Direct Observation of a Lithiated Oxirane: A Synergistic Study Using Spectroscopic, Crystallographic, and Theoretical Methods on the Structure and Stereodynamics of Lithiated *ortho*-Trifluoromethyl Styrene Oxide

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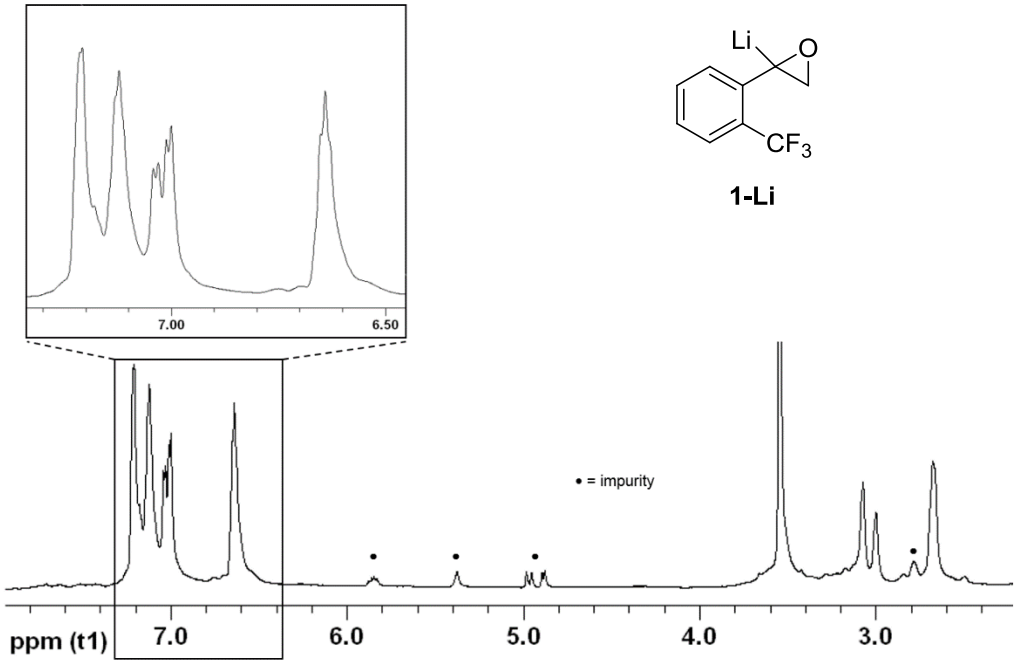

Figure S1. ^{1}H NMR spectrum of 0.2 M solution of **1-Li** in THF-d_8 at 173 K.

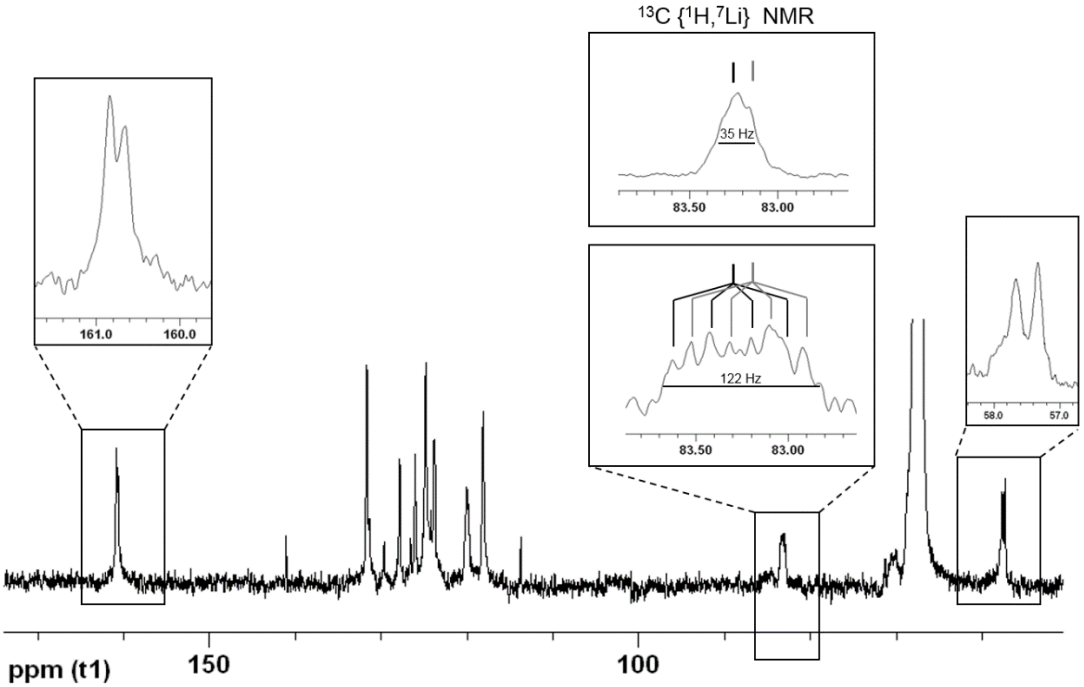

Figure S2. ^{13}C {^{1}H} NMR spectrum of 0.2 M solution of **1-Li** in THF-d_8 at 173 K.

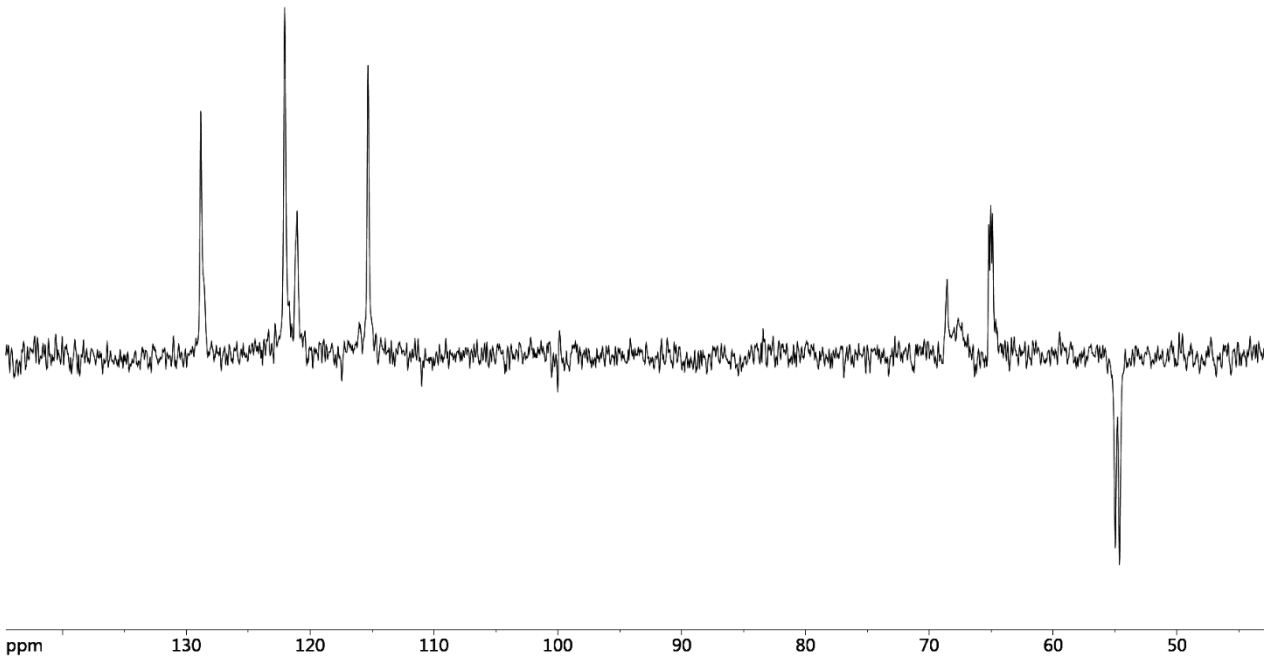

Figure S3. ^{13}C DEPT experiment of 0.2 M solution of **1-Li** in THF-d_8 at 173 K.

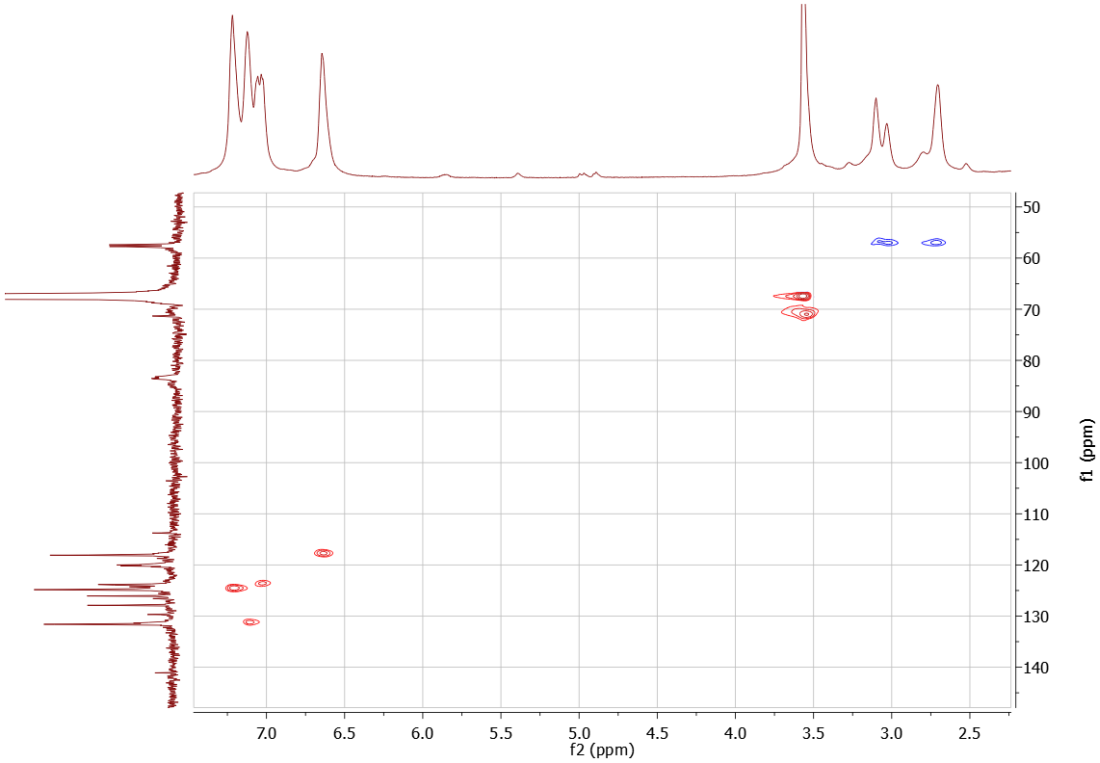

Figure S4. (^{1}H,^{13}C) HSQC-DEPT experiment of 0.2 M solution of **1-Li** in THF-d_8 at 173 K.

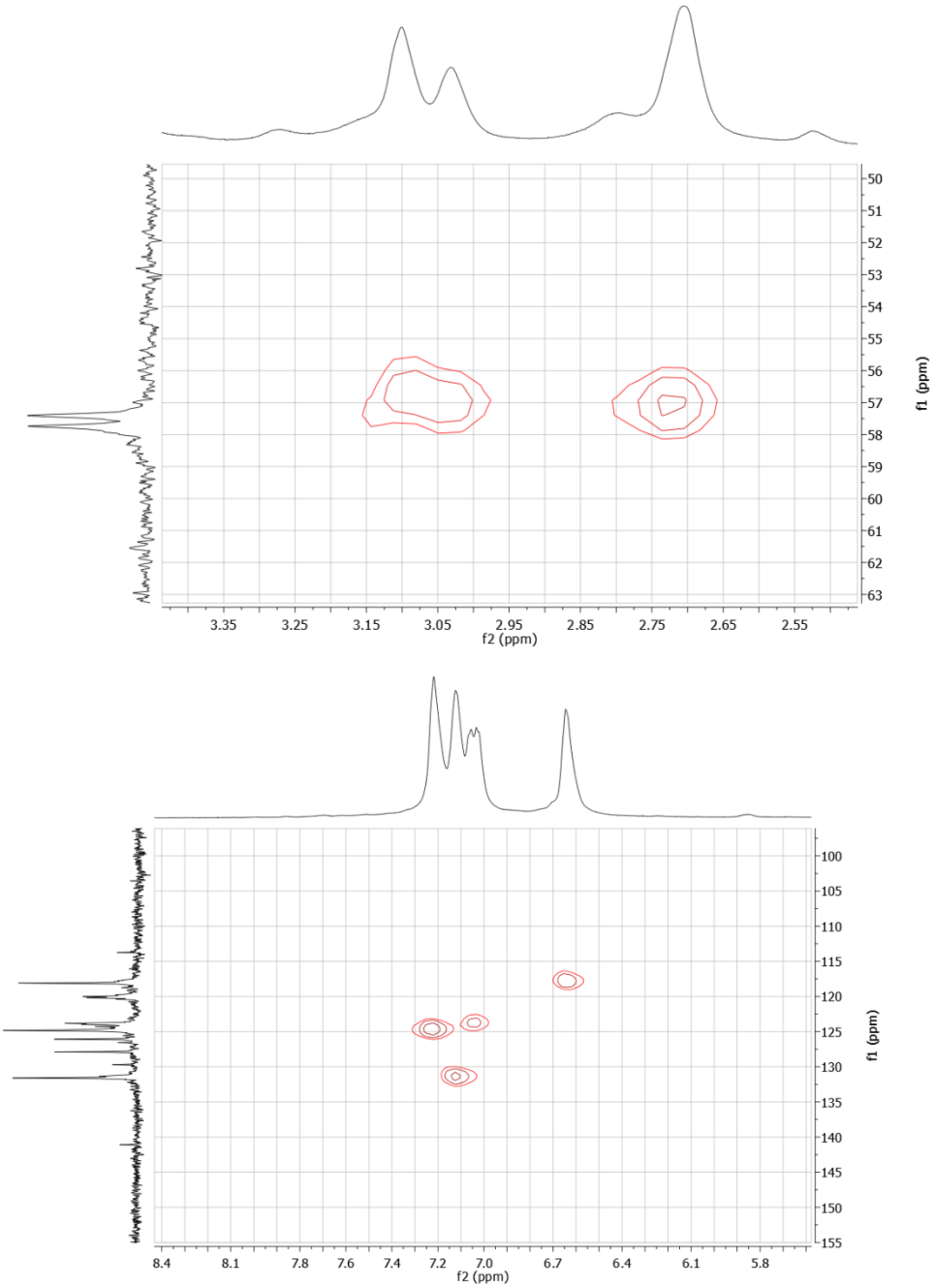

Figure S5. (^{1}H,^{13}C) HSQC-DEPT experiment of 0.2 M solution of **1-Li** in THF-d_8 at 173 K.

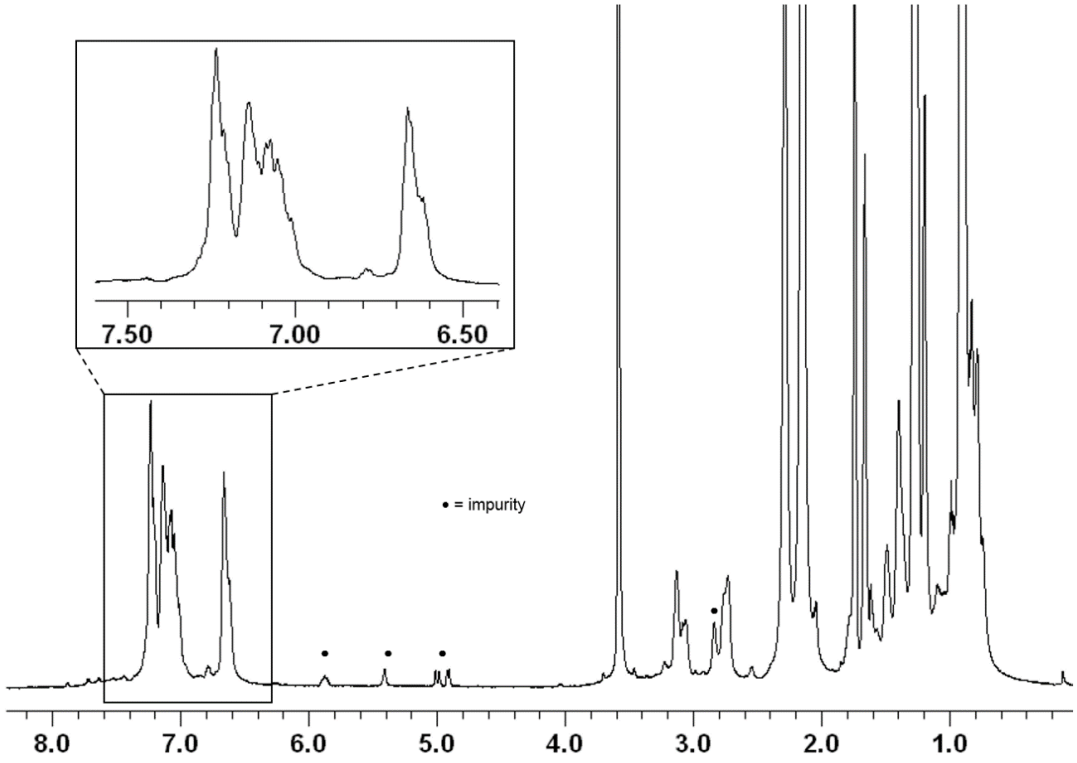

Figure S6. ^{1}H NMR experiment of 0.2 M solution of **1-Li** in THF-d_8 /TMEDA at 173 K.

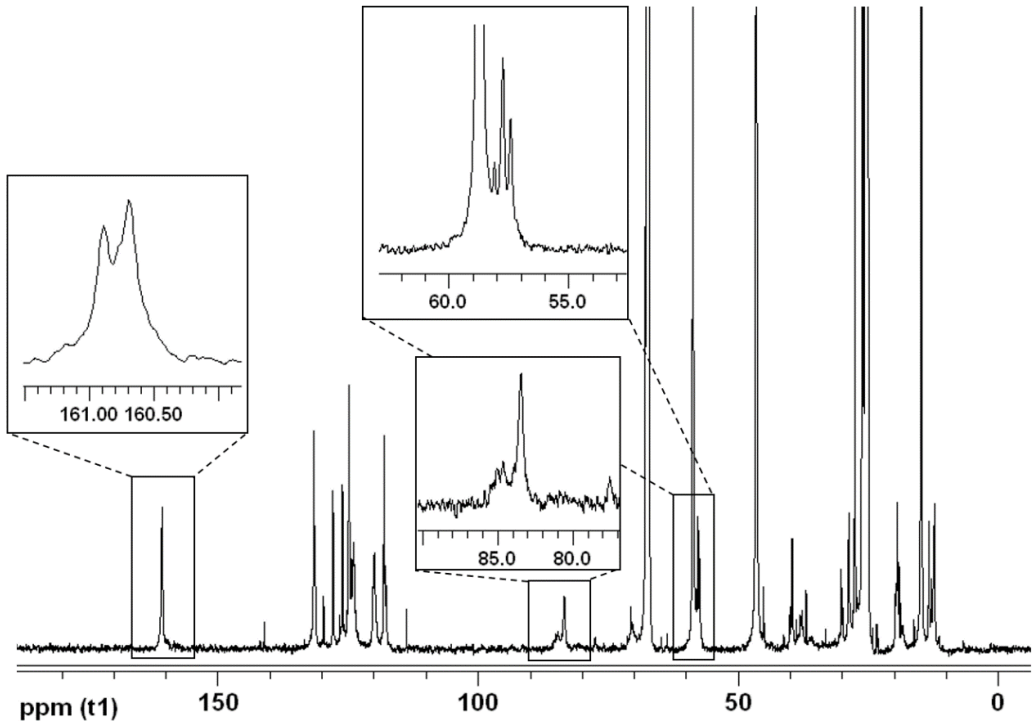

Figure S7. ^{13}C {^{1}H,^{7}Li} NMR spectrum of 0.2 M solution of **1-Li** in THF-d_8/TMEDA at 173 K.

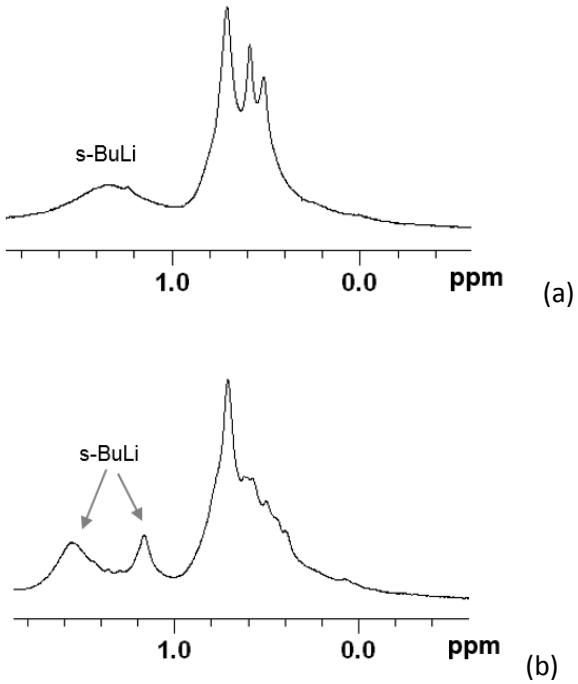

Figure S8. ^{7}Li NMR spectra of 0.2 M solution of **1-Li** in (a) THF-d_8 and (b) THF-d_8 /TMEDA at 173 K.

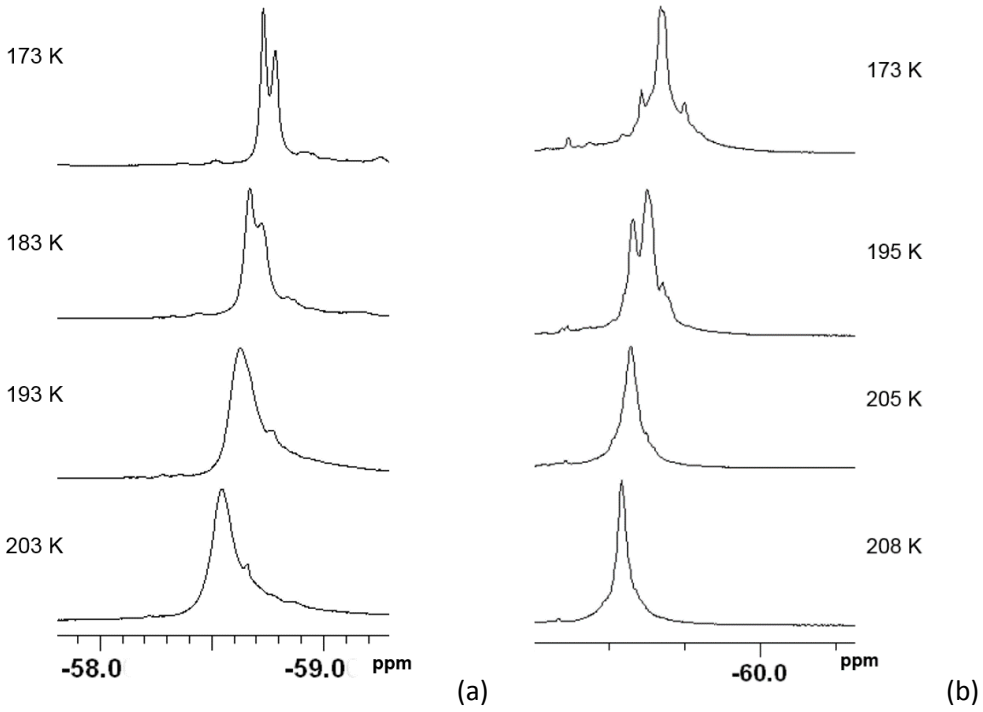

Figure S9. Variable-temperature ^{19}F NMR experiments of 0.2 M solution of **1-Li** in (a) THF-d_8 and (b) THF-d_8/TMEDA.

Table S1. Line shape analysis: rate constants and activation free energies for diastereomeric interconversion of (**1-Li**)$_2$. (A = major diastereoisomer, B = minor diastereoisomer)

$k_{A\rightarrow B}$ (s^{-1})	$\Delta G^{\neq}$(kcal mol^{-1})	T (K)	ln($k_{A\rightarrow B}$/T)	1/T (K^{-1})
21,21	9,10 ±0.4	177	-2,1217	0,00565
71,65	9,17 ±0.4	187	-0,9593	0,00535
234,78	9,23 ±0.4	197	0,17545	0,00508

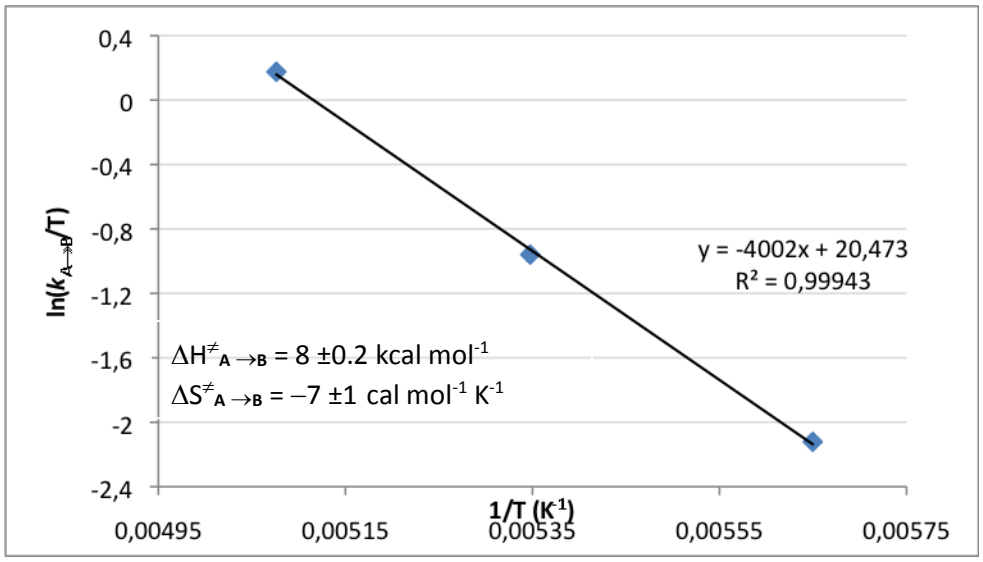

Figure S10. Eyring plot and activation parameters for diastereomeric interconversion of (**1-Li**)$_2$ (A $\rightarrow$ B)

Table S2. Line shape analysis: rate constants and activation free energies for diastereomeric interconversion of (**1-Li**)$_2$. (A = major diastereoisomer, B = minor diastereoisomer)

$k_{B\rightarrow A}$ (s^{-1})	$\Delta G^{\neq}$(kcal mol^{-1})	T (K)	ln($k_{B\rightarrow A}$/T)	1/T (K^{-1})
29,29	8,99 ±0.4	177	-1,798904	0,00565
98,95	9,05 ±0.4	187	-0,636494	0,00535
324,22	9,11 ±0.4	197	0,498219	0,00508

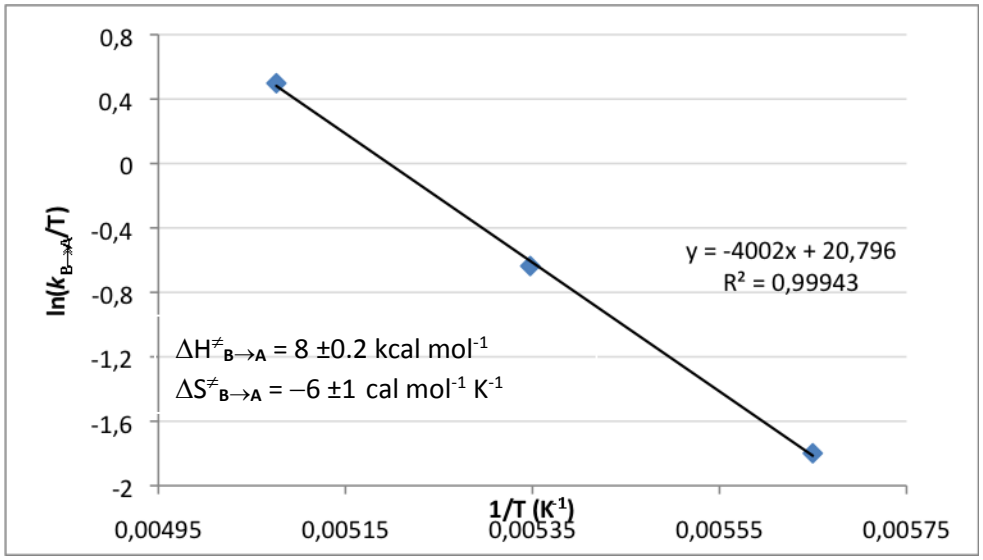

Figure S11. Eyring plot and activation parameters for diastereomeric interconversion of (**1-Li**)$_2$ (B $\rightarrow$ A)

Table S3. Rate constants for the enantiomerization of **1-Li** by line shape analysis.

k_{enant} (s^{-1})	$\Delta G^{\neq}$(kcal mol^{-1})	T (K)	ln(k_{enant}/T)	1/T (K^{-1})
209,90	9,28 ±1.5	197	0,06343	0,00508
312,30	9,38 ±1.5	203	0,43076	0,00493
500,05	9,47 ±1.5	208	0,87717	0,00481

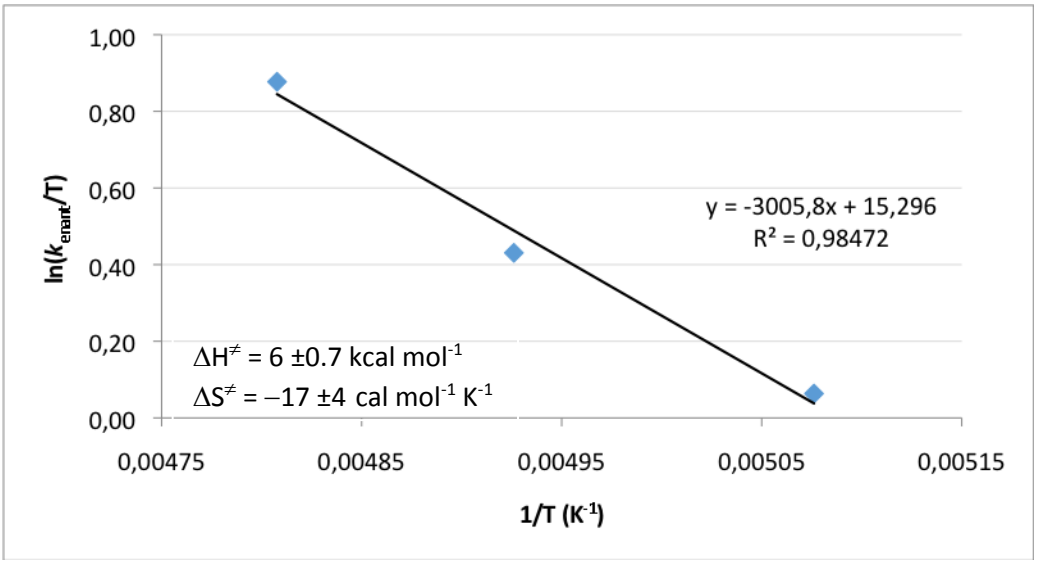

Figure S12. Eyring plot and activation parameters for the enantiomerization of **1-Li**.

Table S4. Crystal data and structure refinement for **(1-Li)$_2$·(TMEDA)$_2$** complex.

Identification code	shelxl	
Empirical formula	C30 H44 F6 Li2 N4 O2	
Formula weight	620.57	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.593(2) Å	α= 90°.
	b = 11.372(2) Å	β= 106.11(2)°.
	c = 15.779(3) Å	γ = 90°.
Volume	1653.7(6) Å^3	
Z	2	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	656	
Crystal size	0.200 x 0.200 x 0.100 mm^3	
Theta range for data collection	2.239 to 26.435°.	
Index ranges	-11<=h<=11, -14<=k<=14, -19<=l<=19	
Reflections collected	41883	
Independent reflections	3391 [R(int) = 0.0351]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6964	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3391 / 0 / 203	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0964	
R indices (all data)	R1 = 0.0452, wR2 = 0.1008	
Extinction coefficient	0	
Largest diff. peak and hole	0.281 and -0.190 e.Å^{-3}	

Table S5. Bond lengths [Å] and angles [°] for $(\mathbf{1\text{-}Li})_2 \cdot (TMEDA)_2$ complex

F(4)-C(5)	1.3433(17)
F(1)-C(5)	1.3436(19)
N(1)-C(2)	1.4653(18)
N(1)-C(8)	1.4657(19)
N(1)-C(11)	1.4657(19)
N(1)-Li(1)	2.165(3)
O(2)-C(20)	1.4319(18)
O(2)-C(7)	1.5300(16)
O(2)-Li(1)	1.898(2)
F(3)-C(5)	1.3405(18)
N(2)-C(15)	1.4583(19)
N(2)-C(14)	1.4659(19)
N(2)-C(13)	1.4731(19)
N(2)-Li(1)	2.141(3)
C(1)-C(3)	1.408(2)
C(1)-C(4)	1.4143(19)
C(1)-C(7)	1.471(2)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-C(9)	1.377(2)
C(3)-H(3)	0.9500
C(4)-C(6)	1.394(2)
C(4)-C(5)	1.487(2)
C(6)-C(10)	1.376(2)
C(6)-H(6)	0.9500
C(7)-C(20)	1.469(2)
C(7)-Li(1)	2.167(3)
C(8)-C(13)	1.514(2)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.384(2)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500

C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
Li(1)-O(2)	1.898(2)

C(2)-N(1)-C(8)	109.70(11)
C(2)-N(1)-C(11)	108.79(11)
C(8)-N(1)-C(11)	111.03(12)
C(2)-N(1)-Li(1)	113.52(10)
C(8)-N(1)-Li(1)	102.23(10)
C(11)-N(1)-Li(1)	111.45(11)
C(20)-O(2)-C(7)	59.36(9)
C(20)-O(2)-Li(1)	140.89(12)
C(7)-O(2)-Li(1)	141.20(11)
C(15)-N(2)-C(14)	109.08(12)
C(15)-N(2)-C(13)	110.58(12)
C(14)-N(2)-C(13)	110.24(12)
C(15)-N(2)-Li(1)	112.63(11)
C(14)-N(2)-Li(1)	113.04(11)
C(13)-N(2)-Li(1)	101.06(10)
C(3)-C(1)-C(4)	115.74(13)
C(3)-C(1)-C(7)	119.64(12)
C(4)-C(1)-C(7)	124.03(13)
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5

N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(9)-C(3)-C(1)	122.39(14)
C(9)-C(3)-H(3)	118.8
C(1)-C(3)-H(3)	118.8
C(6)-C(4)-C(1)	121.35(14)
C(6)-C(4)-C(5)	118.22(13)
C(1)-C(4)-C(5)	120.41(13)
F(3)-C(5)-F(4)	105.03(12)
F(3)-C(5)-F(1)	105.43(14)
F(4)-C(5)-F(1)	104.96(12)
F(3)-C(5)-C(4)	113.94(12)
F(4)-C(5)-C(4)	113.04(13)
F(1)-C(5)-C(4)	113.56(12)
C(10)-C(6)-C(4)	120.92(14)
C(10)-C(6)-H(6)	119.5
C(4)-C(6)-H(6)	119.5
C(20)-C(7)-C(1)	118.46(12)
C(20)-C(7)-O(2)	57.00(8)
C(1)-C(7)-O(2)	110.64(11)
C(20)-C(7)-Li(1)	127.47(12)
C(1)-C(7)-Li(1)	114.06(11)
O(2)-C(7)-Li(1)	105.38(10)
N(1)-C(8)-C(13)	111.24(12)
N(1)-C(8)-H(8A)	109.4
C(13)-C(8)-H(8A)	109.4
N(1)-C(8)-H(8B)	109.4
C(13)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(3)-C(9)-C(10)	120.65(15)
C(3)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(6)-C(10)-C(9)	118.94(14)
C(6)-C(10)-H(10)	120.5
C(9)-C(10)-H(10)	120.5

N(1)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(20)-C(7)	63.65(9)
O(2)-C(20)-H(20A)	117.4
C(7)-C(20)-H(20A)	117.4
O(2)-C(20)-H(20B)	117.4
C(7)-C(20)-H(20B)	117.4
H(20A)-C(20)-H(20B)	114.5
N(2)-C(13)-C(8)	111.33(12)
N(2)-C(13)-H(13A)	109.4
C(8)-C(13)-H(13A)	109.4
N(2)-C(13)-H(13B)	109.4
C(8)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
N(2)-C(14)-H(14A)	109.5
N(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(2)-C(15)-H(15A)	109.5
N(2)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
N(2)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(2)-Li(1)-N(2)	105.56(11)
O(2)-Li(1)-N(1)	108.79(11)
N(2)-Li(1)-N(1)	86.36(9)
O(2)-Li(1)-C(7)	112.89(12)
N(2)-Li(1)-C(7)	123.27(12)
N(1)-Li(1)-C(7)	116.69(11)

Table S6. Torsion angles [°] for $(\mathbf{1\text{-}Li})_2 \cdot (TMEDA)_2$ complex.

C(4)-C(1)-C(3)-C(9)	-0.8(2)
C(7)-C(1)-C(3)-C(9)	170.74(13)
C(3)-C(1)-C(4)-C(6)	1.40(19)
C(7)-C(1)-C(4)-C(6)	-169.75(13)
C(3)-C(1)-C(4)-C(5)	-179.91(12)
C(7)-C(1)-C(4)-C(5)	8.9(2)
C(6)-C(4)-C(5)-F(3)	-119.82(15)
C(1)-C(4)-C(5)-F(3)	61.46(18)
C(6)-C(4)-C(5)-F(4)	0.00(18)
C(1)-C(4)-C(5)-F(4)	-178.72(12)
C(6)-C(4)-C(5)-F(1)	119.44(14)
C(1)-C(4)-C(5)-F(1)	-59.28(17)
C(1)-C(4)-C(6)-C(10)	-1.0(2)
C(5)-C(4)-C(6)-C(10)	-179.68(13)
C(3)-C(1)-C(7)-C(20)	110.50(15)
C(4)-C(1)-C(7)-C(20)	-78.67(17)
C(3)-C(1)-C(7)-O(2)	47.75(16)
C(4)-C(1)-C(7)-O(2)	-141.42(12)
C(3)-C(1)-C(7)-Li(1)	-70.84(15)
C(4)-C(1)-C(7)-Li(1)	99.99(15)
Li(1)-O(2)-C(7)-C(20)	134.64(19)
C(20)-O(2)-C(7)-C(1)	111.26(13)
Li(1)-O(2)-C(7)-C(1)	-114.11(17)
C(20)-O(2)-C(7)-Li(1)	-125.00(13)
Li(1)-O(2)-C(7)-Li(1)	9.6(2)
C(2)-N(1)-C(8)-C(13)	-81.41(14)
C(11)-N(1)-C(8)-C(13)	158.31(12)
Li(1)-N(1)-C(8)-C(13)	39.35(14)
C(1)-C(3)-C(9)-C(10)	-0.2(2)
C(4)-C(6)-C(10)-C(9)	-0.1(2)
C(3)-C(9)-C(10)-C(6)	0.7(2)
Li(1)-O(2)-C(20)-C(7)	-135.02(18)
C(1)-C(7)-C(20)-O(2)	-97.24(13)
Li(1)-C(7)-C(20)-O(2)	84.30(14)

C(15)-N(2)-C(13)-C(8)	164.99(12)
C(14)-N(2)-C(13)-C(8)	-74.31(15)
Li(1)-N(2)-C(13)-C(8)	45.51(14)
N(1)-C(8)-C(13)-N(2)	-62.54(16)

Cartesian coordinates:

(**1a-Li**)$_2$*(THF)$_4$

-2386.33862496502

3	1.133851454	-1.159256326	-0.096148777
1	0.287013851	1.454838905	-2.118475388
6	1.071957694	1.795595537	-1.431972180
8	0.688864003	1.883477737	-0.056783055
6	1.690704616	0.861302882	-0.493023834
6	3.045148447	1.141870492	-0.034893456
3	-1.199108991	1.233961286	-0.083254418
1	1.613137888	2.681717489	-1.782759826
6	5.671368993	1.403514721	1.021713080
6	3.277313608	1.607153954	1.274631809
6	4.192598268	0.839614131	-0.812649206
6	5.477177884	0.971295823	-0.284221935
6	4.556053674	1.732658499	1.793173887
1	2.411605739	1.883345603	1.875453621
1	6.335313715	0.737134716	-0.908548213
1	4.689248784	2.099654720	2.809482124
1	6.676051703	1.499014511	1.424141720
1	-6.247604834	-1.310123867	0.394909648
6	-5.219894186	-1.579710052	0.622204407
6	-4.946586343	-2.417374709	1.695731353
6	-4.192727215	-1.080579417	-0.180799979
6	-3.619264759	-2.760018419	1.953781140
1	-5.754232591	-2.804281694	2.310770826
6	-2.836701830	-1.406681740	0.068575253
6	-2.596315867	-2.268123935	1.158722229
1	-3.383089263	-3.429361783	2.780453891
6	-1.698231787	-0.815991344	-0.641700062

1	-1.563029350	-2.548194363	1.351708819
6	-1.268873910	-1.461578066	-1.891008690
8	-0.568168328	-1.800993510	-0.706497549
1	-1.842749729	-2.295193237	-2.310800788
1	-0.687462914	-0.903137103	-2.634522914
6	4.046739342	0.423122283	-2.243823147
9	3.631219703	1.432299730	-3.039876543
9	5.209153086	-0.013279139	-2.771069854
9	3.164024481	-0.579832387	-2.428343406
6	-4.553093935	-0.108090742	-1.256451825
9	-3.905863875	-0.314386449	-2.416894325
9	-5.866914746	-0.120456747	-1.550863945
9	-4.268201709	1.163723918	-0.887791712
8	-1.808046608	1.713581632	1.745794313
6	-3.047946174	1.376241252	2.361526115
6	-1.116546435	2.530425051	2.683936802
6	-2.672968933	1.046166360	3.800360019
1	-3.489848981	0.545869362	1.802123003
1	-3.725831031	2.245565172	2.304964782
6	-1.442386317	1.939202459	4.062129231
1	-0.055556622	2.521023968	2.408850429
1	-1.487504885	3.566160481	2.600591896
1	-0.602607501	1.354551529	4.454650987
1	-1.652415651	2.729963975	4.789957113
1	-3.495426438	1.235460396	4.497305399
1	-2.412613155	-0.017868240	3.877874307
8	1.054508881	-1.581946081	1.857913326
6	0.934331912	-2.934563151	2.314175150
6	0.558549795	-0.677959583	2.845877631
6	0.203143794	-2.860054205	3.647265022

1	1.946994618	-3.354281362	2.426216974
1	0.407043071	-3.520387285	1.547806637
6	0.580693107	-1.466420932	4.142249592
1	1.208144129	0.206798459	2.841795690
1	-0.463962106	-0.366311118	2.570333402
1	1.591953400	-1.468228173	4.570165662
1	-0.110786669	-1.073239060	4.895855312
1	-0.883712918	-2.918619109	3.495431490
1	0.494303386	-3.663925795	4.330436860
6	-1.755786110	4.925268610	-2.087400378
6	-1.586820035	3.899486620	-3.205447099
6	-2.260419582	2.688292494	-2.592657074
8	-1.900369433	2.735920004	-1.210300871
6	-1.562384905	4.077064185	-0.835016082
1	-2.769559205	5.345707189	-2.115733157
1	-0.522656807	3.694688465	-3.384640296
1	-3.356373274	2.743820483	-2.688178102
1	-2.210468691	4.382452450	-0.002603664
1	-1.932089134	1.722277840	-2.992639559
1	-2.042950726	4.207438729	-4.151449737
1	-1.044528888	5.755001059	-2.143109331
1	-0.519120300	4.075934407	-0.485364602
6	3.722124552	-4.083489222	-1.714957465
6	4.347578886	-3.931929515	-0.330548823
6	3.787516421	-2.587004096	0.085051208
8	2.446274283	-2.592011927	-0.408706943
6	2.325124292	-3.517649713	-1.496934944
1	3.705262428	-5.114560001	-2.081201865
1	5.441633381	-3.953884766	-0.340203213
1	3.747026987	-2.407622272	1.166336824

1	1.602226955	-4.292775663	-1.200976780
1	4.352064430	-1.761336293	-0.377156640
1	3.988493724	-4.721371530	0.345155642
1	4.272389321	-3.470490933	-2.440526127
1	1.926219810	-2.986973058	-2.370229242

(**1b-Li**)$_2$*(THF)$_4$

-2386.33555924835

6	0.975371642	3.133549556	1.369812191
6	-0.002976993	2.768414992	0.425117881
6	-1.306854099	3.280337021	0.626604114
6	-1.607179734	4.074514790	1.733623429
6	-0.629373957	4.389619856	2.669736461
6	0.670715723	3.923995770	2.467786966
6	0.317505489	1.800814805	-0.625380366
6	0.653361821	2.336916576	-1.950615886
8	1.727707112	1.952545800	-1.101885332
3	2.031407215	0.048608328	-0.589433653
8	1.906135474	-1.941691775	-0.137724621
6	1.138653309	-2.709042215	-1.056757432
6	0.402548720	-1.903390827	-0.073627805
6	-0.110066346	-2.641803964	1.086480994
6	-1.449977618	-3.099235315	1.143868690
6	-1.974498305	-3.648255839	2.312204725
6	-1.189153219	-3.785110038	3.452465667
6	0.147550567	-3.397667226	3.396707496
6	0.672033225	-2.842072956	2.237686346
3	-0.862148076	-0.093774620	-0.417244081
1	1.202020410	-2.397045640	-2.104035338
1	1.245431368	-3.790050255	-0.909442194

1	1.720267153	-2.555457880	2.190257932
1	-3.007568060	-3.985167065	2.324895709
1	-1.610082232	-4.212183124	4.358586072
1	0.790287419	-3.533412700	4.265451606
1	0.516384138	1.725526073	-2.851035411
1	0.619933310	3.415171770	-2.138209875
1	-2.615867886	4.461497351	1.854861602
1	-0.874009581	5.007053597	3.529818453
1	1.456606854	4.185737599	3.174803026
1	1.989476875	2.771684567	1.207110742
6	-2.330647336	-3.009313618	-0.064158009
9	-3.497320129	-3.658571417	0.101729193
9	-2.673568800	-1.734830568	-0.382305027
9	-1.763367343	-3.522553694	-1.170671253
6	-2.366076930	3.052708550	-0.403051038
9	-3.590790893	3.419176546	0.018027611
9	-2.134577062	3.746240169	-1.539576769
9	-2.487681409	1.760946640	-0.793524028
8	3.232106343	0.456455046	1.004317138
6	4.532225209	-0.113608386	0.855110672
6	2.736310241	0.169807006	2.322860943
6	4.545375172	-1.298148473	1.800376604
1	5.296082408	0.632815699	1.130306015
1	4.660120777	-0.370754220	-0.203969592
6	3.777076516	-0.725758704	2.990731224
1	2.575411535	1.115907194	2.857573775
1	1.765442931	-0.332740136	2.212847566
1	4.448759541	-0.132506776	3.624883556
1	3.315525131	-1.493419103	3.621851877
1	3.994989114	-2.132754259	1.346640059

1	5.556100744	-1.630483269	2.058353008
8	-1.849189165	0.167130867	1.495244377
6	-1.108596730	0.343803765	2.711613345
6	-3.239862131	0.129811212	1.802491718
6	-2.133853942	0.631752343	3.809862396
1	-0.414836658	1.181768557	2.555968994
1	-0.528688988	-0.569248896	2.913019867
6	-3.381126990	1.019569724	3.019687320
1	-3.791005156	0.469343170	0.918801209
1	-3.547507287	-0.907545359	2.030993255
1	-3.335767407	2.074859160	2.716563291
1	-4.313752978	0.852646658	3.568341180
1	-2.327935058	-0.273775955	4.399762296
1	-1.795055219	1.416536834	4.494297191
6	5.022545600	0.445331800	-3.411628340
6	5.157662677	-1.079769481	-3.239268035
6	3.781704735	-1.513688258	-2.714855303
8	3.120695097	-0.315825327	-2.313349298
6	3.529408999	0.682704544	-3.245014611
1	5.399692914	0.803584050	-4.374628396
1	5.956119575	-1.331876313	-2.533351883
1	3.188256780	-1.998089290	-3.509750732
1	2.987836831	0.529510426	-4.197101522
1	3.809176435	-2.181893336	-1.847092799
1	5.391647719	-1.581638872	-4.184119195
1	5.568928657	0.975092098	-2.622296254
1	3.257739425	1.655380685	-2.827289075
6	-2.273284910	0.648173716	-4.291383414
6	-0.899318202	0.105790229	-4.719856550
6	-0.433140717	-0.700222831	-3.493550677

8	-1.371056516	-0.428788618	-2.461236865
6	-2.619217040	-0.247945741	-3.115265950
1	-3.017698802	0.617468161	-5.093404954
1	-0.203622606	0.914581563	-4.971423115
1	-0.438256647	-1.783513651	-3.704891055
1	-3.005395895	-1.228991677	-3.446605193
1	0.565073181	-0.425968105	-3.125119335
1	-0.979298600	-0.541134854	-5.600935059
1	-2.188872551	1.683249496	-3.937802965
1	-3.322578366	0.183851787	-2.398980366

(**1c-Li**)$_2$*(THF)$_4$

-2386.33995644564

9	2.747550739	-5.742114872	0.423998248
9	2.549820493	-3.888573252	-0.653283895
8	-0.447780783	-1.351737579	1.874934809
9	2.675141193	-3.879004125	1.498785527
6	-0.151067261	-3.513041037	0.768473100
6	-1.547127968	-3.699362214	0.728676428
1	-2.179001034	-2.832885049	0.914962582
6	0.645981372	-4.658381935	0.520878426
6	2.133724302	-4.545526498	0.461432396
6	0.065420418	-5.898531102	0.246014210
1	0.706173014	-6.757007225	0.064327818
6	0.391325054	-2.164116764	0.921425866
6	-2.116502791	-4.930109903	0.447014116
1	-3.200922396	-5.024389642	0.419049494
6	-1.314637690	-6.045721079	0.202511816
1	-1.756813429	-7.013984310	-0.015268199
6	0.860520900	-1.754693555	2.246930624

1	1.595888116	-0.944407564	2.347601404
1	0.873166966	-2.463594871	3.082857764
6	-3.774430507	1.353035171	1.983820225
1	-4.123303398	1.338489093	0.945119116
1	-3.266447952	2.314355230	2.156361008
3	-1.132959518	0.295150091	1.094407503
9	0.003195751	-0.591658754	-5.401353721
9	0.526140853	0.484633232	-3.612450986
8	-1.871851781	1.174115444	-0.438643508
9	-0.978256037	1.269543018	-4.936594446
6	-1.859932129	-0.415564747	-2.286439984
6	-2.969822777	-1.103765166	-1.752846228
1	-3.192676401	-0.963333633	-0.695093094
6	-1.595092235	-0.618020719	-3.658126399
6	-0.516387872	0.125697799	-4.379460377
6	-2.405540369	-1.451528020	-4.435229749
1	-2.183786494	-1.568727850	-5.493638397
6	-1.011235769	0.348908436	-1.361564911
6	-3.764548973	-1.934091785	-2.523485225
1	-4.610273228	-2.444742901	-2.066456399
6	-3.486227992	-2.119571134	-3.879506724
1	-4.105501666	-2.768392766	-4.492776045
6	-1.083220591	1.811671426	-1.430570799
1	-0.261051692	2.429919278	-1.048361436
1	-1.681348852	2.309103459	-2.202550307
3	0.660507837	-1.088022054	-0.946052416
6	1.197273770	2.462208961	3.836701075
6	2.194485879	1.993293391	2.780809105
6	1.330786749	1.957266451	1.528946069
8	-0.002055985	1.683800797	1.982535031

6	-0.055371043	1.718819835	3.410582498
1	3.063439352	2.650485418	2.673124383
1	1.327907118	2.930886742	1.013122851
1	-0.993008187	2.206930248	3.703415407
1	1.042270040	3.546733414	3.763108065
1	1.502149084	2.226802708	4.860943641
1	2.558138445	0.986425897	3.029185519
1	1.619042625	1.179124597	0.806825178
1	-0.064185682	0.685715873	3.795952170
6	-4.089271201	0.343896740	4.105743917
6	-4.859511491	1.085777729	3.016948570
8	-2.808710489	0.303797923	2.154729794
6	-3.158811297	-0.515935694	3.272675292
1	-4.727463196	-0.241704480	4.774850140
1	-5.341336587	2.004366293	3.366080405
1	-3.667515982	-1.425345467	2.913259044
1	-5.638267795	0.434738878	2.598275645
1	-3.509696581	1.051186235	4.716037216
1	-2.232899691	-0.822839075	3.770522459
6	4.797300369	-0.017921339	-0.757728866
6	4.222964332	1.334343633	-1.168652758
6	2.868915013	0.924648583	-1.715840857
8	2.462210614	-0.189312254	-0.911799758
6	3.576404951	-0.697045892	-0.164265382
1	5.629063258	0.049261097	-0.049980896
1	4.831631733	1.870375094	-1.903185157
1	2.091706312	1.696204760	-1.650333668
1	3.440611155	-0.427843350	0.897621932
1	2.940100946	0.601019138	-2.766485450
1	4.102539231	1.980118307	-0.286048116

1	5.145231213	-0.565456839	-1.644751321
1	3.577064836	-1.789651995	-0.237880139
6	1.961329936	-3.648745041	-4.127529056
6	0.455673345	-3.898334565	-4.172778210
6	0.041688425	-3.437303680	-2.791517210
8	0.861921709	-2.288054585	-2.537170396
6	2.054882280	-2.355554315	-3.325157016
1	2.418575774	-3.556516598	-5.117769236
1	0.193444696	-4.943229488	-4.366014888
1	-1.006285818	-3.126884671	-2.708852127
1	2.079341303	-1.469311412	-3.976711065
1	0.242488794	-4.207886092	-2.030873833
1	-0.019844506	-3.270507649	-4.938867352
1	2.461654113	-4.467254127	-3.593978519
1	2.926196605	-2.323371551	-2.655614326

(**1d-Li**)$_2$·(THF)$_4$

-2386.34098445827

9	1.005977302	-0.240574257	5.901526039
9	-0.304371393	-0.909096931	4.328521467
8	1.311894218	-1.565755135	0.452060607
9	1.587312906	-1.890901432	4.640675506
6	1.621727917	0.020966572	2.290237139
6	2.366394459	0.898071466	1.470516691
1	2.370081111	0.704655626	0.397594723
6	1.659530756	0.274743317	3.685698496
6	0.995190623	-0.678211018	4.626514795
6	2.361999321	1.362361063	4.204091257
1	2.375389616	1.522929124	5.279274929
6	0.738338657	-0.961955990	1.681292118

6	3.063796251	1.975011903	1.994072007
1	3.620972833	2.629028318	1.323667667
6	3.056732557	2.228883489	3.367459103
1	3.600298082	3.073659399	3.781764075
6	1.142663767	-2.367617549	1.608734036
1	0.393306936	-3.163358889	1.524659772
1	2.090483703	-2.699954299	2.046440605
6	-3.931332313	-0.011516139	1.674170822
1	-4.547667284	0.029856924	0.766243096
1	-3.620998834	1.012654137	1.925016526
3	-1.019955639	0.241382224	1.342972393
9	0.234584934	0.984349987	-5.787326721
9	1.039593991	-0.097810198	-4.107392080
8	-1.093481969	1.228596269	-0.305166644
9	0.634620743	2.014964914	-3.939502329
6	-1.515061240	0.494747236	-2.594084743
6	-2.827504573	0.129080225	-2.235542347
1	-3.065127548	0.081849133	-1.174601589
6	-1.232042341	0.542057124	-3.982365821
6	0.149365429	0.866103737	-4.449636904
6	-2.205583091	0.237168125	-4.933589052
1	-1.952170924	0.290271277	-5.988749392
6	-0.493401229	0.677022673	-1.563087650
6	-3.790689872	-0.173612892	-3.185769931
1	-4.793817727	-0.448090627	-2.861945024
6	-3.489643722	-0.127749185	-4.546916038
1	-4.242839545	-0.360651590	-5.294522669
6	-0.240145735	2.044386728	-1.089370017
1	0.721783248	2.300836304	-0.626063782
1	-0.756511505	2.897821126	-1.544396709

3	0.902326599	-0.965643635	-1.370580840
6	-1.759101514	3.396568499	4.254110511
6	-0.608068827	3.926698930	3.404867854
6	-0.679060929	3.036532311	2.172519766
8	-1.295166226	1.808265965	2.608198311
6	-1.640430024	1.909621715	3.990261825
1	-0.695725275	4.989256547	3.158288583
1	-1.309242815	3.461938625	1.379172851
1	-2.566000672	1.340157639	4.151164060
1	-2.721379623	3.776389937	3.884727919
1	-1.671521470	3.646556501	5.316007378
1	0.346820900	3.773737982	3.926641037
1	0.309656571	2.804655709	1.753444599
1	-0.845287257	1.461892942	4.606199753
6	-3.525990774	-1.604128918	3.416801333
6	-4.632158988	-0.728156703	2.830631554
8	-2.737605004	-0.761345264	1.398962936
6	-2.739251516	-1.963815071	2.173957995
1	-3.904945413	-2.478313034	3.955116250
1	-5.059971278	-0.027736311	3.555496757
1	-3.231312411	-2.769256487	1.601500645
1	-5.449874081	-1.356439479	2.455312662
1	-2.885665363	-1.030692550	4.100836253
1	-1.692247540	-2.231945173	2.356573163
6	5.153174190	-0.644134505	-1.761755697
6	4.730441926	0.820400299	-1.701298987
6	3.319827800	0.747648499	-2.255736864
8	2.805636795	-0.513940743	-1.811441093
6	3.875192237	-1.345349382	-1.335068098
1	5.999569547	-0.883362662	-1.110670035

1	5.375603824	1.490585506	-2.277988217
1	2.647826651	1.538706116	-1.896983675
1	3.789552527	-1.423963021	-0.240988360
1	3.314412451	0.769649769	-3.355790880
1	4.718379097	1.165332512	-0.657335547
1	5.422492805	-0.918291755	-2.790608005
1	3.748824982	-2.345791156	-1.765932328
6	-1.439219193	-4.027063040	-3.262955318
6	-2.199204604	-3.520905606	-2.040215156
6	-1.081838868	-2.966965005	-1.166115293
8	-0.007219612	-2.627487108	-2.058872042
6	-0.374862763	-2.957854295	-3.402909595
1	-2.066477189	-4.114179425	-4.156230885
1	-2.780099696	-4.297415365	-1.531537241
1	-1.380714885	-2.067873088	-0.603556123
1	-0.778998652	-2.064492614	-3.905406500
1	-0.702189409	-3.713859399	-0.453355041
1	-2.883725864	-2.714051624	-2.335392048
1	-0.979720286	-5.004024897	-3.061452086
1	0.531659961	-3.277875664	-3.927857011

(**1d'-Li**)$_2$·(THF)$_2$

-2386.33996382108

9	4.219084707	1.932799110	3.094818195
9	2.890674652	3.481975181	3.778808105
8	4.301099174	6.102023706	6.829213535
9	4.936641496	3.956442115	3.294469025
6	4.387109817	3.721320349	6.294352644
6	4.816697349	3.387363982	7.595772415
1	4.678148063	4.135390568	8.377201170

6	4.562048992	2.732851597	5.293448610
6	4.157215208	3.024199288	3.881761114
6	5.148670968	1.502355660	5.590629563
1	5.281533875	0.771450727	4.797457420
6	3.685015118	4.976796954	6.068701101
6	5.400764908	2.164323849	7.882948236
1	5.727669889	1.950140772	8.900197812
6	5.574018693	1.207268177	6.880779196
1	6.034231825	0.247731127	7.099967407
6	4.413483417	6.066570395	5.414707767
1	3.878600454	6.859020287	4.878418161
1	5.441966191	5.922189056	5.065896194
3	1.643554384	4.582475756	6.611653154
9	1.464818105	9.082537323	12.476786681
9	2.969518920	8.420500950	11.086552966
8	1.227692588	5.171499422	8.424159542
9	1.689671895	6.981752327	12.056990176
6	0.738635918	7.395642497	9.296181055
6	-0.210228839	7.593648573	8.270294053
1	-0.202833959	6.893617276	7.436337603
6	0.713816972	8.329048571	10.362935878
6	1.692250135	8.202632382	11.485734066
6	-0.195749704	9.386904079	10.381190756
1	-0.189623893	10.077938121	11.219647671
6	1.762066909	6.364778119	9.149211269
6	-1.113944418	8.644396886	8.297299287
1	-1.832342580	8.756646453	7.484823437
6	-1.113872201	9.558027341	9.351931291
1	-1.821336728	10.382311051	9.378165026

6	1.558255179	5.062335221	9.798463597
1	2.416874682	4.417889007	10.024596998
1	0.687152955	4.887004818	10.441713666
3	3.665227869	7.059949807	8.395575152
6	5.870647407	4.925763693	10.952181201
6	7.073323894	5.293004938	10.080233522
6	6.519891466	6.361077972	9.127816740
8	5.215926812	6.708367302	9.617849461
6	5.079513364	6.217707350	10.950376830
1	6.151625551	4.597657647	11.958097789
1	7.482997455	4.434080698	9.538367335
1	7.147254025	7.263042157	9.109474097
1	5.498734034	6.949419038	11.661556120
1	6.385421673	6.002206894	8.099662353
1	7.876635055	5.707598658	10.701604383
1	5.275938679	4.125650032	10.488089146
1	4.009872268	6.106965609	11.154092271
6	2.755244933	11.140429875	7.338876581
6	1.797852049	10.247546751	6.555490211
6	2.556026355	8.929023991	6.508946586
8	3.413976864	8.921625342	7.659038032
6	3.279504195	10.159545405	8.367634629
1	2.264942499	12.006672372	7.794289359
1	1.557770609	10.626469078	5.556356748
1	1.895496354	8.047711083	6.554158077
1	2.558768292	10.034539143	9.191071946
1	3.189200661	8.848674535	5.612425699
1	0.858510267	10.125730202	7.113872427
1	3.570450668	11.498241329	6.695804261

1	4.258092869	10.410938714	8.789994105
6	-1.659388996	6.560124475	4.759748930
6	-0.436373928	7.411344297	4.377274511
6	0.686426329	6.389255387	4.377936813
8	0.354917422	5.534581139	5.465193289
6	-1.049319248	5.296367315	5.391124114
1	-2.255441379	6.301908147	3.877384622
1	-0.239325275	8.172269507	5.145200953
1	0.711770694	5.806528181	3.441737793
1	-1.229065492	4.403591101	4.773294454
1	1.689089564	6.788744319	4.564689244
1	-0.552214034	7.920424814	3.415223956
1	-2.321265126	7.086647257	5.455697821
1	-1.398741212	5.088501522	6.409369376
6	1.838754342	0.715751445	7.275686672
6	1.237877335	1.419991797	8.507027231
6	0.183233267	2.326532763	7.894066053
8	0.760369395	2.727407041	6.651482721
6	1.290674358	1.523841682	6.091481080
1	1.528674234	-0.332999858	7.209973262
1	2.000382207	2.030861376	9.007259621
1	-0.751822757	1.774598491	7.691760536
1	0.474437736	0.987375726	5.580983328
1	-0.045901808	3.230354600	8.465748192
1	0.822004658	0.724712353	9.243440465
1	2.934000317	0.737620100	7.298607718
1	2.044579808	1.800178335	5.349404182