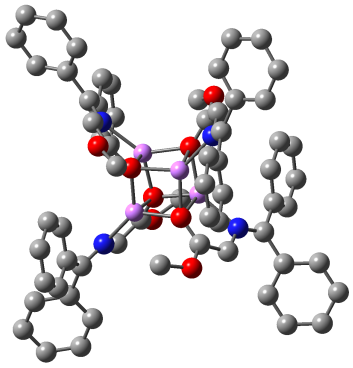
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.19800	1.29500	-1.25700	C	-4.80600	-1.50200	2.04300
Li	-0.67600	-2.27200	-0.45300	H	-3.02600	-2.26000	3.86500
Li	1.97300	0.01500	-0.71900	C	-1.30200	-2.02100	2.59700
Li	0.44400	1.95400	0.72000	O	-0.37100	-2.40000	3.52600
Li	-2.14600	-0.42800	0.69100	C	-0.78100	-2.69200	4.86000
Li	1.20600	-1.43400	1.42300	H	0.13300	-2.93300	5.40500
O	1.25400	-1.83100	-0.53000	H	-1.26900	-1.82500	5.32000
N	3.74900	-1.03600	-1.52400	H	-1.46100	-3.55100	4.88600
C	3.30200	-2.33600	-1.62700	N	3.17800	-1.52800	2.41100
C	4.88400	-0.65900	-2.05300	C	3.44500	-0.18900	2.63700
H	3.92000	-3.09300	-2.09200	C	4.05600	-2.45600	2.67900
C	2.07400	-2.66200	-1.09100	H	4.30800	0.10600	3.22100
O	1.57900	-3.93300	-1.11900	C	2.60300	0.75300	2.08100
C	2.37600	-4.99900	-1.63200	O	2.74200	2.09200	2.30600
H	1.76600	-5.89800	-1.52500	C	3.70900	2.55300	3.24700
H	2.61500	-4.84000	-2.69000	H	3.58000	3.63400	3.29600
H	3.30000	-5.10800	-1.05400	H	3.53800	2.10700	4.23400
N	-0.36600	3.80100	1.60300	H	4.72700	2.31900	2.91400
C	-1.65300	3.43500	1.92900	N	-2.06500	-3.35800	-1.85600
C	0.18100	4.90300	2.04300	C	-2.26800	-2.32900	-2.76300
H	-2.28000	4.08800	2.52300	C	-2.51800	-4.56000	-2.08400
C	-2.14000	2.24500	1.42600	H	-2.65200	-2.53500	-3.75500
O	-3.41000	1.81100	1.65900	C	-2.01700	-1.03900	-2.34900
C	-4.33700	2.65800	2.33400	O	-2.15900	0.04700	-3.17500
H	-5.28000	2.11000	2.34800	C	-2.43200	-0.13900	-4.56100
H	-4.01200	2.86000	3.36200	H	-2.40800	0.85800	-5.00400
H	-4.46800	3.60200	1.79500	H	-1.66900	-0.77300	-5.02600
N	-3.51000	-1.54700	1.90200	H	-3.42200	-0.58500	-4.71200
C	-2.65100	-1.95700	2.89500	O	0.76700	1.45300	-1.26300

N	-1.12000	3.18200	-2.33000
C	0.17100	3.13900	-2.82300
C	-1.95400	4.14000	-2.62400
H	0.48600	3.81500	-3.60800
C	1.04800	2.22900	-2.26300
O	2.32600	2.07000	-2.70400
C	2.79400	2.83500	-3.81000
H	3.83200	2.53600	-3.95700
H	2.20700	2.62300	-4.71300
H	2.74900	3.90900	-3.59500
O	-1.63600	-0.68400	-1.16900
O	-0.76700	-1.71700	1.46200
O	1.62800	0.48700	1.27100
O	-1.45900	1.40400	0.71500
C	-5.64500	-1.18600	0.86400
C	-6.95800	-0.69800	1.01100
C	-5.16000	-1.39100	-0.44300
C	-7.75100	-0.42000	-0.10300
H	-7.36000	-0.53600	2.00600
C	-5.95200	-1.10900	-1.55200
H	-4.16300	-1.79600	-0.57900
C	-7.25500	-0.62400	-1.39100
H	-8.76100	-0.04200	0.03900
H	-5.55200	-1.28200	-2.54800
H	-7.87500	-0.41400	-2.25900
C	-5.49600	-1.78500	3.34300
C	-5.26300	-0.97600	4.46700
C	-6.39600	-2.85600	3.46600
C	-5.90800	-1.23000	5.67800
H	-4.57200	-0.14100	4.38300
C	-7.03500	-3.11600	4.67800
H	-6.59100	-3.48700	2.60300
C	-6.79400	-2.30400	5.78800
H	-5.72000	-0.58800	6.53500
H	-7.72300	-3.95400	4.75600
H	-7.29600	-2.50400	6.73100
C	-3.33500	-4.89800	-3.30000
C	-2.80700	-5.72300	-4.30400
C	-4.64300	-4.41000	-3.44900
C	-3.56100	-6.04200	-5.43500
H	-1.80000	-6.11700	-4.19400
C	-5.40000	-4.73700	-4.57400
H	-5.06700	-3.77900	-2.67200
C	-4.86000	-5.55100	-5.57200
H	-3.13400	-6.67900	-6.20600
H	-6.41500	-4.35900	-4.66800
H	-5.45000	-5.80400	-6.44900
C	-2.25000	-5.66300	-1.13200
C	-1.11800	-5.66200	-0.29800
C	-3.13200	-6.75800	-1.04900
C	-0.88200	-6.71300	0.58600
H	-0.39700	-4.85700	-0.37500
C	-2.90100	-7.80100	-0.15400
H	-4.01300	-6.78500	-1.68300
C	-1.77300	-7.78600	0.66800
H	0.01400	-6.69700	1.19900
H	-3.60500	-8.62800	-0.10200
H	-1.58600	-8.60600	1.35700
C	5.40600	0.70100	-1.79600
C	6.30500	1.31000	-2.69500
C	5.04500	1.41800	-0.63900
C	6.80700	2.58900	-2.45400
H	6.60800	0.77700	-3.59000
C	5.54700	2.69400	-0.40000
H	4.38900	0.95100	0.08700
C	6.43000	3.28900	-1.30700
H	7.49500	3.03700	-3.16600
H	5.24700	3.22800	0.49600
H	6.82600	4.28300	-1.11400
C	5.72000	-1.56400	-2.91100
C	6.99800	-1.96900	-2.49600
C	5.24800	-2.01000	-4.15600
C	7.77900	-2.80300	-3.29700
H	7.37900	-1.62600	-1.53800
C	6.03200	-2.83600	-4.96200
H	4.26100	-1.70200	-4.49000
C	7.29900	-3.23800	-4.53400
H	8.76300	-3.11200	-2.95600
H	5.65300	-3.16400	-5.92700
H	7.90800	-3.88300	-5.16100
C	3.66100	-3.88300	2.60200
C	2.35100	-4.28500	2.91900
C	4.59600	-4.87800	2.25500
C	1.99400	-5.63300	2.89600
H	1.62100	-3.53700	3.20800
C	4.23000	-6.22200	2.21500
H	5.61400	-4.59000	2.01000
C	2.92800	-6.60900	2.54200
H	0.98200	-5.92000	3.17300
H	4.96800	-6.97000	1.93500
H	2.65000	-7.65900	2.53200
C	5.46700	-2.16100	3.09200
C	5.98800	-2.67200	4.29100
C	6.30900	-1.39100	2.27100

C	7.30500	-2.41000	4.66900	C	-1.68400	7.48400	4.95800
H	5.35200	-3.28000	4.93000	H	-1.62700	8.99200	3.41700
C	7.62900	-1.13800	2.64300	H	-1.59300	5.78200	6.28000
H	5.92200	-0.99300	1.33700	H	-2.14900	8.13500	5.69300
C	8.13100	-1.64300	3.84500	C	-3.34800	4.07200	-2.12100
H	7.68700	-2.80800	5.60500	C	-4.06400	5.25200	-1.83900
H	8.26700	-0.54500	1.99200	C	-3.99200	2.84000	-1.90300
H	9.15900	-1.44300	4.13600	C	-5.36200	5.20000	-1.33400
C	1.49200	5.32800	1.50600	H	-3.59000	6.21500	-2.00100
C	2.34700	6.16500	2.25100	C	-5.29100	2.78900	-1.40100
C	1.91100	4.93700	0.21900	H	-3.47900	1.91800	-2.15900
C	3.57500	6.58000	1.73700	C	-5.98200	3.96800	-1.11200
H	2.04400	6.49000	3.24200	H	-5.88900	6.12500	-1.11400
C	3.13700	5.35400	-0.29200	H	-5.76800	1.82500	-1.24800
H	1.25200	4.32400	-0.38800	H	-6.99800	3.92700	-0.72700
C	3.97800	6.17700	0.46300	C	-1.57600	5.33900	-3.44300
H	4.21700	7.22200	2.33500	C	-2.26900	5.64000	-4.62600
H	3.43900	5.03500	-1.28600	C	-0.54300	6.20000	-3.03500
H	4.93000	6.50900	0.05700	C	-1.93000	6.75700	-5.39100
C	-0.47600	5.79800	3.05200	H	-3.08200	4.99200	-4.94400
C	-0.78500	7.13100	2.73900	C	-0.21100	7.32300	-3.79300
C	-0.77900	5.32600	4.34000	H	-0.00400	5.99000	-2.11600
C	-1.38900	7.96500	3.68100	C	-0.90000	7.60300	-4.97600
H	-0.54800	7.51200	1.75000	H	-2.47400	6.96800	-6.30800
C	-1.37400	6.16200	5.28500	H	0.58400	7.98300	-3.45700
H	-0.54200	4.29700	4.59700	H	-0.63900	8.47700	-5.56700

Table 19. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated D_{2d} tetramer **1a** with free energies and coordinates.



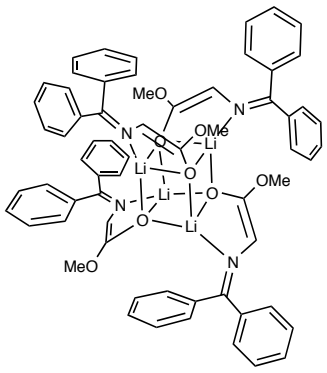


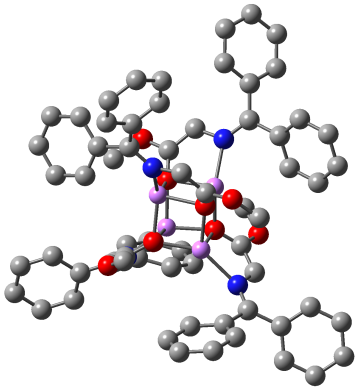
G = -3322.870678
G_{MP2} = -3312.395581

Atom	X	Y	Z	Atom	X	Y	Z
H	2.24200	-5.22800	-0.92700	H	3.43400	7.38800	0.75600
H	3.41800	-7.39600	-0.75700	H	5.85000	7.54400	1.33400
H	5.83300	-7.55700	-1.33400	H	7.06400	5.51400	2.10500
H	7.05200	-5.52900	-2.10400	H	5.87200	3.35500	2.30300
H	5.86500	-3.36700	-2.30100	Li	1.05200	0.87900	0.95000
Li	1.05000	-0.88100	-0.94800	O	0.90200	-1.06200	1.10600
O	0.90500	1.05900	-1.10500	Li	-1.05300	-0.88000	0.94700
C	1.63600	2.09500	-1.38200	N	-2.55500	-2.27500	0.79200
C	2.45600	2.75900	-0.48600	C	-2.45600	-2.75900	-0.48900
H	3.01400	3.62500	-0.82600	C	-1.63700	-2.09400	-1.38400
N	2.55500	2.27300	0.79400	O	-0.90700	-1.05800	-1.10700
C	3.27000	2.82100	1.74500	Li	-1.05100	0.88200	-0.94700
C	3.40000	2.07800	3.02300	N	-2.54900	2.28100	-0.79200
C	3.49400	2.75200	4.25600	C	-2.44900	2.76600	0.48800
C	3.59400	2.04300	5.45200	C	-1.63200	2.09900	1.38400
C	3.61500	0.64600	5.44600	O	-0.90400	1.06000	1.10700
C	3.54200	-0.03700	4.23000	O	-1.61300	2.61000	2.64500
C	3.43800	0.67000	3.03200	C	-0.63700	2.10600	3.55900
H	3.42300	0.13400	2.08800	H	0.38100	2.32400	3.21800
H	3.57800	-1.12300	4.20400	H	-0.82000	2.63500	4.49500
H	3.70200	0.09600	6.38000	H	-0.75300	1.03000	3.71800
H	3.65500	2.58500	6.39300	H	-3.00400	3.63300	0.82900
H	3.48000	3.83800	4.27200	C	-3.26300	2.83100	-1.74300
C	3.98100	4.12800	1.61600	C	-3.39500	2.09100	-3.02100
C	5.34100	4.23600	1.95500	C	-3.48700	2.76500	-4.25400
C	6.01000	5.45400	1.84800	C	-3.58900	2.05800	-5.45000
C	5.32900	6.59300	1.41300	C	-3.61600	0.66100	-5.44600
C	3.97500	6.50400	1.08500	C	-3.54500	-0.02300	-4.23000
C	3.30800	5.28300	1.18200	C	-3.43900	0.68300	-3.03200
H	2.25400	5.22200	0.92600	H	-3.42600	0.14600	-2.08800

H	-3.58500	-1.10900	-4.20500	C	-3.54400	0.03200	4.22900
H	-3.70500	0.11200	-6.37900	C	-3.43900	-0.67500	3.03100
H	-3.64800	2.60000	-6.39100	H	-3.42500	-0.13800	2.08700
H	-3.46900	3.85100	-4.26900	H	-3.58100	1.11700	4.20500
C	-3.97000	4.14000	-1.61200	H	-3.70400	-0.10300	6.37900
C	-5.33000	4.25200	-1.95200	H	-3.65500	-2.59200	6.39000
C	-5.99600	5.47200	-1.84300	H	-3.48000	-3.84300	4.26900
C	-5.31200	6.60900	-1.40800	C	-3.98100	-4.13100	1.61100
C	-3.95800	6.51600	-1.08000	C	-5.34000	-4.24000	1.95100
C	-3.29500	5.29400	-1.17700	C	-6.00900	-5.45800	1.84200
H	-2.24100	5.22900	-0.92100	C	-5.32800	-6.59700	1.40700
H	-3.41500	7.39800	-0.75000	C	-3.97400	-6.50700	1.07900
H	-5.83000	7.56100	-1.32800	C	-3.30700	-5.28600	1.17700
H	-7.05000	5.53500	-2.10100	H	-2.25300	-5.22400	0.92100
H	-5.86400	3.37300	-2.30000	H	-3.43300	-7.39000	0.74900
O	-1.61900	-2.60500	-2.64600	H	-5.84800	-7.54800	1.32600
C	-0.64200	-2.10200	-3.55900	H	-7.06400	-5.51900	2.10000
H	0.37600	-2.32300	-3.21800	H	-5.87300	-3.35900	2.29900
H	-0.82500	-2.63200	-4.49500	O	1.61800	2.60700	-2.64300
H	-0.75600	-1.02700	-3.71800	C	0.64200	2.10600	-3.55600
H	-3.01400	-3.62500	-0.83000	H	-0.37600	2.32600	-3.21500
C	-3.27000	-2.82400	1.74200	H	0.82500	2.63600	-4.49300
C	-3.40100	-2.08300	3.02000	H	0.75500	1.03000	-3.71600
C	-3.49500	-2.75700	4.25300	H	-0.38300	-2.32800	3.21500
C	-3.59500	-2.05000	5.45000	H	0.81700	-2.64000	4.49200
C	-3.61700	-0.65200	5.44500	H	0.75100	-1.03400	3.71700

Table 20. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated S_4 tetramer **1a** with free energies and coordinates.



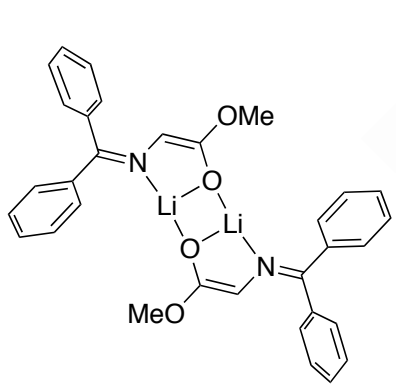


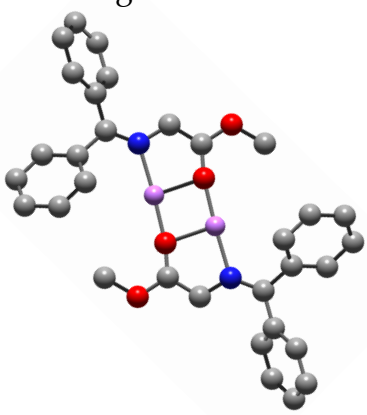
G = -3322.870294
G_{MP2} = -3312.392614

Atom	X	Y	Z	Atom	X	Y	Z
C	0.90500	-3.69500	1.80700	O	0.72700	1.14000	-1.02300
O	1.74500	-2.68900	2.37500	C	1.63600	1.42000	-1.90800
C	1.63500	-1.42100	1.90800	C	2.54000	0.51400	-2.44300
C	2.53900	-0.51700	2.44300	H	3.30000	0.87800	-3.12600
H	3.29900	-0.88100	3.12600	N	2.42800	-0.81300	-2.10900
N	2.42800	0.81100	2.10900	C	3.28800	-1.74100	-2.45000
C	3.28900	1.73800	2.45000	C	2.95600	-3.15300	-2.13700
C	2.95800	3.15000	2.13700	C	3.96300	-4.07300	-1.78200
C	3.96600	4.06900	1.78300	C	3.65100	-5.39500	-1.47100
C	3.65500	5.39100	1.47200	C	2.32700	-5.84100	-1.52000
C	2.33200	5.83800	1.52000	C	1.31800	-4.94700	-1.88400
C	1.32200	4.94500	1.88300	C	1.62900	-3.62100	-2.18800
C	1.63100	3.61900	2.18800	H	0.83800	-2.95500	-2.51400
H	0.84000	2.95300	2.51400	H	0.28600	-5.28100	-1.95100
H	0.29000	5.28000	1.95000	H	2.08800	-6.87500	-1.28800
H	2.09300	6.87300	1.28800	H	4.44600	-6.08000	-1.18900
H	4.45000	6.07600	1.19000	H	4.99500	-3.74000	-1.74000
H	4.99800	3.73600	1.74100	C	4.58400	-1.46500	-3.13900
C	4.58500	1.46100	3.14000	C	4.94700	-2.18300	-4.29200
C	4.94700	2.17900	4.29300	C	6.16000	-1.94000	-4.93500
C	6.16000	1.93500	4.93600	C	7.04300	-0.98400	-4.42900
C	7.04300	0.97800	4.43000	C	6.70200	-0.27200	-3.27700
C	6.70200	0.26700	3.27800	C	5.48400	-0.50700	-2.64100
C	5.48500	0.50300	2.64100	H	5.22600	0.05000	-1.74500
H	5.22600	-0.05400	1.74500	H	7.38800	0.46700	-2.87000
H	7.38700	-0.47200	2.87100	H	7.99100	-0.79700	-4.92700
H	7.99100	0.79100	4.92900	H	6.41700	-2.49900	-5.83100
H	6.41700	2.49400	5.83200	H	4.26800	-2.93600	-4.68500
H	4.27000	2.93200	4.68600	Li	0.80100	-0.90300	-0.90600
Li	0.80200	0.90200	0.90600	O	0.72600	-1.14100	1.02300

Li	-1.26300	-1.01800	0.87100	H	-5.84500	4.16300	-1.85800
N	-2.67300	-2.52500	0.51000	O	-1.76300	-2.22400	-2.94000
C	-2.56400	-2.79600	-0.83300	C	-1.09100	-1.30400	-3.81000
C	-1.81600	-1.93300	-1.61200	H	-0.04200	-1.16700	-3.53200
O	-1.14900	-0.91600	-1.15900	H	-1.14900	-1.75900	-4.80000
Li	-1.26200	1.01800	-0.87100	H	-1.59300	-0.33300	-3.82400
N	-2.67000	2.52700	-0.51000	H	-3.07900	-3.62700	-1.30400
C	-2.56100	2.79800	0.83200	C	-3.32700	-3.27400	1.36300
C	-1.81400	1.93400	1.61200	C	-3.54600	-2.73700	2.72900
O	-1.14800	0.91600	1.15900	C	-3.55200	-3.58000	3.85700
O	-1.76100	2.22400	2.94000	C	-3.76800	-3.06500	5.13400
C	-1.09000	1.30400	3.81000	C	-4.00300	-1.69900	5.31400
H	-0.04100	1.16700	3.53200	C	-4.01800	-0.85300	4.20300
H	-1.14700	1.75900	4.80000	C	-3.78900	-1.36400	2.92500
H	-1.59200	0.33300	3.82400	H	-3.83500	-0.70800	2.06000
H	-3.07500	3.62900	1.30300	H	-4.22300	0.20800	4.32600
C	-3.32300	3.27700	-1.36300	H	-4.18600	-1.30100	6.30800
C	-3.54300	2.74100	-2.72900	H	-3.75400	-3.73200	5.99100
C	-3.54700	3.58300	-3.85700	H	-3.37900	-4.64400	3.72800
C	-3.76400	3.06800	-5.13400	C	-3.90900	-4.61000	1.03700
C	-4.00100	1.70300	-5.31400	C	-5.24100	-4.91200	1.37000
C	-4.01700	0.85700	-4.20300	C	-5.78700	-6.16100	1.08000
C	-3.78700	1.36800	-2.92500	C	-5.00700	-7.14200	0.46400
H	-3.83400	0.71200	-2.06100	C	-3.67800	-6.86300	0.13900
H	-4.22300	-0.20300	-4.32600	C	-3.13600	-5.60900	0.41900
H	-4.18400	1.30500	-6.30800	H	-2.10100	-5.39900	0.16300
H	-3.75000	3.73600	-5.99200	H	-3.06100	-7.62300	-0.33200
H	-3.37300	4.64700	-3.72800	H	-5.43100	-8.11800	0.24100
C	-3.90300	4.61400	-1.03700	H	-6.82200	-6.37000	1.33700
C	-5.23400	4.91800	-1.37000	H	-5.85000	-4.15600	1.85800
C	-5.77800	6.16800	-1.08000	O	1.74700	2.68700	-2.37500
C	-4.99700	7.14800	-0.46400	C	0.90700	3.69400	-1.80800
C	-3.66800	6.86600	-0.13900	H	1.08200	3.80300	-0.73400
C	-3.12800	5.61200	-0.41900	H	1.18500	4.61700	-2.32000
H	-2.09400	5.40000	-0.16400	H	-0.15200	3.48300	-1.98700
H	-3.05000	7.62600	0.33100	H	1.08000	-3.80500	0.73400
H	-5.41900	8.12500	-0.24100	H	1.18200	-4.61800	2.31900
H	-6.81400	6.37800	-1.33700	H	-0.15500	-3.48400	1.98700

Table 21. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated dimer **1a** with free energies and coordinates.



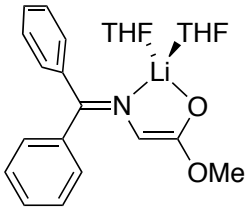


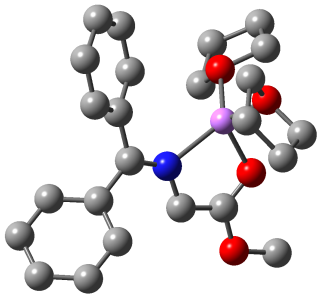
G = -1661.419638
G_{MP2} = -1656.15668

Atom	X	Y	Z	Atom	X	Y	Z
C	0.36500	3.86600	-0.65700	O	-0.33900	1.36000	-0.08000
O	-1.00900	3.50200	-0.52800	Li	1.21000	0.39200	0.02900
C	-1.29200	2.20100	-0.27500	O	0.33900	-1.35900	-0.08300
C	-2.64700	1.87400	-0.26000	C	1.29200	-2.20000	-0.27600
H	-3.38800	2.64400	-0.44000	C	2.64700	-1.87300	-0.26000
N	-2.96800	0.57800	0.03000	N	2.96800	-0.57800	0.02900
C	-4.17000	0.05400	0.07900	C	4.17000	-0.05400	0.07800
C	-4.26200	-1.34800	0.55100	C	5.42000	-0.77300	-0.29700
C	-5.22200	-2.24000	0.03400	C	6.54900	-0.72600	0.54000
C	-5.26400	-3.56900	0.45000	C	7.72500	-1.39200	0.19600
C	-4.35700	-4.04400	1.40200	C	7.80200	-2.10900	-1.00000
C	-3.41400	-3.16800	1.94300	C	6.69300	-2.15400	-1.84800
C	-3.37100	-1.83800	1.52800	C	5.51500	-1.49600	-1.50000
H	-2.67300	-1.14800	1.99800	H	4.66000	-1.53100	-2.16900
H	-2.72400	-3.51400	2.71000	H	6.74600	-2.70000	-2.78700
H	-4.39700	-5.08000	1.73000	H	8.71800	-2.62600	-1.27000
H	-6.00600	-4.24000	0.02500	H	8.58200	-1.35100	0.86300
H	-5.92900	-1.88600	-0.71100	H	6.49800	-0.16500	1.46900
C	-5.42000	0.77200	-0.29700	C	4.26200	1.34800	0.55000
C	-6.55000	0.72600	0.53900	C	5.22300	2.24000	0.03300
C	-7.72500	1.39100	0.19400	C	5.26500	3.56900	0.44900
C	-7.80200	2.10800	-1.00200	C	4.35900	4.04400	1.40100
C	-6.69300	2.15300	-1.84900	C	3.41400	3.16900	1.94200
C	-5.51400	1.49500	-1.50000	C	3.37100	1.83800	1.52700
H	-4.65900	1.53000	-2.16900	H	2.67300	1.14900	1.99700
H	-6.74600	2.69900	-2.78800	H	2.72500	3.51500	2.70800
H	-8.71900	2.62400	-1.27200	H	4.39800	5.08000	1.72800
H	-8.58300	1.35000	0.86100	H	6.00800	4.24000	0.02400
H	-6.49900	0.16500	1.46800	H	5.92900	1.88500	-0.71100
Li	-1.21000	-0.39100	0.03100	H	3.38800	-2.64400	-0.44000

O	1.00800	-3.50100	-0.52900	H	-0.92700	-3.67100	0.26000
C	-0.36600	-3.86500	-0.65900	H	0.84100	3.33200	-1.48700
H	-0.84100	-3.33100	-1.48900	H	0.36100	4.93700	-0.86600
H	-0.36200	-4.93600	-0.86800	H	0.92600	3.67200	0.26200

Table 22. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for THF-disolvated monomer **1a** with free energies and coordinates.

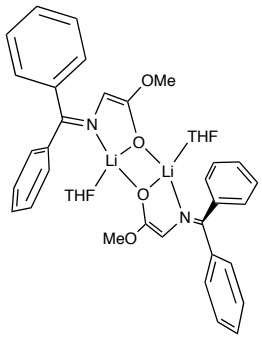


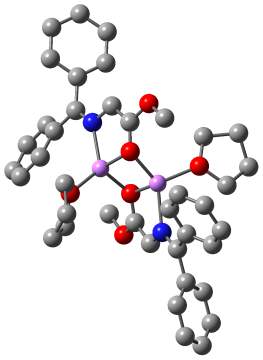


G = -1295.40975
G_{MP2} = -1291.234565

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.08000	4.60100	-0.05400	O	-1.92500	1.97900	0.15100
O	-0.84200	3.93700	-0.28600	O	-1.78400	-0.56400	2.06400
C	-0.85300	2.57600	-0.16100	C	-1.03500	-1.65500	2.63600
C	0.39800	1.97400	-0.39300	C	0.11700	-0.98600	3.40100
H	1.25200	2.59900	-0.63300	C	-0.43600	0.42500	3.74800
N	0.47100	0.61900	-0.31600	C	-1.82600	0.45500	3.08400
C	1.57400	-0.09400	-0.43900	H	-2.07300	1.39200	2.58500
C	1.46300	-1.56700	-0.41400	H	-2.61900	0.19900	3.80200
C	2.52000	-2.37300	0.06300	H	0.20600	1.20500	3.32900
C	2.40400	-3.76000	0.12400	H	-0.50700	0.59500	4.82600
C	1.23100	-4.39500	-0.29300	H	0.99600	-0.90800	2.75700
C	0.17900	-3.61700	-0.78400	H	0.39800	-1.56100	4.28900
C	0.29500	-2.22900	-0.85100	H	-1.69600	-2.22000	3.31000
H	-0.51800	-1.64800	-1.27200	H	-0.71700	-2.30200	1.81700
H	-0.73200	-4.09400	-1.13800	O	-2.85400	-0.71000	-0.99000
H	1.14400	-5.47700	-0.24900	C	-2.99400	-0.03400	-2.25600
H	3.23400	-4.34900	0.50700	C	-4.26900	-0.62900	-2.86200
H	3.43700	-1.89900	0.40000	C	-5.14300	-0.94900	-1.62000
C	2.93200	0.51100	-0.59400	C	-4.17900	-0.77200	-0.42400
C	3.77400	0.12000	-1.65000	H	-4.18800	-1.60000	0.28700
C	5.04600	0.67100	-1.79900	H	-4.38000	0.16300	0.11600
C	5.51100	1.62300	-0.89000	H	-5.54000	-1.96700	-1.66900
C	4.69100	2.01700	0.16900	H	-5.99500	-0.26800	-1.53300
C	3.41700	1.46900	0.31400	H	-4.03400	-1.54500	-3.41200
H	2.78600	1.78300	1.14000	H	-4.75500	0.06400	-3.55600
H	5.04500	2.75200	0.88800	H	-3.08300	1.04500	-2.07500
H	6.50300	2.05200	-1.00400	H	-2.08600	-0.22700	-2.83200
H	5.67500	0.35700	-2.62900	H	-2.44800	4.41900	0.96200
H	3.42100	-0.62400	-2.35900	H	-1.87300	5.66400	-0.19000
Li	-1.49400	0.12500	0.22600	H	-2.84800	4.27700	-0.76400

Table 23. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for THF-solvated dimer **1a** with free energies and coordinates.



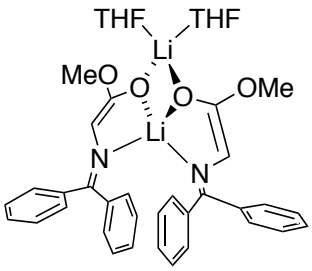


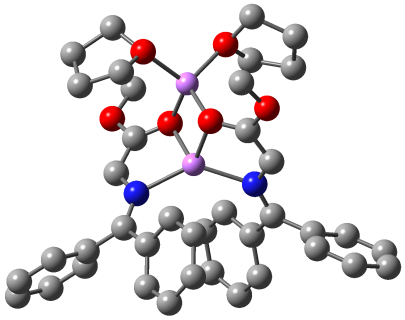
G = -2126.133993
G_{MP2} = -2119.340707

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.97500	-2.63800	-2.66300	Li	-1.17300	-0.63900	0.54800
O	0.41300	-2.55500	-2.32400	N	-3.03900	0.29600	0.51700
C	0.78700	-1.53700	-1.50300	C	-2.75000	1.58000	0.89100
C	2.16200	-1.45100	-1.26500	H	-3.50800	2.35300	0.96400
H	2.82700	-2.17300	-1.72800	C	-1.42900	1.90100	1.19000
N	2.60300	-0.45500	-0.44200	O	-0.42700	1.10200	1.15100
C	3.85900	-0.23300	-0.13000	O	-1.23300	3.21200	1.53600
C	4.16400	0.83400	0.84900	C	0.05900	3.56500	2.02900
C	5.40800	1.49900	0.83700	H	0.84100	3.38800	1.28500
C	5.69400	2.51500	1.74700	H	-0.00100	4.63000	2.26200
C	4.75100	2.89500	2.70400	H	0.30200	3.00400	2.93800
C	3.51600	2.24200	2.73600	C	-4.22000	-0.11900	0.12900
C	3.22600	1.22800	1.82600	C	-5.39900	0.78600	-0.04300
H	2.27000	0.71600	1.88200	C	-6.61000	0.51500	0.61600
H	2.77900	2.51200	3.48800	C	-7.71600	1.34900	0.45700
H	4.97800	3.68000	3.42000	C	-7.63900	2.46800	-0.37500
H	6.66000	3.01300	1.70600	C	-6.44500	2.74500	-1.04600
H	6.15300	1.21900	0.09800	C	-5.33700	1.91500	-0.87900
C	5.00000	-1.01500	-0.70100	H	-4.41200	2.13500	-1.40400
C	5.91700	-1.66300	0.14400	H	-6.37800	3.60800	-1.70300
C	6.98300	-2.39600	-0.37800	H	-8.50100	3.11600	-0.50300
C	7.16100	-2.48900	-1.75900	H	-8.64100	1.12400	0.98300
C	6.26500	-1.84300	-2.61300	H	-6.67900	-0.35900	1.25800
C	5.19600	-1.11700	-2.08900	C	-4.40500	-1.55900	-0.16100
H	4.50300	-0.61900	-2.76200	C	-5.34200	-1.99100	-1.12100
H	6.39900	-1.90300	-3.69000	C	-5.49600	-3.34300	-1.42200
H	7.99300	-3.05800	-2.16700	C	-4.72700	-4.30700	-0.76600
H	7.67500	-2.89500	0.29600	C	-3.80500	-3.89800	0.20000
H	5.78800	-1.58900	1.22100	C	-3.64900	-2.54600	0.50300
Li	0.88200	0.77900	-0.24800	H	-2.95100	-2.24900	1.28000
O	-0.09700	-0.74800	-1.02600	H	-3.21600	-4.63900	0.73700

H	-4.85300	-5.36200	-0.99700	O	1.14100	2.38600	-1.35400
H	-6.21900	-3.64500	-2.17600	C	2.29600	2.58400	-2.20800
H	-5.94400	-1.25500	-1.64500	C	1.82300	3.48500	-3.35500
O	-0.62700	-1.93000	1.97300	C	0.64600	4.24400	-2.72100
C	-0.43800	-1.41600	3.31400	C	0.02100	3.16600	-1.83900
C	0.89300	-2.00200	3.78200	H	-0.64800	2.51200	-2.41300
C	0.88500	-3.38200	3.10600	H	-0.51800	3.54900	-0.97000
C	0.22800	-3.08300	1.75400	H	-0.05800	4.64300	-3.45700
H	-0.39200	-3.90500	1.38200	H	1.00900	5.07600	-2.10700
H	0.96600	-2.81900	0.98900	H	1.47200	2.88000	-4.20000
H	0.27600	-4.08600	3.68500	H	2.61800	4.14300	-3.71900
H	1.88400	-3.81300	2.99100	H	3.08200	3.05600	-1.60700
H	0.96700	-2.05500	4.87300	H	2.65000	1.60500	-2.54100
H	1.72700	-1.39600	3.41000	H	-1.32700	-1.70500	-3.11500
H	-0.45100	-0.32700	3.24900	H	-1.04600	-3.45400	-3.38500
H	-1.27200	-1.75500	3.94400	H	-1.59300	-2.86300	-1.79000

Table 24. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for THF-disolvated unsymmetric dimer **1a** with free energies and coordinates.



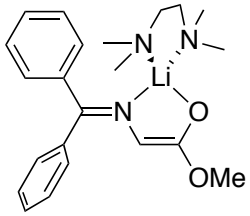


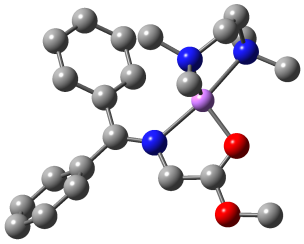
G = -2126.131169
G_{MP2} = -2119.342935

Atom	X	Y	Z	Atom	X	Y	Z
C	1.92200	2.95300	3.31100	C	-2.57300	0.29400	-0.95300
O	2.64000	2.04800	2.47900	C	-1.91400	1.37100	-1.53100
C	1.91400	1.37000	1.53100	O	-0.72100	1.76100	-1.25800
C	2.57300	0.29300	0.95300	Li	0.00000	3.01500	0.00000
H	3.56300	0.02300	1.30400	O	0.72200	1.76100	1.25700
N	1.92100	-0.40100	-0.03500	O	-1.29400	4.17300	0.96000
C	2.38700	-1.47200	-0.62400	C	-2.25100	5.01500	0.29200
C	1.61600	-2.05700	-1.74500	C	-3.59400	4.26200	0.36600
C	1.72800	-3.42400	-2.06800	C	-3.39300	3.25100	1.53100
C	0.98300	-3.98300	-3.10500	C	-1.99800	3.58700	2.07500
C	0.10800	-3.19200	-3.85300	H	-1.41200	2.72700	2.40400
C	-0.00600	-1.83200	-3.55400	H	-2.04600	4.32800	2.88800
C	0.74100	-1.27000	-2.52000	H	-3.41400	2.22700	1.14800
H	0.66000	-0.20700	-2.31900	H	-4.16000	3.34100	2.30600
H	-0.67300	-1.20000	-4.13600	H	-3.79600	3.73300	-0.56800
H	-0.47000	-3.62800	-4.66400	H	-4.42200	4.95300	0.54900
H	1.08200	-5.04300	-3.32400	H	-2.29900	5.98000	0.81800
H	2.39500	-4.05600	-1.48900	H	-1.88300	5.18700	-0.72200
C	3.66200	-2.14000	-0.21400	O	1.29400	4.17300	-0.96000
C	4.71200	-2.31300	-1.13000	C	2.25100	5.01500	-0.29200
C	5.89900	-2.93800	-0.74800	C	3.59500	4.26200	-0.36600
C	6.05400	-3.41200	0.55600	C	3.39500	3.25100	-1.53100
C	5.01300	-3.25700	1.47500	C	1.99900	3.58800	-2.07600
C	3.82900	-2.62500	1.09500	H	1.41400	2.72800	-2.40400
H	3.01800	-2.51100	1.80900	H	2.04800	4.32800	-2.88800
H	5.12100	-3.63300	2.48900	H	3.41500	2.22800	-1.14800
H	6.97700	-3.90300	0.85400	H	4.16200	3.34300	-2.30500
H	6.70400	-3.05600	-1.47000	H	3.79600	3.73200	0.56900
H	4.59100	-1.95400	-2.14900	H	4.42300	4.95400	-0.54800
Li	0.00000	0.38900	0.00000	H	2.30000	5.98000	-0.81700
N	-1.92100	-0.40000	0.03500	H	1.88300	5.18700	0.72200

O	-2.63900	2.04800	-2.47900	H	0.67200	-1.19900	4.13600
C	-1.92200	2.95400	-3.31100	H	-0.66100	-0.20600	2.31900
H	-2.66000	3.36100	-4.00600	C	-3.66200	-2.13900	0.21400
H	-1.46800	3.76900	-2.73700	C	-4.71300	-2.31100	1.13000
H	-1.13300	2.44000	-3.87300	C	-5.90000	-2.93600	0.74800
H	-3.56300	0.02400	-1.30400	C	-6.05400	-3.41100	-0.55600
C	-2.38700	-1.47100	0.62400	C	-5.01300	-3.25600	-1.47500
C	-1.61700	-2.05700	1.74500	C	-3.83000	-2.62400	-1.09500
C	-0.74100	-1.27000	2.52000	H	-3.01900	-2.51100	-1.80900
C	0.00600	-1.83100	3.55400	H	-5.12200	-3.63200	-2.48900
C	-0.10900	-3.19200	3.85300	H	-6.97800	-3.90100	-0.85400
C	-0.98400	-3.98200	3.10500	H	-6.70400	-3.05400	1.47000
C	-1.72900	-3.42400	2.06800	H	-4.59200	-1.95300	2.14900
H	-2.39600	-4.05500	1.48900	H	1.13500	2.43900	3.87300
H	-1.08300	-5.04200	3.32500	H	2.66100	3.36000	4.00500
H	0.46900	-3.62700	4.66400	H	1.46800	3.76800	2.73700

Table 25. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for TMEDA-chelated monomer **1a** with free energies and coordinates.

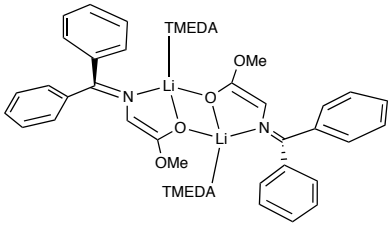


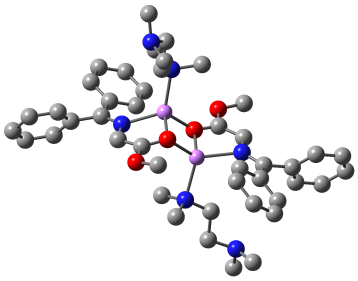


G = -1178.256299
G_{MP2} = -1174.391174

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.80300	4.77600	-0.82100	Li	-1.54300	0.32000	-0.18800
O	-0.58200	4.04700	-0.74100	N	-2.02600	-0.22100	1.83100
C	-0.69600	2.69200	-0.60800	C	-3.46500	-0.52100	1.74200
C	0.54000	2.02000	-0.53300	C	-3.80800	-1.36600	0.51100
H	1.46200	2.59100	-0.57000	N	-3.41800	-0.71500	-0.75400
N	0.50800	0.66700	-0.45400	C	-4.33600	0.38200	-1.10500
C	1.55700	-0.12400	-0.31900	H	-3.99700	0.85000	-2.03200
C	1.32700	-1.58100	-0.39100	H	-5.36900	0.01600	-1.24100
C	2.11100	-2.49200	0.35000	H	-4.32400	1.15400	-0.33500
C	1.86300	-3.86300	0.30700	C	-3.38700	-1.69400	-1.84700
C	0.83200	-4.37400	-0.48700	H	-4.37900	-2.14000	-2.03900
C	0.06000	-3.49100	-1.24600	H	-3.05000	-1.20300	-2.76600
C	0.30500	-2.11900	-1.20300	H	-2.68500	-2.49600	-1.60500
H	-0.26700	-1.44400	-1.83300	H	-4.88900	-1.59900	0.52500
H	-0.71600	-3.87900	-1.90300	H	-3.28000	-2.32400	0.56600
H	0.64700	-5.44400	-0.52800	H	-3.82700	-1.04300	2.64600
H	2.47700	-4.53600	0.90000	H	-4.00100	0.43200	1.69600
H	2.91300	-2.11300	0.97500	C	-1.25300	-1.37500	2.31300
C	2.95000	0.36500	-0.10700	H	-1.54300	-1.66300	3.33900
C	4.01500	-0.15200	-0.86800	H	-1.39200	-2.23500	1.65400
C	5.32400	0.28600	-0.66800	H	-0.18900	-1.12600	2.30200
C	5.60300	1.24900	0.30400	C	-1.77800	0.94700	2.68800
C	4.56000	1.76900	1.07300	H	-2.11300	0.78300	3.72700
C	3.25100	1.33400	0.86800	H	-0.70600	1.16300	2.69600
H	2.44800	1.74600	1.47300	H	-2.29500	1.81700	2.27500
H	4.76500	2.51300	1.83800	O	-1.84000	2.15500	-0.54800
H	6.62300	1.59100	0.46000	H	-2.41100	4.63900	0.07900
H	6.12700	-0.12500	-1.27500	H	-1.51200	5.82400	-0.91800
H	3.80800	-0.90400	-1.62400	H	-2.39400	4.47100	-1.69100

Table 26. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for TMEDA-disolvated(η^1) symmetric dimer **1a** with free energies and coordinates.



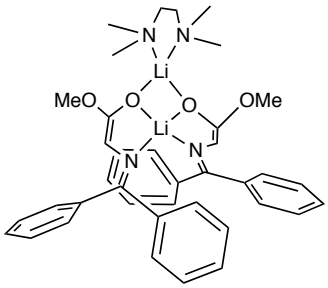


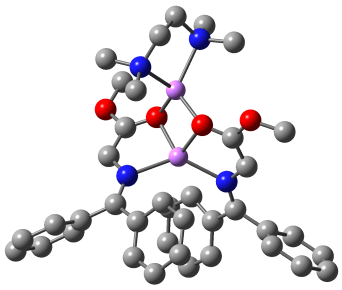
G = -2356.506792
G_{MP2} = -2348.784786

Atom	X	Y	Z	Atom	X	Y	Z
C	0.45300	1.76400	-3.65800	O	0.71900	0.82200	-1.17400
O	1.44300	0.78700	-3.35000	N	-2.61800	0.54900	0.66700
C	1.59900	0.45200	-2.03100	C	-2.31200	0.08100	1.92100
C	2.75000	-0.28500	-1.76500	H	-3.05600	0.07700	2.70800
H	3.42300	-0.52300	-2.58200	C	-1.00600	-0.35400	2.14000
N	2.97700	-0.68700	-0.47700	O	-0.57300	-0.75300	3.37500
C	4.01400	-1.37900	-0.07200	C	-1.48100	-0.72900	4.47300
C	4.05900	-1.81000	1.34500	H	-0.91200	-1.07000	5.33900
C	5.28600	-2.03300	2.00200	H	-1.85800	0.28400	4.65800
C	5.32800	-2.39500	3.34700	H	-2.32900	-1.40400	4.30400
C	4.14600	-2.55100	4.07500	C	-3.81800	0.93700	0.31700
C	2.92000	-2.34700	3.43600	C	-5.01500	0.80100	1.21100
C	2.87500	-1.99100	2.09000	C	-5.69800	1.93600	1.67400
H	1.91100	-1.86400	1.60800	C	-6.81200	1.81100	2.50500
H	1.98600	-2.47200	3.97800	C	-7.26900	0.54600	2.87800
H	4.18000	-2.83600	5.12400	C	-6.60500	-0.59200	2.41500
H	6.28900	-2.55100	3.83000	C	-5.48600	-0.46800	1.59100
H	6.21500	-1.90500	1.45400	H	-4.98100	-1.35900	1.22700
C	5.14800	-1.76800	-0.96800	H	-6.96100	-1.58100	2.69300
C	5.52700	-3.11500	-1.09600	H	-8.13900	0.44700	3.52200
C	6.58100	-3.48800	-1.92900	H	-7.32400	2.70200	2.85800
C	7.28600	-2.51900	-2.64600	H	-5.35000	2.92200	1.37800
C	6.92800	-1.17500	-2.52100	C	-4.01300	1.54200	-1.01800
C	5.86900	-0.80400	-1.69300	C	-2.95700	2.19700	-1.68600
H	5.59800	0.24400	-1.60100	C	-3.14700	2.76100	-2.94600
H	7.47700	-0.41200	-3.06800	C	-4.39200	2.69000	-3.57700
H	8.10900	-2.80800	-3.29400	C	-5.45000	2.05300	-2.92500
H	6.85200	-4.53700	-2.01900	C	-5.26600	1.49300	-1.66200
H	4.98700	-3.87200	-0.53400	H	-6.10000	1.00600	-1.16600
Li	1.51300	0.34300	0.61400	H	-6.42600	1.99300	-3.40100
O	-0.10900	-0.42400	1.23400	H	-4.53900	3.13700	-4.55600
Li	-0.88700	-0.04400	-0.50000	H	-2.32400	3.28100	-3.43000

H	-1.99400	2.28600	-1.19100	C	2.59900	3.00000	0.58900
N	-1.40900	-1.82600	-1.62400	H	1.72600	3.07900	-0.06600
C	-2.71700	-2.25100	-1.08300	H	3.39400	2.52500	0.00400
H	-2.63800	-2.26000	0.00900	C	3.08600	4.39900	1.01300
H	-3.43300	-1.46600	-1.33900	H	2.26900	4.96000	1.51000
C	-3.26300	-3.62100	-1.52800	H	3.88800	4.29100	1.75200
H	-3.24800	-3.72400	-2.62900	N	3.64200	5.15100	-0.11400
H	-2.61700	-4.41100	-1.13000	C	2.62800	5.54800	-1.08500
N	-4.61100	-3.83300	-0.98800	H	1.84500	6.20200	-0.65000
C	-5.63700	-3.14900	-1.76900	H	3.10700	6.09300	-1.90500
H	-5.71700	-3.53700	-2.80400	H	2.13800	4.66900	-1.51400
H	-6.61000	-3.27400	-1.28300	C	4.39400	6.31100	0.34500
H	-5.43100	-2.07600	-1.82500	H	4.85300	6.81400	-0.51300
C	-4.93100	-5.25000	-0.85900	H	3.77000	7.05500	0.88100
H	-5.91700	-5.36200	-0.39400	H	5.19500	5.99200	1.02000
H	-4.95100	-5.78500	-1.82900	C	1.08800	2.54300	2.47600
H	-4.19500	-5.74100	-0.21400	H	0.25300	2.79600	1.81600
C	-1.45000	-1.55000	-3.06700	H	0.76400	1.74000	3.14500
H	-2.24500	-0.82700	-3.27700	H	1.33200	3.42600	3.08900
H	-0.49400	-1.11800	-3.37800	C	3.35600	1.70200	2.53900
H	-1.62800	-2.45100	-3.67600	H	3.05400	0.88700	3.20200
C	-0.32500	-2.76800	-1.30100	H	4.18600	1.34500	1.92300
H	0.63300	-2.32600	-1.59200	H	3.71100	2.53900	3.16300
H	-0.30500	-2.94100	-0.22100	H	0.63800	2.70100	-3.11800
H	-0.43000	-3.73500	-1.81800	H	0.54000	1.93800	-4.73300
N	2.22500	2.06800	1.67500	H	-0.55600	1.41400	-3.42300

Table 27. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for TMEDA-solvated unsymmetric dimer **1a** with free energies and coordinates.



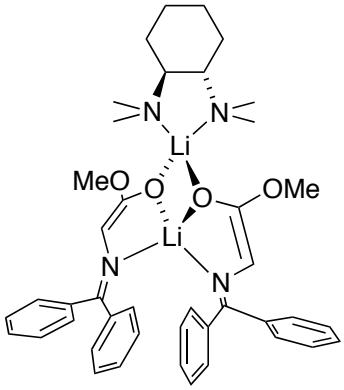


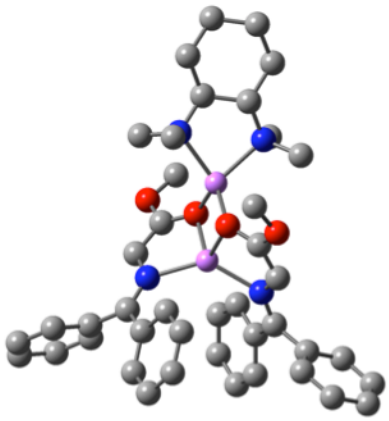
G = -2008.976949
G_{MP2} = -2002.49425

Atom	X	Y	Z	Atom	X	Y	Z
Li	-2.95800	-0.83900	0.22700	C	-1.92500	1.53100	1.58900
O	-1.50900	-1.52700	-0.74700	O	-1.99800	0.25600	1.46100
C	-0.75700	-2.53800	-0.97900	O	-2.67700	2.15400	2.55100
C	0.52100	-2.70500	-0.46100	C	-3.42100	1.32000	3.42900
H	1.13700	-3.56100	-0.71000	H	-3.84000	1.98900	4.18400
N	0.97900	-1.73100	0.39600	H	-4.23800	0.80600	2.90700
C	2.17100	-1.71000	0.92700	H	-2.78500	0.56800	3.90800
C	2.47800	-0.66000	1.92600	H	-1.12300	3.44600	1.06200
C	3.79800	-0.20900	2.12700	C	0.52500	2.49600	-0.86500
C	4.08000	0.80400	3.04100	C	1.25600	1.77800	-1.93300
C	3.05400	1.38900	3.78700	C	0.74600	0.59200	-2.50000
C	1.74100	0.94200	3.61100	C	1.45000	-0.09400	-3.48700
C	1.45700	-0.07200	2.70000	C	2.67900	0.38700	-3.94700
H	0.43800	-0.43200	2.59700	C	3.19300	1.56700	-3.40500
H	0.93500	1.37700	4.19700	C	2.49200	2.25400	-2.41600
H	3.27500	2.17600	4.50300	H	2.91200	3.16400	-1.99800
H	5.10500	1.14100	3.16700	H	4.14800	1.95500	-3.75100
H	4.60400	-0.64700	1.54600	H	3.22300	-0.14400	-4.72400
C	3.24500	-2.69300	0.57600	H	1.02700	-1.00300	-3.90700
C	3.83500	-3.49900	1.56300	H	-0.21800	0.21600	-2.17300
C	4.83500	-4.41400	1.23500	C	0.79000	3.95800	-0.68200
C	5.27200	-4.53100	-0.08600	C	0.56200	4.86700	-1.72800
C	4.70200	-3.72700	-1.07600	C	0.80700	6.23000	-1.55900
C	3.69500	-2.81800	-0.74900	C	1.29300	6.70900	-0.34100
H	3.25900	-2.18800	-1.52000	C	1.53400	5.81500	0.70500
H	5.04600	-3.80300	-2.10500	C	1.28300	4.45400	0.53800
H	6.05600	-5.24000	-0.34200	H	1.47600	3.76100	1.35200
H	5.27600	-5.03400	2.01200	H	1.92200	6.17900	1.65300
H	3.50500	-3.40200	2.59400	H	1.48800	7.77100	-0.20900
Li	-0.44900	-0.22200	0.27600	H	0.61900	6.91800	-2.38000
N	-0.32400	1.82800	-0.12400	H	0.19300	4.49600	-2.68100
C	-1.12100	2.38400	0.84100	O	-1.32800	-3.45700	-1.82300

C	-0.59200	-4.62200	-2.17600	C	-3.68100	0.40200	-2.38800
H	-0.34600	-5.22500	-1.29300	H	-3.17200	-0.49200	-2.75400
H	-1.24000	-5.19800	-2.84100	H	-4.39300	0.75900	-3.15300
H	0.33400	-4.36500	-2.70400	H	-2.92700	1.17700	-2.22400
N	-4.55000	-2.22200	0.74200	H	-6.50000	-2.39100	-0.12500
C	-5.71600	-1.63300	0.05500	H	-6.15300	-0.88500	0.72600
C	-5.34400	-0.97100	-1.27600	C	-4.82500	-2.41300	2.17200
H	-4.91700	-1.72000	-1.95000	H	-5.65800	-3.11600	2.35000
H	-6.26500	-0.59700	-1.75900	H	-3.93000	-2.80600	2.66400
N	-4.34600	0.10000	-1.11100	H	-5.07400	-1.45400	2.63400
C	-4.93200	1.32500	-0.55100	C	-4.15300	-3.50400	0.13600
H	-4.14200	2.06400	-0.39600	H	-3.84300	-3.36400	-0.90000
H	-5.69900	1.75700	-1.21800	H	-3.29200	-3.90400	0.67700
H	-5.39500	1.12300	0.41900	H	-4.97300	-4.24400	0.17800

Table 28. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for (*S,S*)-TMCDA-solvated unsymmetric dimer **1a** with free energies and coordinates.



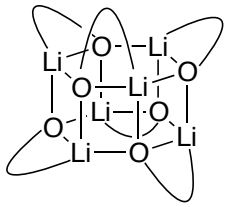


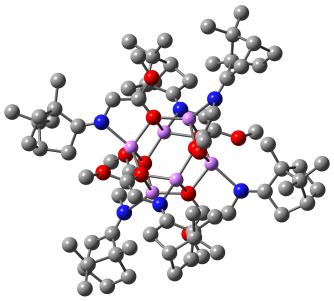
G = -2164.929157
G_{MP2} = -2157.903251

Atom	X	Y	Z	Atom	X	Y	Z
Li	2.39100	0.00000	-0.00100	H	-2.54100	4.42100	2.48800
O	1.17100	0.83000	-1.21200	Li	-0.19300	0.00000	0.00000
C	0.70700	2.00900	-1.43100	N	-0.99700	-1.89600	-0.20700
C	-0.36200	2.60700	-0.77800	C	-0.36200	-2.60700	0.77800
H	-0.68400	3.59600	-1.08600	C	0.70700	-2.00900	1.43100
N	-0.99700	1.89600	0.20600	O	1.17100	-0.83100	1.21100
C	-2.06200	2.30200	0.84900	O	1.27800	-2.78800	2.40700
C	-2.59100	1.46200	1.94800	C	2.13700	-2.14300	3.33600
C	-3.95000	1.51900	2.31700	H	2.33300	-2.88000	4.11800
C	-4.45500	0.70500	3.32900	H	3.08700	-1.84600	2.87700
C	-3.61800	-0.18400	4.00700	H	1.66800	-1.25500	3.77300
C	-2.26500	-0.24400	3.66100	H	-0.68300	-3.59700	1.08600
C	-1.75600	0.57200	2.65200	C	-2.06200	-2.30200	-0.84900
H	-0.69800	0.53300	2.41400	C	-2.59200	-1.46200	-1.94700
H	-1.59800	-0.92200	4.18800	C	-1.75700	-0.57200	-2.65200
H	-4.01200	-0.81600	4.79800	C	-2.26600	0.24400	-3.66100
H	-5.51000	0.76300	3.58600	C	-3.61900	0.18400	-4.00600
H	-4.61700	2.19600	1.79300	C	-4.45600	-0.70500	-3.32800
C	-2.77800	3.57500	0.52100	C	-3.95100	-1.51900	-2.31600
C	-2.94200	4.57800	1.49100	H	-4.61700	-2.19600	-1.79200
C	-3.61200	5.76300	1.18800	H	-5.51100	-0.76200	-3.58400
C	-4.14200	5.96300	-0.08800	H	-4.01400	0.81600	-4.79700
C	-3.99500	4.97000	-1.05900	H	-1.59900	0.92200	-4.18700
C	-3.31800	3.78800	-0.75900	H	-0.69900	-0.53300	-2.41400
H	-3.21000	3.01500	-1.51600	C	-2.77900	-3.57500	-0.52100
H	-4.41300	5.11300	-2.05300	C	-2.94300	-4.57800	-1.49000
H	-4.66800	6.88500	-0.32400	C	-3.61300	-5.76300	-1.18700
H	-3.72300	6.53000	1.95100	C	-4.14200	-5.96300	0.08900

C	-3.99500	-4.96900	1.06000	H	2.89600	-1.27600	-2.53300
C	-3.31800	-3.78800	0.76000	H	5.18100	-1.19600	0.94200
H	-3.21000	-3.01500	1.51600	C	6.49700	-1.26200	-0.75400
H	-4.41200	-5.11300	2.05400	C	7.76300	-0.76500	-0.04400
H	-4.66800	-6.88400	0.32500	C	7.76300	0.76500	0.04500
H	-3.72400	-6.53000	-1.95000	C	6.49700	1.26200	0.75500
H	-2.54200	-4.42000	-2.48800	H	6.51900	0.90200	1.79300
O	1.27700	2.78800	-2.40800	H	6.49300	2.35700	0.80500
C	2.13600	2.14200	-3.33700	H	8.65300	1.12200	0.57800
H	1.66600	1.25500	-3.77500	H	7.81400	1.19000	-0.96800
H	2.33200	2.88000	-4.11900	H	8.65300	-1.12200	-0.57600
H	3.08600	1.84500	-2.87800	H	7.81300	-1.19100	0.96900
N	3.94800	1.26300	0.71800	H	6.49400	-2.35800	-0.80400
C	5.19900	0.77300	0.07200	H	6.52000	-0.90300	-1.79200
C	5.19900	-0.77300	-0.07200	H	5.18200	1.19600	-0.94200
N	3.94800	-1.26200	-0.71900	C	3.91900	1.11700	2.18200
C	3.63900	-2.65600	-0.36100	H	4.57700	1.83400	2.69700
H	2.65700	-2.92000	-0.76400	H	2.89500	1.27700	2.53100
H	4.37800	-3.37400	-0.75600	H	4.21400	0.10600	2.47200
H	3.59000	-2.76200	0.72500	C	3.63900	2.65600	0.36000
C	3.92000	-1.11600	-2.18300	H	3.59000	2.76200	-0.72700
H	4.21600	-0.10500	-2.47300	H	2.65600	2.92000	0.76100
H	4.57900	-1.83300	-2.69800	H	4.37700	3.37400	0.75400

Table 29. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated S_6 hexamer **3a** with free energies and coordinates.





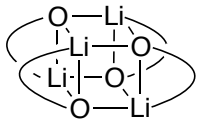
G = -4319.721311
G_{MP2} = -4305.562363

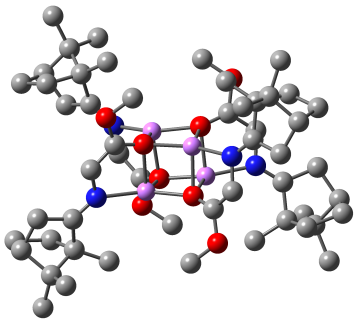
Atom	X	Y	Z	Atom	X	Y	Z
N	3.03800	-1.95100	-1.74700	H	4.25400	-6.63500	-3.43200
C	3.40400	-0.75500	-2.35900	C	5.89300	-2.56100	-3.11400
H	4.16600	-0.72300	-3.12300	H	5.54100	-1.98700	-3.97800
C	2.75400	0.38700	-1.95200	H	6.16300	-1.85100	-2.32600
O	1.86200	0.44900	-1.01000	H	6.80800	-3.07700	-3.43200
Li	1.26500	-1.44200	-0.78300	C	6.54300	-5.54600	-2.19500
Li	0.63700	1.95500	-0.75700	H	7.47600	-4.97200	-2.23700
Li	-2.04400	-0.44100	-0.79100	H	6.71900	-6.39600	-1.52400
Li	-0.68200	-1.92600	1.01700	H	6.36100	-5.95000	-3.19400
Li	1.98200	0.42000	1.00200	C	5.84600	-4.11900	-0.29200
Li	-1.38600	1.52900	0.95900	H	6.78600	-3.56500	-0.40400
O	-0.62900	-1.81900	-1.00300	H	5.11900	-3.43700	0.15800
O	0.55300	1.81400	1.23200	H	6.03400	-4.93400	0.41900
O	-1.27100	1.36600	-1.03200	N	0.05800	3.71000	-1.81400
O	-1.91600	-0.38600	1.21500	C	-1.04900	3.21400	-2.50700
O	1.24100	-1.40500	1.21400	C	0.51000	4.88500	-2.07700
O	3.00500	1.61200	-2.51700	H	-1.44200	3.75800	-3.35800
C	3.88000	1.69000	-3.63400	C	-1.63000	2.04600	-2.07500
H	3.87200	2.73400	-3.95000	C	1.68200	5.57000	-1.37700
H	4.90200	1.39900	-3.36200	C	0.05000	5.88700	-3.08700
H	3.53000	1.05300	-4.45600	O	-2.68700	1.46700	-2.73400
C	3.61300	-3.09300	-1.86800	C	1.01000	6.64700	-0.46000
C	4.85600	-3.57900	-2.64600	C	2.23900	6.46800	-2.55000
C	3.05000	-4.32700	-1.16000	C	2.66400	4.66100	-0.65700
C	4.27600	-4.45700	-3.80500	C	0.84900	7.11700	-2.84100
C	5.38900	-4.68600	-1.64900	H	0.03000	5.50900	-4.11500
C	4.02500	-5.43800	-1.59700	H	-1.11400	6.09700	-2.91300
H	3.03000	-4.18800	-0.07300	C	-3.10900	2.00900	-3.97800
H	2.01500	-4.52400	-1.46500	C	0.44400	7.69900	-1.46300
C	3.73800	-5.73300	-3.08900	H	0.23600	6.19500	0.16800
H	3.49900	-3.91600	-4.35400	H	1.75400	7.08900	0.21300
H	5.06400	-4.70100	-4.52800	C	3.31900	7.48000	-2.13000
H	4.00800	-6.32600	-0.95600	C	2.81100	5.65700	-3.72700
H	2.66800	-5.89400	-3.26300	H	2.19400	4.16000	0.19500

H	3.05600	3.88200	-1.31800
H	3.50800	5.24100	-0.26200
H	0.83700	7.84700	-3.65700
H	-3.89100	1.34300	-4.34700
H	-3.51900	3.02000	-3.85500
H	-2.27900	2.04100	-4.69500
H	-0.64300	7.81100	-1.38300
H	0.87700	8.69000	-1.29900
H	4.23700	6.96300	-1.82700
H	3.57600	8.12800	-2.97700
H	3.02100	8.13000	-1.30300
H	3.78400	5.23000	-3.45600
H	2.16700	4.82800	-4.03300
H	2.97100	6.30300	-4.60000
N	-3.32600	-1.87600	-1.74400
C	-2.37700	-2.71600	-2.33100
C	-4.57800	-2.06500	-1.97300
H	-2.68400	-3.44600	-3.07100
C	-1.06800	-2.61800	-1.92600
C	-5.72900	-1.25300	-1.38100
C	-5.20700	-3.16400	-2.83000
O	-0.07200	-3.38600	-2.47500
C	-6.36800	-2.20700	-0.31700
C	-6.78200	-1.34600	-2.55400
C	-5.38300	0.12600	-0.84700
C	-6.71400	-2.90400	-2.62000
H	-4.91000	-3.07500	-3.88400
H	-4.90000	-4.16600	-2.50200
C	-0.38000	-4.23500	-3.57100
C	-7.04200	-3.32700	-1.16600
H	-5.60400	-2.58900	0.36800
H	-7.10100	-1.66200	0.29000
C	-8.18000	-0.80300	-2.20900
C	-6.32800	-0.64300	-3.84700
H	-4.75100	0.06100	0.04500
H	-4.84600	0.72800	-1.58700
H	-6.29400	0.66300	-0.55600
H	-7.35500	-3.36800	-3.37800
H	0.56600	-4.68200	-3.88200
H	-1.07900	-5.02900	-3.27700
H	-0.80900	-3.66600	-4.40500
H	-6.64200	-4.32200	-0.94200
H	-8.12200	-3.37300	-0.99300
H	-8.15300	0.28700	-2.08900
H	-8.87900	-1.02100	-3.02600
H	-8.60500	-1.22300	-1.29500
H	-6.38800	0.44500	-3.73000
H	-5.29900	-0.88400	-4.12900
H	-6.98200	-0.91700	-4.68500
N	-0.09600	-3.78600	1.92900
C	1.21500	-3.50600	2.32300
C	-0.59300	-4.94800	2.17800
H	1.75800	-4.22600	2.92200
C	1.79600	-2.31800	1.95000
C	-2.00700	-5.41800	1.85200
C	0.11900	-6.13000	2.83800
O	3.07400	-1.98600	2.32900
C	-2.70500	-5.56800	3.24700
C	-1.72500	-6.92800	1.48200
C	-2.78900	-4.57900	0.85600
C	-0.97700	-7.21600	2.82200
H	1.01200	-6.41700	2.26600
H	0.46200	-5.90100	3.85600
C	3.79000	-2.86400	3.18800
C	-2.01800	-6.81100	3.89200
H	-2.57800	-4.65900	3.84300
H	-3.78300	-5.72200	3.11800
C	-2.98600	-7.78500	1.27800
C	-0.85000	-7.10200	0.22700
H	-2.95400	-3.56900	1.24200
H	-2.26800	-4.48600	-0.10200
H	-3.77300	-5.02600	0.66500
H	-0.59400	-8.23600	2.93200
H	4.75300	-2.38700	3.37300
H	3.26000	-3.00800	4.13700
H	3.95300	-3.84000	2.71400
H	-1.53800	-6.57600	4.84900
H	-2.73500	-7.61500	4.08600
H	-3.50800	-7.49200	0.35900
H	-2.70900	-8.84200	1.17000
H	-3.70600	-7.71800	2.09800
H	-1.42200	-6.85200	-0.67500
H	0.04200	-6.46900	0.22700
H	-0.52500	-8.14600	0.12700
N	3.24200	1.78400	2.06800
C	2.29600	2.65800	2.60900
C	4.48600	1.93500	2.36400
H	2.59800	3.37500	3.36200
C	1.00000	2.61000	2.15500
C	5.63900	1.07000	1.86500
C	5.10200	3.02400	3.24200
O	0.02800	3.44200	2.65000
C	6.14400	0.30600	3.13600
C	6.76300	2.16800	1.69700
C	5.33700	0.17700	0.67500
C	6.60700	2.68800	3.16100
H	4.86700	4.02200	2.84900
H	4.72600	2.99800	4.27400

C	0.36800	4.35600	3.68500	O	-3.11900	-1.60800	2.62600
C	6.82200	1.40900	4.00500	C	-3.47600	5.24800	2.97800
H	5.31000	-0.18200	3.65000	C	-5.22800	4.87600	1.33000
H	6.85400	-0.47900	2.85000	C	-2.68500	4.60300	0.60100
C	8.16200	1.61100	1.38400	C	-5.76800	4.49700	2.74600
C	6.44100	3.22200	0.62200	H	-6.04400	2.31900	2.43500
H	4.56200	-0.55600	0.91900	H	-5.23900	2.72200	3.94700
H	4.98600	0.75500	-0.18500	C	-4.10600	-1.74500	3.64000
H	6.23200	-0.38000	0.36900	C	-4.86000	5.31900	3.69100
H	7.26400	3.52100	3.43300	H	-2.71400	4.75300	3.58800
H	-0.54900	4.89600	3.92600	H	-3.09300	6.24500	2.72900
H	0.72900	3.82900	4.57600	C	-5.38600	6.36700	0.98600
H	1.13300	5.06800	3.35000	C	-5.86500	4.07400	0.18200
H	6.36500	1.50100	4.99700	H	-1.70300	4.30100	0.98000
H	7.88500	1.20300	4.16400	H	-2.89200	4.00500	-0.29200
H	8.19100	1.18600	0.37300	H	-2.61100	5.65400	0.29600
H	8.90400	2.41900	1.41600	H	-6.84000	4.66200	2.89700
H	8.49500	0.83400	2.07600	H	-4.10100	-2.79800	3.92500
H	6.54800	2.79100	-0.38100	H	-3.86600	-1.12500	4.51200
H	5.42400	3.61700	0.69300	H	-5.10100	-1.47200	3.26400
H	7.14000	4.06500	0.69100	H	-4.83600	4.89100	4.69900
N	-3.24000	1.98800	1.93600	H	-5.21100	6.35100	3.79200
C	-3.58000	0.74500	2.47800	H	-4.94200	6.58700	0.00800
C	-4.00000	3.00400	2.15000	H	-6.45000	6.62800	0.92600
H	-4.39300	0.67500	3.19100	H	-4.92500	7.04200	1.71200
C	-2.86900	-0.36700	2.09700	H	-5.40700	4.34800	-0.77600
C	-3.75000	4.43000	1.66900	H	-5.75200	2.99300	0.29400
C	-5.33500	3.02100	2.89500	H	-6.93700	4.29800	0.10600

Table 30. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated D_{2d} tetramer **3a** with free energies and coordinates.



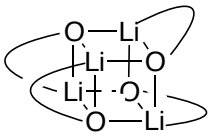


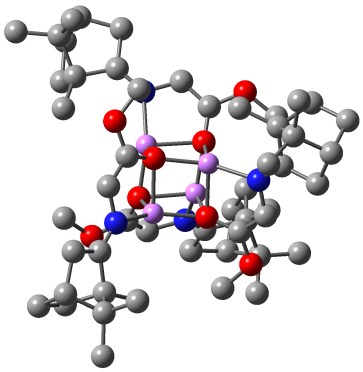
G = -2879.808634
G_{MP2} = -2870.355573

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.88400	3.63000	2.10600	Li	-0.98600	0.87400	-0.96400
O	-2.04100	2.80500	2.12900	O	-0.89400	1.16100	0.99000
C	-1.88000	1.48700	1.78000	Li	1.06100	1.00800	0.82800
C	-2.83300	0.63400	2.27400	O	0.96400	1.01600	-1.13500
H	-3.61200	1.03700	2.91300	C	1.92700	1.23000	-1.98700
N	-2.81400	-0.71400	1.91400	C	2.86400	0.31400	-2.39200
C	-3.80300	-1.47900	2.22700	H	3.62400	0.62400	-3.10200
C	-3.95300	-2.94900	1.84300	N	2.85900	-0.97200	-1.85100
C	-5.03300	-2.94300	0.70900	Li	1.06000	-1.00900	-0.83000
C	-6.35400	-2.57200	1.45000	O	-0.89500	-1.16200	-0.99000
C	-5.89100	-2.39400	2.91800	C	-1.88000	-1.48800	-1.78000
C	-5.07600	-1.08400	2.97000	C	-2.83300	-0.63500	-2.27400
H	-4.85900	-0.76400	3.99800	H	-3.61300	-1.03700	-2.91300
H	-5.59200	-0.24400	2.48500	N	-2.81500	0.71400	-1.91500
C	-4.78700	-3.48800	3.07000	C	-3.80400	1.47900	-2.22700
C	-4.02200	-3.42800	4.40600	C	-3.95400	2.94800	-1.84300
H	-4.70100	-3.60800	5.24800	C	-5.03300	2.94300	-0.70800
H	-3.25000	-4.20700	4.44100	C	-6.35400	2.57200	-1.44900
H	-3.52200	-2.47000	4.57700	C	-5.89200	2.39400	-2.91700
C	-5.31300	-4.92500	2.91100	C	-5.07700	1.08400	-2.97000
H	-4.48800	-5.64700	2.93500	H	-4.86000	0.76400	-3.99800
H	-5.98200	-5.17200	3.74500	H	-5.59200	0.24400	-2.48500
H	-5.86900	-5.09200	1.98600	C	-4.78800	3.48800	-3.07000
H	-6.70000	-2.44400	3.65400	C	-4.02300	3.42800	-4.40500
H	-6.80900	-1.65400	1.06200	H	-4.70300	3.60800	-5.24700
H	-7.10600	-3.36300	1.35700	H	-3.25200	4.20700	-4.44100
H	-4.76500	-2.23400	-0.08100	H	-3.52400	2.47000	-4.57700
H	-5.09300	-3.93200	0.24100	C	-5.31500	4.92500	-2.91000
C	-2.67700	-3.68400	1.47500	H	-4.48900	5.64600	-2.93400
H	-2.22200	-3.24900	0.58000	H	-5.98400	5.17200	-3.74400
H	-1.94400	-3.64800	2.28800	H	-5.87000	5.09200	-1.98500
H	-2.88500	-4.73700	1.25300	H	-6.70100	2.44400	-3.65200
Li	-0.98500	-0.87400	0.96400	H	-6.80900	1.65400	-1.06100

H	-7.10600	3.36200	-1.35500
H	-4.76500	2.23400	0.08100
H	-5.09300	3.93200	-0.24000
C	-2.67800	3.68400	-1.47500
H	-2.22200	3.24800	-0.58000
H	-1.94500	3.64700	-2.28900
H	-2.88500	4.73700	-1.25200
O	-2.04200	-2.80500	-2.12900
C	-0.88500	-3.63000	-2.10600
H	-0.45900	-3.71300	-1.10100
H	-1.21700	-4.61500	-2.44100
H	-0.11700	-3.25500	-2.79500
O	0.96400	-1.01600	1.13300
C	1.92800	-1.23000	1.98600
C	2.86400	-0.31400	2.39100
H	3.62300	-0.62400	3.10100
N	2.85900	0.97200	1.85000
C	3.82000	1.78900	2.11700
C	3.98000	3.19600	1.54900
C	5.16000	3.07100	0.52600
C	6.41700	2.85400	1.42300
C	5.82300	2.85000	2.85300
C	5.03600	1.53000	3.00200
H	4.73800	1.33000	4.04000
H	5.61100	0.65600	2.67000
C	4.68600	3.91800	2.76200
C	3.80700	4.00600	4.02300
H	4.40200	4.33200	4.88500
H	3.00900	4.74600	3.88400
H	3.32700	3.05900	4.28600
C	5.19300	5.33900	2.45900
H	4.35200	6.03300	2.33700
H	5.79700	5.70800	3.29700
H	5.80800	5.40600	1.55800
H	6.55900	3.02000	3.64600
H	6.93200	1.91300	1.20200
H	7.15000	3.65600	1.29300
H	4.98100	2.25000	-0.17500
H	5.24000	3.98700	-0.07100
C	2.73100	3.83500	0.96800
H	2.37100	3.27000	0.10200
H	1.92600	3.88600	1.70800
H	2.93900	4.85500	0.62300
O	2.08000	-2.48900	2.50900
C	0.92200	-3.31000	2.57600
H	0.51800	-3.53400	1.58400
H	1.24400	-4.23800	3.05400
H	0.13800	-2.84300	3.18800
C	3.82000	-1.78900	-2.11700
C	3.98000	-3.19600	-1.54900
C	5.15900	-3.07100	-0.52500
C	6.41600	-2.85300	-1.42100
C	5.82400	-2.85000	-2.85100
C	5.03700	-1.53000	-3.00100
H	4.74000	-1.33000	-4.04000
H	5.61100	-0.65500	-2.66800
C	4.68700	-3.91800	-2.76200
C	5.19400	-5.33800	-2.45800
H	4.35300	-6.03200	-2.33700
H	5.79900	-5.70700	-3.29600
H	5.80800	-5.40600	-1.55700
C	3.80900	-4.00600	-4.02400
H	4.40500	-4.33100	-4.88500
H	3.01100	-4.74600	-3.88500
H	3.32900	-3.05900	-4.28700
H	6.56100	-3.02000	-3.64400
H	6.93200	-1.91200	-1.20000
H	7.14900	-3.65600	-1.29000
H	4.97900	-2.25000	0.17600
H	5.23900	-3.98700	0.07100
C	2.73100	-3.83500	-0.97000
H	2.36900	-3.27000	-0.10400
H	1.92600	-3.88600	-1.71000
H	2.93800	-4.85500	-0.62400
O	2.07900	2.48900	-2.51100
C	0.92100	3.31000	-2.57800
H	0.51800	3.53400	-1.58500
H	1.24200	4.23800	-3.05600
H	0.13700	2.84200	-3.18900
H	-0.45900	3.71300	1.10100
H	-1.21600	4.61500	2.44100
H	-0.11500	3.25500	2.79400

Table 31. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated S_4 tetramer **3a** with free energies and coordinates.



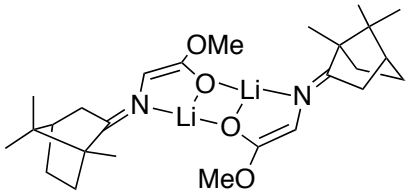


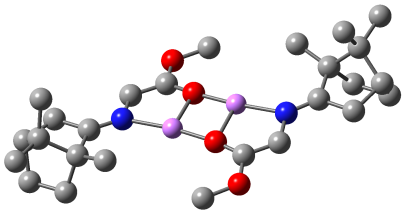
G = -2879.81497
G_{MP2} = -2870.359641

Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.10700	1.25400	-0.34000	H	4.58800	0.82600	6.62400
O	0.85100	1.41900	-0.48000	H	5.60900	3.27600	4.74000
Li	0.94100	-0.37700	-1.26600	H	3.11800	4.01100	5.50900
N	2.30800	-1.82200	-1.90700	H	3.97800	2.95300	6.62000
C	2.26200	-2.76600	-0.88200	H	1.55100	2.24000	5.06900
C	1.50100	-2.52200	0.23300	H	2.42800	1.21300	6.19600
O	0.85100	-1.41900	0.48000	C	2.61000	-0.31000	3.93800
Li	0.94100	0.37700	1.26600	H	1.52200	-0.26900	3.79700
N	2.30800	1.82100	1.90700	H	3.04600	-0.80200	3.06100
C	2.26200	2.76600	0.88200	H	2.79600	-0.94200	4.81500
C	1.50100	2.52200	-0.23300	O	-1.03200	0.46700	1.44600
O	1.39300	3.57000	-1.10800	C	-1.72200	0.16500	2.51200
C	0.97200	3.29700	-2.44400	C	-2.50800	-0.94900	2.66900
H	0.02200	2.75700	-2.47500	H	-3.07500	-1.06600	3.58700
H	0.85200	4.27500	-2.91400	N	-2.51100	-1.93800	1.68600
H	1.73400	2.72800	-2.98700	Li	-1.10700	-1.25400	0.34000
H	2.78700	3.71200	0.96400	O	-1.03200	-0.46700	-1.44600
C	3.06300	2.01400	2.93300	C	-1.72200	-0.16500	-2.51200
C	3.18100	1.08200	4.13200	C	-2.50800	0.94900	-2.66900
C	2.54800	1.87000	5.32800	H	-3.07500	1.06700	-3.58700
C	3.56700	3.01700	5.60700	N	-2.51100	1.93800	-1.68600
C	4.65500	2.78000	4.53200	C	-3.25400	2.98300	-1.80800
C	4.02900	3.17000	3.17400	C	-3.32500	4.13500	-0.81100
H	4.76800	3.23600	2.36500	C	-4.71900	3.97300	-0.11900
H	3.52200	4.14500	3.21200	C	-5.74000	4.32900	-1.24300
C	4.72300	1.22000	4.44400	C	-4.82700	4.64800	-2.45300
C	5.63000	0.69300	3.31700	C	-4.23400	3.30400	-2.93200
H	6.67000	0.99400	3.48900	H	-3.72300	3.39000	-3.90100
H	5.61000	-0.40300	3.28900	H	-4.99600	2.52200	-3.05200
H	5.33800	1.04600	2.32400	C	-3.59800	5.34500	-1.78800
C	5.17900	0.54500	5.75000	C	-2.43700	5.63100	-2.75700
H	5.13300	-0.54700	5.65700	H	-2.75300	6.33600	-3.53700
H	6.22300	0.80600	5.96200	H	-1.59700	6.09200	-2.22300

H	-2.05400	4.73400	-3.25100
C	-3.94100	6.67100	-1.08700
H	-3.06500	7.06700	-0.55900
H	-4.23600	7.42200	-1.83100
H	-4.75500	6.59300	-0.36200
H	-5.31800	5.22400	-3.24500
H	-6.42400	3.50300	-1.46500
H	-6.35900	5.18900	-0.96800
H	-4.84900	2.95600	0.26800
H	-4.80300	4.65300	0.73700
C	-2.15400	4.24700	0.14900
H	-2.09300	3.35900	0.78800
H	-1.19700	4.34600	-0.37400
H	-2.27100	5.11300	0.81200
O	-1.63200	-0.97000	-3.61600
C	-1.27400	-2.33700	-3.43200
H	-2.08200	-2.88900	-2.93600
H	-1.13400	-2.74000	-4.43800
H	-0.34900	-2.45100	-2.86000
C	-3.25400	-2.98300	1.80800
C	-3.32500	-4.13500	0.81100
C	-4.71900	-3.97200	0.11800
C	-5.74000	-4.32900	1.24200
C	-4.82800	-4.64700	2.45300
C	-4.23500	-3.30400	2.93200
H	-3.72400	-3.39000	3.90100
H	-4.99700	-2.52200	3.05100
C	-3.59900	-5.34500	1.78800
C	-3.94100	-6.67100	1.08700
H	-3.06600	-7.06700	0.55900
H	-4.23700	-7.42200	1.83100
H	-4.75500	-6.59300	0.36100
C	-2.43800	-5.63100	2.75700
H	-2.75400	-6.33600	3.53700
H	-1.59800	-6.09200	2.22400
H	-2.05500	-4.73400	3.25100
H	-5.31900	-5.22300	3.24500
H	-6.42400	-3.50300	1.46400
H	-6.36000	-5.18800	0.96700
H	-4.84800	-2.95600	-0.26800
H	-4.80200	-4.65300	-0.73700
C	-2.15400	-4.24700	-0.14900
H	-2.09200	-3.35900	-0.78800
H	-1.19700	-4.34600	0.37400
H	-2.27000	-5.11300	-0.81200
O	-1.63200	0.97000	3.61600
C	-1.27300	2.33700	3.43200
H	-2.08100	2.88900	2.93700
H	-1.13400	2.74000	4.43800
H	-0.34900	2.45100	2.86000
O	1.39300	-3.57000	1.10800
C	0.97200	-3.29700	2.44400
H	0.02300	-2.75700	2.47500
H	0.85200	-4.27500	2.91400
H	1.73400	-2.72800	2.98700
H	2.78700	-3.71200	-0.96400
C	3.06300	-2.01400	-2.93300
C	3.18100	-1.08200	-4.13200
C	2.54900	-1.87100	-5.32800
C	3.56800	-3.01700	-5.60700
C	4.65600	-2.78000	-4.53100
C	4.02900	-3.17000	-3.17400
H	4.76900	-3.23600	-2.36500
H	3.52300	-4.14500	-3.21100
C	4.72300	-1.22000	-4.44400
C	5.17900	-0.54500	-5.74900
H	5.13300	0.54600	-5.65700
H	6.22400	-0.80600	-5.96200
H	4.58800	-0.82600	-6.62400
C	5.62900	-0.69300	-3.31700
H	5.33700	-1.04600	-2.32400
H	6.67000	-0.99400	-3.48900
H	5.61000	0.40300	-3.28900
H	5.60900	-3.27600	-4.74000
H	3.11800	-4.01100	-5.50800
H	3.97900	-2.95400	-6.62000
H	1.55100	-2.24000	-5.06800
H	2.42900	-1.21300	-6.19600
C	2.60900	0.31000	-3.93800
H	1.52200	0.26900	-3.79700
H	3.04600	0.80200	-3.06200
H	2.79500	0.94100	-4.81500

Table 32. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for unsolvated dimer **3a** with free energies and coordinates.

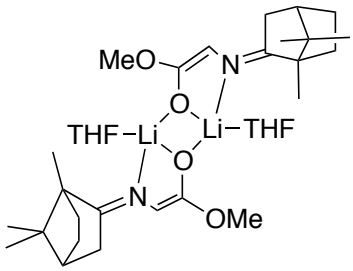


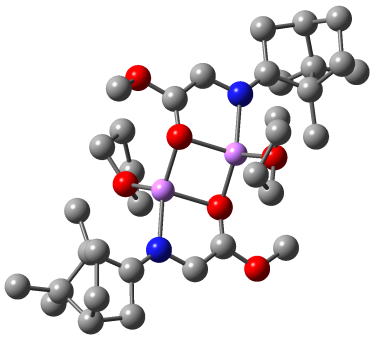


G = -1439.889472
G_{MP2} = -1435.140233

Atom	X	Y	Z	Atom	X	Y	Z
C	0.84200	3.86500	-0.56500	H	6.66100	-0.82900	-2.20200
O	-0.56200	3.65000	-0.53400	H	7.70200	0.34400	-1.40700
C	-1.00200	2.36600	-0.38500	H	4.87000	0.77300	-2.16900
C	-2.37300	2.21300	-0.35900	H	5.93700	1.92300	-1.36800
H	-3.01100	3.08600	-0.44800	C	3.93100	1.75300	0.49000
N	-2.90000	0.93600	-0.21000	H	3.16500	1.96800	-0.26500
Li	-1.23300	-0.20500	-0.22300	H	3.41800	1.50600	1.42700
O	-0.14500	1.40300	-0.28400	H	4.49500	2.68000	0.64500
Li	1.23300	0.20500	-0.22100	C	-4.17200	0.73600	-0.13100
N	2.90000	-0.93600	-0.21000	C	-4.84000	-0.62400	0.03300
C	2.37300	-2.21300	-0.35900	C	-5.56300	-0.89200	-1.32900
C	1.00200	-2.36600	-0.38500	C	-6.72500	0.14700	-1.34800
O	0.14500	-1.40300	-0.28200	C	-6.54000	0.89800	-0.00600
O	0.56200	-3.64900	-0.53500	C	-5.28000	1.78000	-0.15900
C	-0.84200	-3.86500	-0.56500	H	-5.16500	2.50300	0.66000
H	-1.31600	-3.33400	-1.39900	H	-5.28600	2.36300	-1.08900
H	-0.97000	-4.94100	-0.70200	C	-6.05600	-0.23000	0.96100
H	-1.32000	-3.55700	0.37200	C	-7.09100	-1.34700	1.17700
H	3.01100	-3.08600	-0.45000	H	-6.67000	-2.15500	1.78700
C	4.17200	-0.73600	-0.13100	H	-7.95900	-0.95300	1.72100
C	4.84000	0.62400	0.03400	H	-7.46200	-1.79300	0.25100
C	5.56200	0.89400	-1.32900	C	-5.63000	0.27400	2.35200
C	6.72500	-0.14600	-1.34900	H	-6.48300	0.72600	2.87400
C	6.54100	-0.89800	-0.00700	H	-5.27700	-0.55800	2.97200
C	5.28000	-1.77900	-0.16000	H	-4.82700	1.01600	2.31900
H	5.16600	-2.50300	0.65800	H	-7.42800	1.44500	0.32700
H	5.28500	-2.36200	-1.09200	H	-6.66200	0.83200	-2.20000
C	6.05600	0.23000	0.96100	H	-7.70300	-0.34200	-1.40600
C	5.63100	-0.27600	2.35200	H	-4.87100	-0.77100	-2.17000
H	6.48500	-0.72900	2.87300	H	-5.93800	-1.92200	-1.36900
H	5.27800	0.55600	2.97300	C	-3.93100	-1.75300	0.48800
H	4.82900	-1.01800	2.31800	H	-3.16600	-1.96800	-0.26800
C	7.09100	1.34700	1.17800	H	-3.41700	-1.50700	1.42500
H	6.67000	2.15400	1.78900	H	-4.49600	-2.68000	0.64200
H	7.95900	0.95200	1.72000	H	1.31500	3.33400	-1.39900
H	7.46100	1.79400	0.25200	H	0.97000	4.94100	-0.70200
H	7.42900	-1.44500	0.32500	H	1.32000	3.55700	0.37200

Table 33. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for THF-disolvated dimer **3a** with free energies and coordinates.



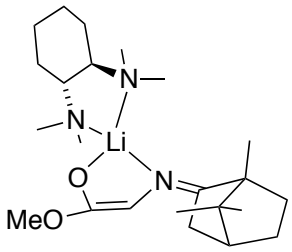


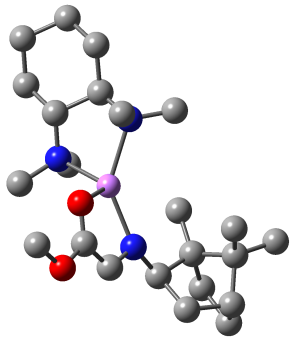
G = -1904.602584
G_{MP2} = -1898.323025

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.77600	-0.44300	-3.98300	C	-5.96200	-1.83100	0.97800
O	0.34600	-1.07700	-3.37600	H	-5.14400	-1.71800	1.69500
C	0.81700	-0.50200	-2.21100	H	-6.87900	-2.04500	1.54200
C	2.17700	-0.63200	-2.02300	H	-5.74100	-2.71700	0.37100
H	2.77700	-1.09900	-2.79800	H	-7.36900	0.71800	1.45700
N	2.75300	-0.12500	-0.86200	H	-6.19700	2.79100	0.16100
Li	1.07700	0.76600	0.09200	H	-7.38200	1.87700	-0.76400
O	-0.01600	0.07000	-1.41400	H	-4.46900	1.99300	-1.30900
Li	-1.16100	-0.57500	-0.00200	H	-5.68100	1.08700	-2.21100
N	-2.82200	0.32700	0.94800	C	-4.01500	-0.95000	-1.45100
C	-2.26800	0.75900	2.14500	H	-3.12000	-0.43200	-1.81400
C	-0.90700	0.62500	2.34200	H	-3.68100	-1.85700	-0.93600
O	-0.06200	0.14600	1.49400	H	-4.60400	-1.24400	-2.32900
O	-0.46700	1.04500	3.57300	O	-1.17300	-2.57700	0.08300
C	0.91000	0.86000	3.87300	C	-0.78000	-3.45800	-0.98900
H	1.55000	1.49500	3.25100	C	0.49000	-4.13200	-0.47800
H	1.02100	1.15000	4.92100	C	0.15600	-4.34900	1.00900
H	1.21700	-0.18300	3.74300	C	-0.76200	-3.15600	1.35000
H	-2.88200	1.16300	2.94500	H	-0.24900	-2.36600	1.90400
C	-4.09300	0.39800	0.74200	H	-1.65500	-3.46100	1.90600
C	-4.81100	-0.04200	-0.53100	H	1.04600	-4.37600	1.64400
C	-5.29700	1.28400	-1.20300	H	-0.37800	-5.29600	1.14400
C	-6.41900	1.79900	-0.24900	H	1.33700	-3.44800	-0.59900
C	-6.44800	0.72300	0.86400	H	0.71700	-5.06300	-1.00700
C	-5.16300	0.91100	1.70000	H	-1.58000	-4.19100	-1.17200
H	-5.17500	0.33000	2.63300	H	-0.63400	-2.85000	-1.88300
H	-5.00200	1.95900	1.99100	O	1.18800	2.75400	-0.03100
C	-6.15700	-0.59700	0.07900	C	0.03300	3.53800	0.36000
C	-7.23800	-0.95300	-0.95600	C	-0.45600	4.19500	-0.92800
H	-6.94400	-1.83700	-1.53500	C	0.86700	4.47200	-1.66000
H	-8.17900	-1.20000	-0.44700	C	1.71500	3.24800	-1.29200
H	-7.45300	-0.15200	-1.66700	H	2.77500	3.48300	-1.15500

H	1.62400	2.44400	-2.02900	H	7.75600	-1.21500	1.73300
H	1.32700	5.39100	-1.27700	H	7.43400	0.51600	1.61600
H	0.74900	4.58100	-2.74200	C	5.28400	-2.16200	1.12600
H	-1.04500	5.09800	-0.74100	H	4.43800	-2.46200	0.50000
H	-1.07200	3.49100	-1.49800	H	6.05200	-2.94300	1.05300
H	-0.69100	2.86400	0.82200	H	4.93200	-2.15100	2.16400
H	0.34900	4.28700	1.09900	H	7.16400	-1.39100	-1.00900
C	4.02100	-0.23100	-0.65700	H	6.69100	1.10600	-1.94500
C	4.77500	0.33000	0.54400	H	7.73000	1.00300	-0.53000
C	5.63600	1.50500	-0.03000	H	5.01400	2.19500	-0.61000
C	6.72000	0.79300	-0.89600	H	6.08300	2.08600	0.78500
C	6.35500	-0.70300	-0.74300	C	3.92100	0.71800	1.73800
C	5.05200	-0.92500	-1.54300	H	3.24100	1.53600	1.47500
H	4.80800	-1.98900	-1.67400	H	3.31000	-0.12200	2.08600
H	5.10100	-0.49300	-2.55100	H	4.54400	1.06300	2.57200
C	5.86900	-0.79200	0.74000	H	-0.54000	0.59300	-4.26100
C	6.96300	-0.45800	1.77000	H	-0.99000	-1.01800	-4.88700
H	6.55400	-0.46800	2.78800	H	-1.65300	-0.44300	-3.33200

Table 34. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for (*R,R*)-TMCDA monomer of **3a** with free energies and coordinates.



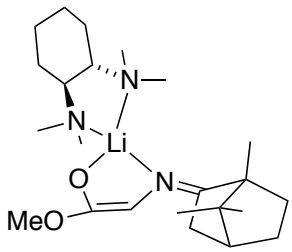


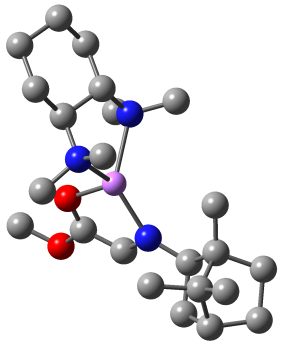
G = -1224.010821
G_{MP2} = -1219.832348

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.80900	5.00600	-0.81100	C	-1.55000	-0.84200	2.36800
O	0.33700	4.32800	-0.31300	H	-1.44200	-1.81700	1.88400
C	0.25100	2.95700	-0.26400	H	-0.56400	-0.53900	2.73200
O	-0.80800	2.36100	-0.63000	H	-2.21500	-0.95700	3.23900
C	1.41400	2.31600	0.21200	C	-2.19200	1.45800	2.08700
N	1.46300	0.96700	0.27600	H	-2.43700	2.22500	1.34900
Li	-0.52000	0.54300	-0.10100	H	-2.96800	1.43400	2.87100
N	-2.02100	0.16400	1.40800	H	-1.24300	1.73900	2.55500
C	-3.23500	-0.23000	0.64100	C	2.72800	0.44400	0.78400
C	-4.38600	-0.77400	1.52100	C	2.93400	-1.10900	0.65400
H	-4.04500	-1.67300	2.05000	C	4.06100	-1.44800	1.67500
C	-5.63400	-1.14000	0.70800	C	5.35300	-0.86300	1.02700
H	-6.05100	-0.23800	0.23700	C	4.82000	-0.26100	-0.29400
H	-6.41200	-1.53300	1.37500	C	4.01800	1.00400	0.06900
C	-5.28300	-2.16300	-0.37700	H	3.73300	1.56900	-0.82300
H	-6.16600	-2.41000	-0.97900	H	4.59500	1.68000	0.71000
H	-4.95400	-3.10000	0.09600	C	3.70300	-1.26400	-0.71300
C	-4.17200	-1.61800	-1.28200	C	2.91000	-0.82300	-1.95800
C	-2.89700	-1.23200	-0.49600	H	3.58100	-0.73500	-2.82300
H	-2.51500	-2.14600	-0.02300	H	2.15500	-1.57700	-2.21300
N	-1.78100	-0.74100	-1.35700	H	2.38900	0.12600	-1.82400
C	-1.08300	-1.84700	-2.02400	C	4.22500	-2.68400	-1.00400
H	-1.71600	-2.38200	-2.75300	H	3.39300	-3.37200	-1.20100
H	-0.21600	-1.45000	-2.56000	H	4.85300	-2.67500	-1.90400
H	-0.72500	-2.56800	-1.28200	H	4.82100	-3.11600	-0.19600
C	-2.18900	0.25500	-2.36500	H	5.59700	-0.08700	-1.04800
H	-1.29100	0.70100	-2.80100	H	5.82700	-0.09800	1.65200
H	-2.79100	-0.18400	-3.17600	H	6.10400	-1.63900	0.85000
H	-2.74900	1.06600	-1.89700	H	3.84800	-1.01500	2.65900
H	-3.91800	-2.35200	-2.05600	H	4.14000	-2.53200	1.82000
H	-4.55700	-0.73200	-1.80500	C	1.68500	-1.95300	0.85900
H	-4.63700	-0.03400	2.29100	H	1.28900	-1.82400	1.87300
H	-3.58700	0.69700	0.16800	H	0.89400	-1.67800	0.15600

H	1.90500	-3.02000	0.72700	H	-0.55200	6.06800	-0.79900
H	2.78000	0.69500	1.85900	H	-1.04900	4.69300	-1.83300
H	2.25800	2.94600	0.49600	H	-1.68800	4.83200	-0.17900

Table 35. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for (*S,S*)-TMCDA monomer of **3a** with free energies and coordinates.



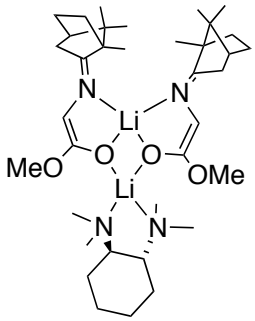


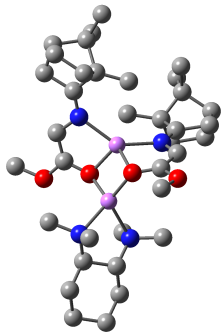
G = -1224.010058
G_{MP2} = -1219.831969

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.48400	0.39600	0.04500	C	1.89200	-1.84600	1.04200
N	1.44600	1.00800	0.31600	H	1.56400	-1.63900	2.06800
C	1.28800	2.34700	0.24400	H	1.03300	-1.69200	0.38300
C	0.04200	2.88600	-0.13900	H	2.16900	-2.90700	0.99500
O	-0.99000	2.19800	-0.41100	H	2.92500	0.90800	1.77300
O	0.00900	4.25800	-0.20500	N	-1.93900	-0.29400	1.55300
C	-1.23400	4.83400	-0.58300	C	-3.02800	-0.97200	0.78800
H	-1.06800	5.91400	-0.59200	C	-3.01500	-0.57900	-0.71400
H	-1.54700	4.49800	-1.57800	N	-1.66300	-0.76200	-1.31800
H	-2.02700	4.58800	0.13200	C	-1.51800	-0.02600	-2.58500
H	2.09900	3.04400	0.46000	H	-0.47800	-0.10500	-2.92000
C	2.78300	0.58900	0.72500	H	-2.16200	-0.41900	-3.38900
C	3.06500	-0.95500	0.66200	H	-1.73600	1.03000	-2.41600
C	4.30600	-1.17100	1.57900	C	-1.25900	-2.16100	-1.50600
C	5.48900	-0.55700	0.77100	H	-1.35900	-2.72300	-0.57400
C	4.79500	-0.06600	-0.52000	H	-1.83500	-2.68000	-2.28900
C	3.95900	1.17400	-0.14700	H	-0.20500	-2.18400	-1.79900
H	3.55300	1.67000	-1.03400	H	-3.20700	0.50000	-0.77500
H	4.55400	1.91800	0.39400	C	-4.14300	-1.31500	-1.47500
C	3.70400	-1.15200	-0.76600	C	-5.52600	-1.09800	-0.84800
C	2.76900	-0.83000	-1.94800	C	-5.52200	-1.53800	0.62000
H	3.35000	-0.74100	-2.87600	C	-4.43600	-0.78300	1.39700
H	2.05100	-1.64800	-2.09900	H	-4.69300	0.28300	1.39900
H	2.19500	0.08600	-1.80600	H	-4.42400	-1.10500	2.44600
C	4.27800	-2.55800	-1.02700	H	-6.50100	-1.36100	1.08200
H	3.47300	-3.30200	-1.08000	H	-5.33900	-2.62100	0.67700
H	4.79700	-2.57800	-1.99400	H	-6.28400	-1.65100	-1.41700
H	4.98800	-2.89800	-0.27000	H	-5.80100	-0.03500	-0.91000
H	5.48200	0.10200	-1.35800	H	-4.15100	-0.99200	-2.52300
H	5.97800	0.26800	1.30200	H	-3.93400	-2.39400	-1.48200
H	6.26500	-1.30100	0.56000	H	-2.80000	-2.04400	0.84300
H	4.16500	-0.69200	2.55400	C	-2.30200	1.02500	2.10200
H	4.46400	-2.23800	1.77300	H	-3.03100	0.96000	2.92600

H	-1.39400	1.50100	2.48700	H	-1.06500	-2.09400	2.22500
H	-2.69200	1.67000	1.31400	H	-0.58100	-0.64200	3.11400
C	-1.42500	-1.14500	2.63200	H	-2.18100	-1.36000	3.40800

Table 36. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for (*R,R*)-TMCDA-solvated unsymmetric dimer **3a** with free energies and coordinates.



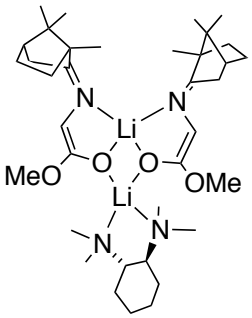


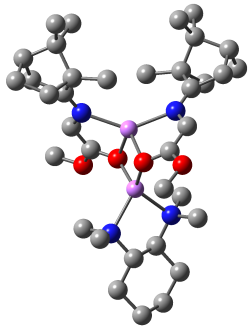
G = -1943.400516
G_{MP2} = -1936.88612

Atom	X	Y	Z	Atom	X	Y	Z
C	1.50100	-0.61000	4.30000	N	-1.49900	-1.78500	-0.68400
O	0.92000	0.60100	3.83300	C	-0.74600	-2.04400	-1.82900
C	0.46700	0.61000	2.53500	C	0.44100	-1.35500	-1.98200
C	-0.32500	1.69200	2.20200	O	0.90400	-0.49400	-1.15000
H	-0.55400	2.44400	2.95200	Li	2.09800	-0.40400	0.31600
N	-0.80400	1.78100	0.90100	O	0.80600	-0.35100	1.74400
C	-1.47400	2.80300	0.49500	N	3.74000	-1.76300	0.22200
C	-1.87100	4.03800	1.29900	C	4.86100	-0.96600	-0.35200
C	-2.58600	4.89200	0.22800	C	4.90200	0.46800	0.24000
C	-1.48600	5.42100	-0.72600	C	6.05800	1.28400	-0.38200
C	-1.06300	4.14200	-1.51100	C	7.41600	0.58700	-0.23500
C	-1.98200	3.01600	-0.92900	C	7.36900	-0.81100	-0.86100
C	-3.31200	3.81600	-0.64500	C	6.24500	-1.64500	-0.23200
C	-4.00100	4.39500	-1.89300	H	6.20700	-2.63900	-0.69300
H	-4.43100	3.59300	-2.50500	H	6.48300	-1.80100	0.82900
H	-4.82700	5.05400	-1.59500	H	7.20400	-0.72100	-1.94400
H	-3.33600	4.97700	-2.53600	H	8.33000	-1.32600	-0.73300
C	-4.37000	3.00200	0.12200	H	8.20100	1.19400	-0.70300
H	-5.18300	3.65400	0.46700	H	7.67900	0.50200	0.83000
H	-4.81700	2.24400	-0.53200	H	5.86100	1.43700	-1.45100
H	-3.96600	2.48100	0.99400	H	6.08900	2.28000	0.07600
C	-2.05900	1.77400	-1.80200	H	5.11300	0.37200	1.31400
H	-1.06600	1.33200	-1.94000	N	3.57200	1.13200	0.16100
H	-2.70100	1.00400	-1.36000	C	3.24900	1.70200	-1.15900
H	-2.45500	2.01900	-2.79500	H	3.38900	0.95600	-1.94400
H	-0.00600	3.88800	-1.37700	H	2.19200	1.98100	-1.16800
H	-1.23000	4.25400	-2.58900	H	3.85000	2.59500	-1.39600
H	-1.87000	6.19800	-1.39500	C	3.39600	2.15300	1.20300
H	-0.65500	5.86500	-0.16700	H	3.58100	1.71400	2.18900
H	-3.23500	5.67200	0.64100	H	4.06600	3.02100	1.07300
H	-1.00200	4.55200	1.73400	H	2.36200	2.50800	1.18900
H	-2.52800	3.77700	2.14000	H	4.62600	-0.87300	-1.42000
Li	-0.45000	-0.18600	0.20900	C	3.97000	-2.25300	1.58800

H	3.02600	-2.64100	1.98400	C	-4.88900	-2.47900	0.18000
H	4.72100	-3.05900	1.63900	C	-5.29400	-1.42000	-0.86200
H	4.29400	-1.43700	2.23900	H	-6.19700	-1.73600	-1.39900
C	3.34400	-2.87800	-0.65100	H	-5.52600	-0.46800	-0.37000
H	4.12400	-3.65200	-0.74000	H	-4.51500	-1.22000	-1.60200
H	2.44600	-3.34900	-0.23800	C	-6.03100	-2.56600	1.20700
H	3.09400	-2.49700	-1.64400	H	-6.22000	-1.58500	1.65900
O	1.26100	-1.54200	-3.07500	H	-6.96000	-2.87800	0.71000
C	0.82200	-2.39600	-4.12200	H	-5.84400	-3.27100	2.02100
H	1.59000	-2.34700	-4.89700	H	-5.28500	-4.36400	-0.99900
H	0.71800	-3.43500	-3.78100	H	-3.30400	-5.46100	0.48700
H	-0.13700	-2.05900	-4.53500	H	-4.80000	-5.11100	1.34400
H	-1.09000	-2.77400	-2.55200	H	-2.19000	-3.76100	1.77700
C	-2.58700	-2.42600	-0.43800	H	-3.70100	-3.45000	2.62700
C	-3.45700	-2.24100	0.80100	C	-3.21900	-0.97000	1.59800
C	-3.25500	-3.55400	1.63000	H	-2.20600	-0.95000	2.01600
C	-3.97700	-4.65100	0.78800	H	-3.33500	-0.07300	0.98100
C	-4.49100	-3.85800	-0.43900	H	-3.91800	-0.89700	2.44000
C	-3.25100	-3.50400	-1.29000	H	0.81400	-1.45700	4.18700
H	-3.51500	-3.12000	-2.28500	H	2.43400	-0.84600	3.77800
H	-2.59500	-4.37100	-1.45400	H	1.70900	-0.44500	5.36000

Table 37. Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for (*S,S*)-TMCDA-solvated unsymmetric dimer **3a** with free energies and coordinates.





G = -1943.399557
G_{MP2} = -1936.884642

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.43900	-0.11600	0.17900	H	-3.18600	-3.92600	2.46500
N	-0.90600	1.80300	0.93300	C	-2.97100	-1.30900	1.71500
C	-0.38100	1.72900	2.21700	H	-1.92500	-1.25900	2.04000
C	0.45200	0.67000	2.52200	H	-3.20900	-0.35800	1.22700
O	0.81300	-0.26600	1.71300	H	-3.58800	-1.39300	2.61800
Li	2.09100	-0.29000	0.28300	H	-1.05000	-2.50300	-2.75500
O	0.92000	-0.30200	-1.20000	O	1.22600	-1.11500	-3.24300
C	0.45600	-1.08800	-2.10200	C	0.79100	-1.89800	-4.34400
C	-0.69500	-1.84400	-1.97100	H	1.52700	-1.74400	-5.13700
N	-1.38800	-1.74900	-0.76600	H	0.74900	-2.96600	-4.09000
C	-2.42700	-2.46900	-0.52800	H	-0.19800	-1.57800	-4.69700
C	-3.19500	-2.49500	0.79100	N	3.54900	1.22000	0.05600
C	-2.82400	-3.87500	1.43100	C	4.76700	0.50700	-0.42100
C	-3.53700	-4.92000	0.51900	C	6.05900	1.35400	-0.35700
C	-4.22300	-4.03400	-0.54900	C	7.28700	0.60100	-0.88500
C	-3.09800	-3.48200	-1.45300	C	7.48300	-0.71100	-0.11700
H	-3.48300	-2.99700	-2.36100	C	6.22000	-1.57700	-0.20800
H	-2.40500	-4.26600	-1.78800	C	4.96100	-0.84600	0.31300
C	-4.65800	-2.77500	0.27000	H	5.13100	-0.61900	1.37400
C	-5.23300	-1.63800	-0.59300	N	3.72100	-1.67200	0.28500
H	-6.15500	-1.96200	-1.09200	C	3.65900	-2.61700	1.40700
H	-5.48900	-0.77400	0.03200	H	2.67700	-3.09900	1.41500
H	-4.54000	-1.28700	-1.36200	H	4.42900	-3.40600	1.35100
C	-5.68900	-3.07900	1.37100	H	3.77800	-2.08000	2.35200
H	-5.89200	-2.18200	1.96700	C	3.48700	-2.39000	-0.98000
H	-6.64000	-3.38900	0.91900	H	3.50700	-1.70000	-1.82600
H	-5.38300	-3.86900	2.06100	H	4.21500	-3.19900	-1.15300
H	-5.02900	-4.53400	-1.09700	H	2.48700	-2.83300	-0.94900
H	-2.83500	-5.62500	0.06100	H	6.35900	-2.51100	0.34900
H	-4.26500	-5.51700	1.07800	H	6.06900	-1.85800	-1.25800
H	-1.73800	-4.00900	1.46600	H	7.70800	-0.48800	0.93600

H	8.34400	-1.26500	-0.51000	C	-1.84600	5.41700	-0.62900
H	7.15700	0.38100	-1.95500	C	-1.37800	4.17200	-1.44300
H	8.17800	1.23500	-0.80200	C	-2.21000	2.98900	-0.84300
H	6.25300	1.64300	0.68500	C	-3.57300	3.70800	-0.50400
H	5.91400	2.28400	-0.91800	C	-4.33800	4.25700	-1.72100
H	4.56900	0.28100	-1.47700	H	-4.74000	3.43600	-2.32800
C	3.03700	2.17400	-0.94000	H	-5.19100	4.86100	-1.38800
H	3.73200	3.01100	-1.12800	H	-3.73100	4.88300	-2.37900
H	2.83300	1.65100	-1.87700	C	-4.55400	2.82700	0.29100
H	2.09100	2.58700	-0.57800	H	-5.38200	3.43100	0.68300
C	3.68600	1.88100	1.36300	H	-4.99100	2.05800	-0.35700
H	2.69700	2.21400	1.69100	H	-4.08500	2.31300	1.13400
H	4.06700	1.17800	2.11000	C	-2.24500	1.75500	-1.72800
H	4.35300	2.75800	1.33800	H	-1.23300	1.37900	-1.91200
O	0.91200	0.65000	3.81900	H	-2.81900	0.94100	-1.27100
C	1.66600	-0.48400	4.21700	H	-2.69500	1.98500	-2.70200
H	1.13900	-1.42000	4.00200	H	-0.30400	3.97900	-1.35000
H	2.64700	-0.51600	3.72700	H	-1.58900	4.28500	-2.51400
H	1.80900	-0.37900	5.29600	H	-2.29600	6.17700	-1.27500
H	-0.62200	2.46300	2.98000	H	-1.02200	5.90200	-0.09300
C	-1.64200	2.79200	0.56000	H	-3.55700	5.55400	0.79900
C	-2.08000	3.99400	1.39100	H	-1.22800	4.55300	1.80200
C	-2.88000	4.81600	0.35500	H	-2.69200	3.68600	2.25100

VII. Full author list for reference 20:

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