Electronic Supplementary Information (ESI)

Syntheses and Crystal Structures of Phenyllithium Derivaties

Alexander Bodach†, René Hebestreit, Michael Bolte, and Lothar Fink*

Goethe-Universität Frankfurt, Institut für Anorganische und Analytische Chemie, Max-von-Laue-Strasse 7, D-60438 Frankfurt/Main, Germany.

Corresponding Author
*fink@chemie.uni-frankfurt.de
Present Addresses
†Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim/Ruhr, Germany

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Table 1. Selected crystallographic data of *p*-TolLi, *o*-TolLi, [(5-*m*-XyLi)$_3$·MTBE$_3$·LiBr] (XRPD & SC), as well as PhLi[1], MesLi[2] and [(PhLi)$_3$(Et$_2$O)$_3$LiBr][3] for comparison.

	p-TolLi	*o*-TolLi	[(5-*m*-XyLi)$_3$·MTBE$_3$·LiBr]		PhLi[1]	MesLi[2]	[(PhLi)$_3$(Et$_2$O)$_3$LiBr][3]
Sum formula	C_7H_7Li	C_7H_7Li	$C_{39}H_{63}O_3Li_4Br$		C_6H_5Li	$C_9H_{11}Li$	$C_{30}H_{45}O_3Li_4Br$
MW / g·mol^{-1}	98.07	98.07	687.56		84.05	126.13	561,34
Crystal system	monoclinic	orthorhombic	cubic		monoclinic	monoclinic	monoclinic
Space group (No)	$P2_1/a$ (14)	$P2_12_12_1$ (19)	$Pa\bar{3}$ (205)		$P2_1/n$ (14)	$P2_1/n$ (14)	$P2_1/c$ (14)
T / °C	20	20	20	-100	20	25	-138
a / Å	11.8833(2)	19.1387(5)	20.71358(6)	20.5485(6)	11.528(1)	15.2796(7)	18.632(4)
b / Å	4.72773(6)	14.2328(4)	-	-	4.555(1)	10.6181(5)	7.709(2)
c / Å	10.1676(2)	4.55022(8)	-	-	10.406(1)	4.7461(2)	22.253(8)
β / °	91.606(2)	-	-	-	114.24(1)	96.596(2)	94.63(1)
V / Å^3	571.00(2)	1239.47(5)	8887.21(7)	8676.4(8)	498.22(2)	764.91(6)	3185.9(2)
Z	4 (monomer)	8 (monomer)	8 (cage)		4 (monomer)	4 (monomer)	4 (cage)
Z'	1	2	1		1	1	1
ρ_{calc} /Mg·m^{-3}	1.141	1.051	1.028	1.053	1.121	1.095	1.17
2*θ* / °	2–100	3–80	3–100	4.4–50	5–49	2–100	up to 55
Radiation type	Cu-$K_{\alpha1}$	Cu-$K_{\alpha1}$	Cu-$K_{\alpha1}$	Mo-K_α	synchrotron	Cu-$K_{\alpha1}$	Mo-K_α
λ / Å	1.540598	1.540598	1.540598	0.71073	1.14966(2)	1.540598	0.71073
Reflections[a]	18	18	-	124239(2569)	-	-	4812
Parameters	91	153	154	144	30	112	344
Restraints	36	80	99	-	rigid body	39	-
R_{wp}[b] / %	2.10	2.22	2.50	14.12	4.68	2.06	-
R_{esp} / %	1.60	1.05	1.81	-	-	1.36	-
R'_{wp}[c] / %	10.23	10.43	9.14	-	-	-	-
R'_{exp} / %	7.77	4.92	6.61	-	-	-	-
R_{Bragg}[d] / %	0.836	1.358	1.20	9.30	-	9.12	4.1
R_{int} / %	-	-	-	10.24	-	-	-
gof	1.32	2.12	1.38	1.46	-	1.52	-
B_{iso}[e]	4.09(5)	4.27(9)	6.96(4)	-	-	-	-
d(Li-C) / Å	2.163(5)	2.237(6)	2.094(4)	2.109(5)	2.24(2)	2.146(9)	2.148(8)
d(Li-C) / Å	2.273(6)	2.245(7)	2.289(6)	2.279(7)	2.32(2)	2.172(8)	2.28(4)
d(Li-Li) / Å	2.427(8)	2.588(6)	2.434(5)	2.447(1)	2.39(3)	2.13(2)	2.47(4)
d(Li-*X*)[f] / Å	2.24(2)	2.16(2)	3.063(6)	3.02(2)	2.25(2)	2.10(2)	2,96(3)
Φ(C-Li-C) / °	113.7(2)	109.6(2)	100.3(2)	102.6(3)	116.8(4)	121.0(3)	104(1)
Φ(C-Li-C) / °			116.8(2)	114.9(3)			114(1)

a used for indexing (XRPD); used for refinement (thereof independent, SC)
b mind the different definitions for XRPD and SC data
c R'-values indicate background corrected *R*-values according to TOPAS[4, 5]
d equals R_1
e anisotropic atomic displacement parameter used for SC data
f X marks either another Li atom or the centre of a phenyl ring

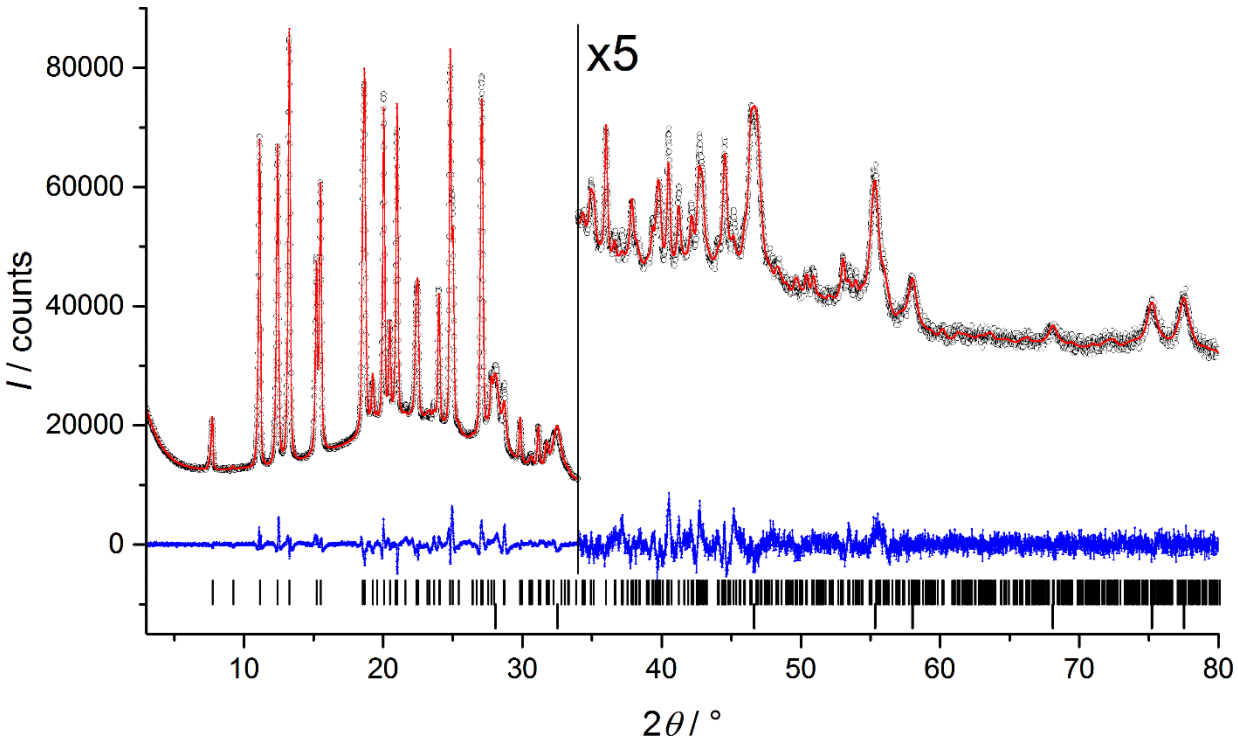

Fig. S1. Rietveld-Plot of the crystal structure of *o*-TolLi (*trans* isomer). I_{exp} (black circles), I_{calc} (red), I_{exp}-I_{calc} (blue), positions of Bragg reflections of *o*-TolLi (upper tick marks) and LiBr (quantitative phase analysis yielded 3.5%, lower tick marks).

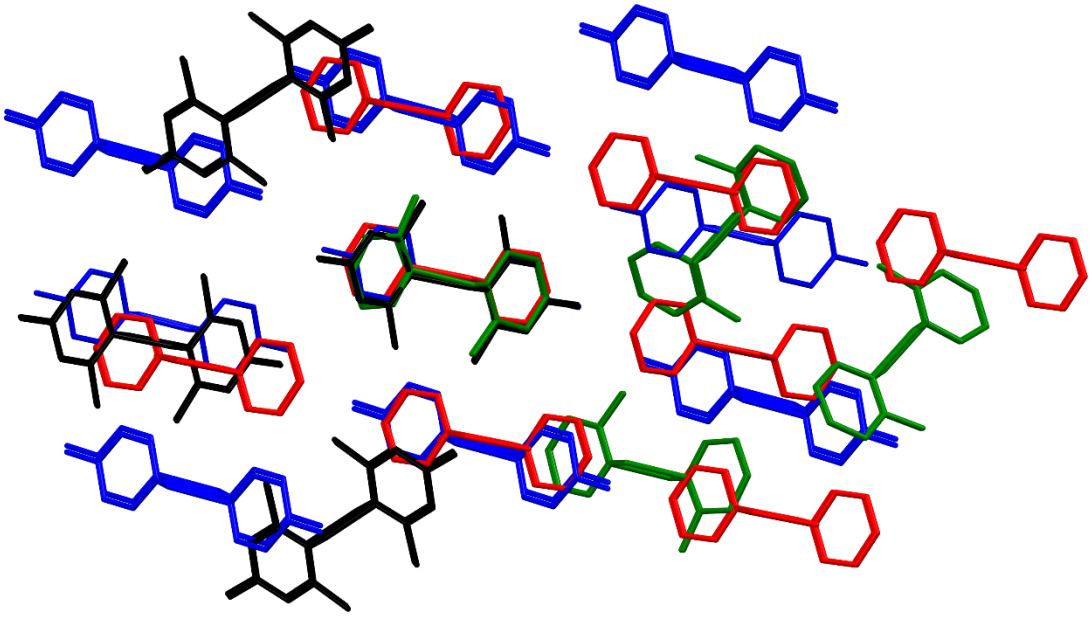

Fig. S2. Packing motifs of *p*-TolLi (blue), *o*-TolLi (green), MesLi[2] (black) and PhLi[1] (red), view along the superimposed zigzag-chains, parallel to *b* (for *p*-TolLi and PhLi), H atoms omitted for clarity.

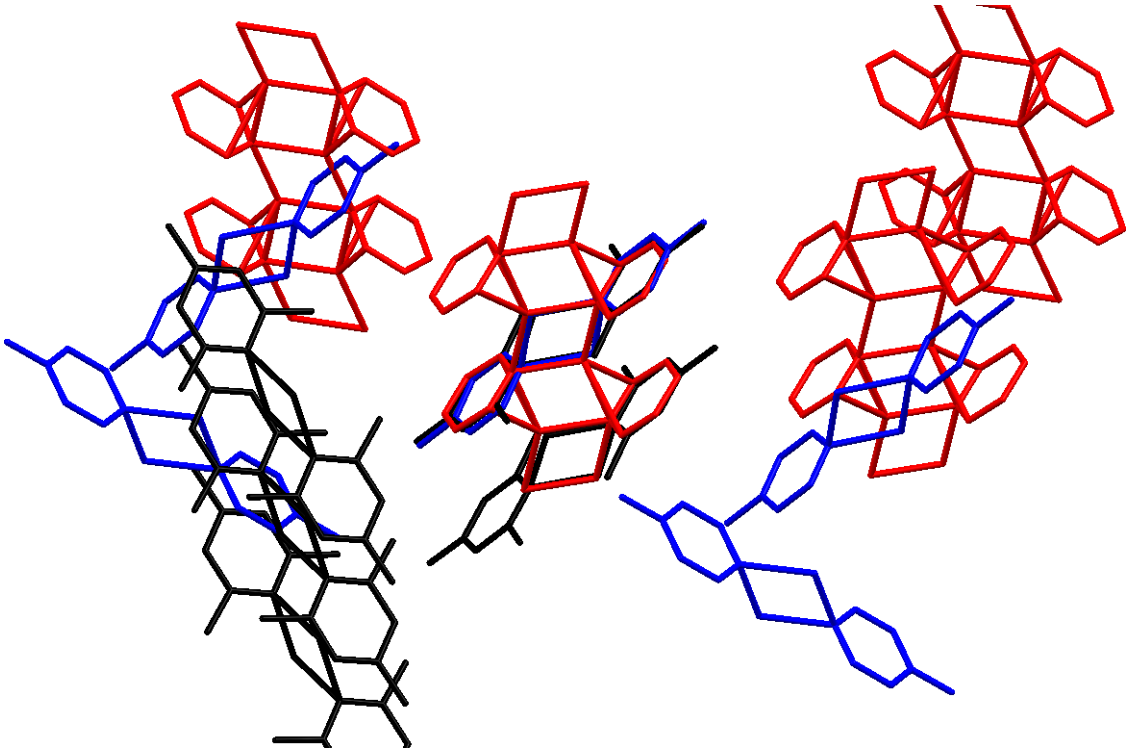

Fig. S3. Packing motifs of *p*-TolLi (blue), *o*-TolLi (green), MesLi[2] (black) and PhLi[1] (red), perpendicular to the zigzag-chains shown in Fig S2, H atoms omitted for clarity.

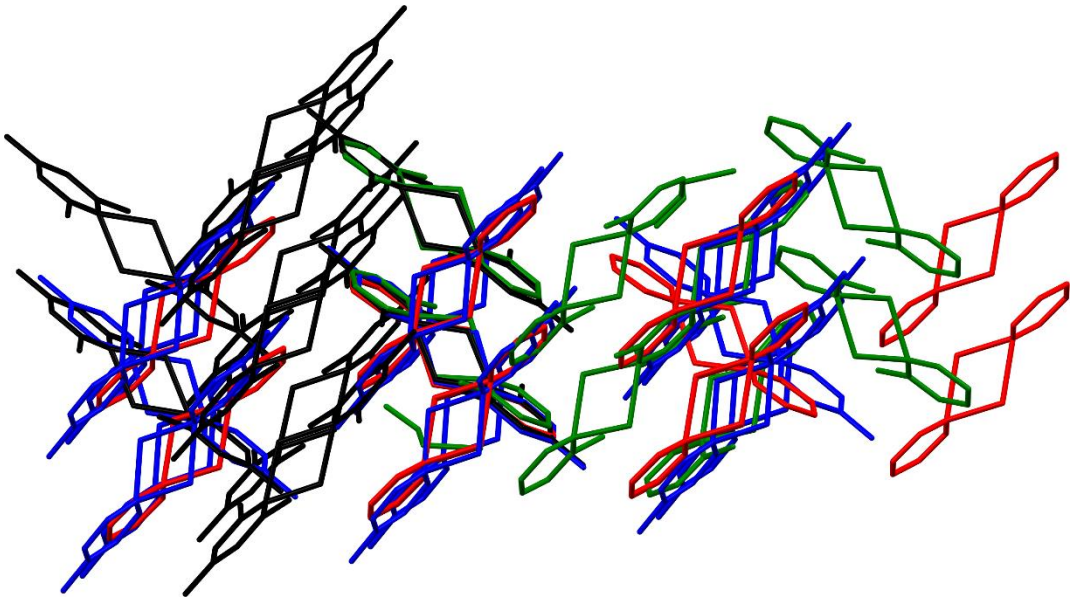

Fig. S4. Packing motifs of *p*-TolLi (blue), *o*-TolLi (green), MesLi[2] (black) and PhLi[1] (red), perpendicular to the zigzag-chains shown in Fig S2 and S3, H atoms omitted for clarity.

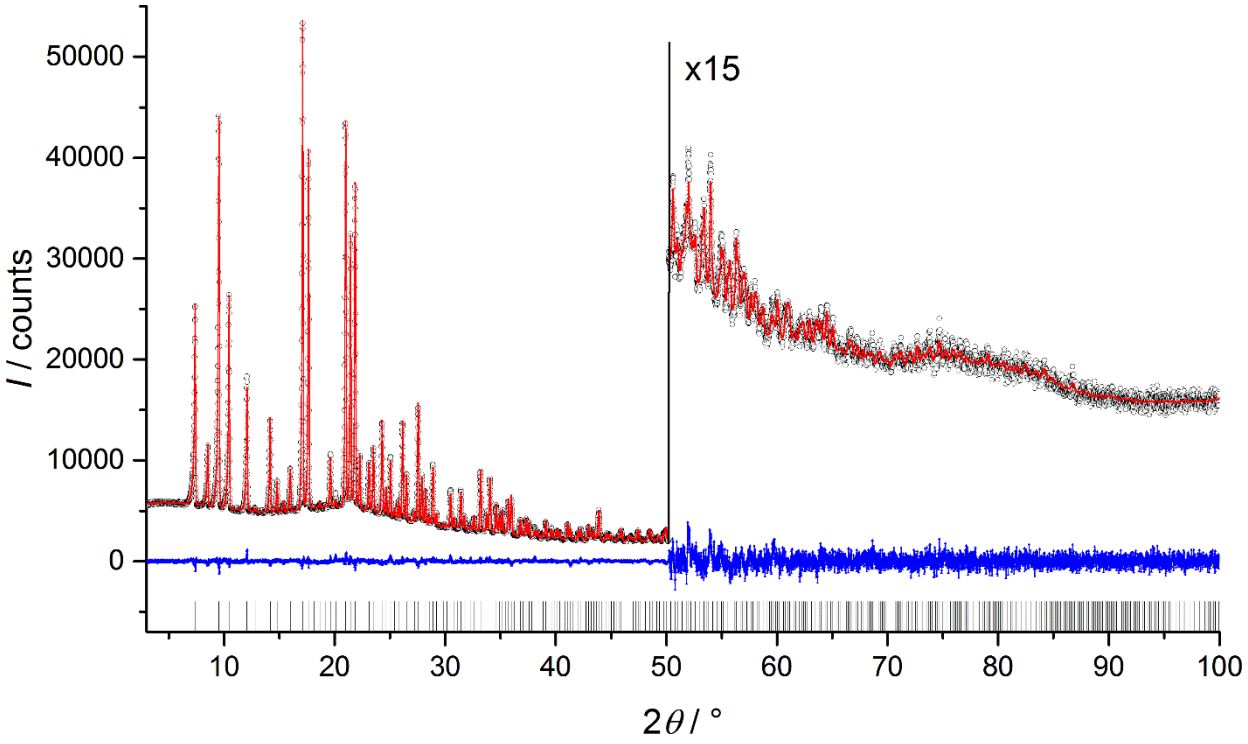

Fig. S5. Plot of the Rietveld refinement of the crystal structure of [(5-*m*-XyLi)$_3$(MTBE)$_3$LiBr]. I_{exp} (black circles), I_{calc} (red), I_{exp}-I_{calc} (blue), positions of Bragg reflections (tick marks).

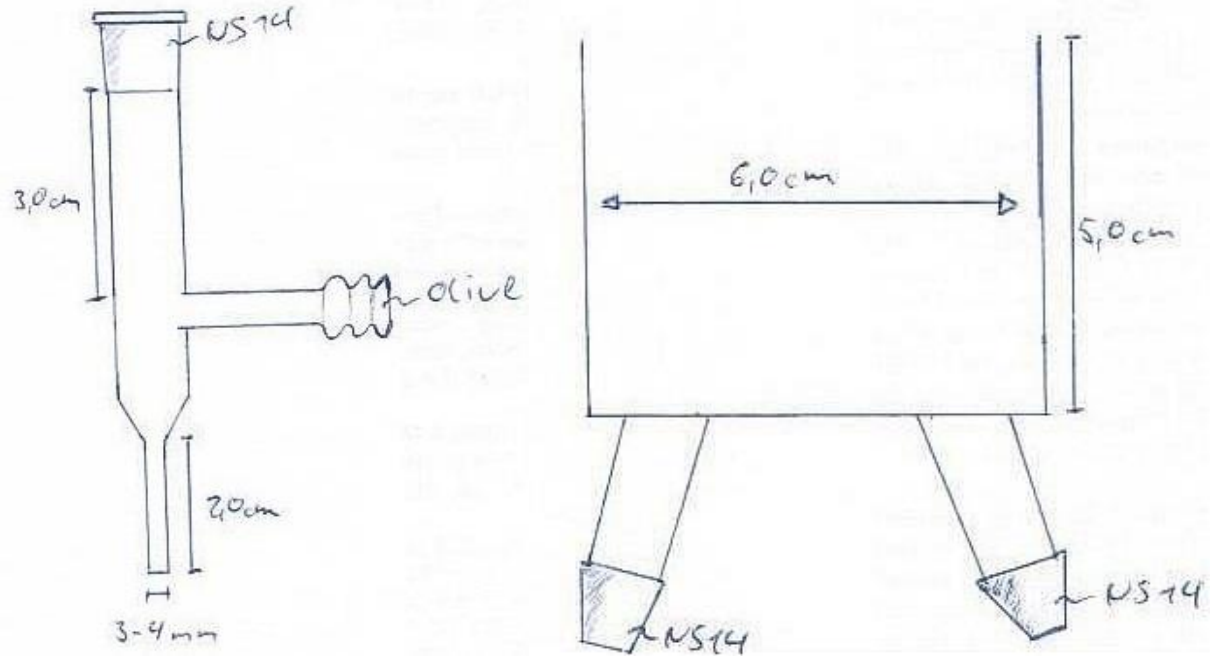

Fig. S6. Sketch of applied capillary station and glass trousers.

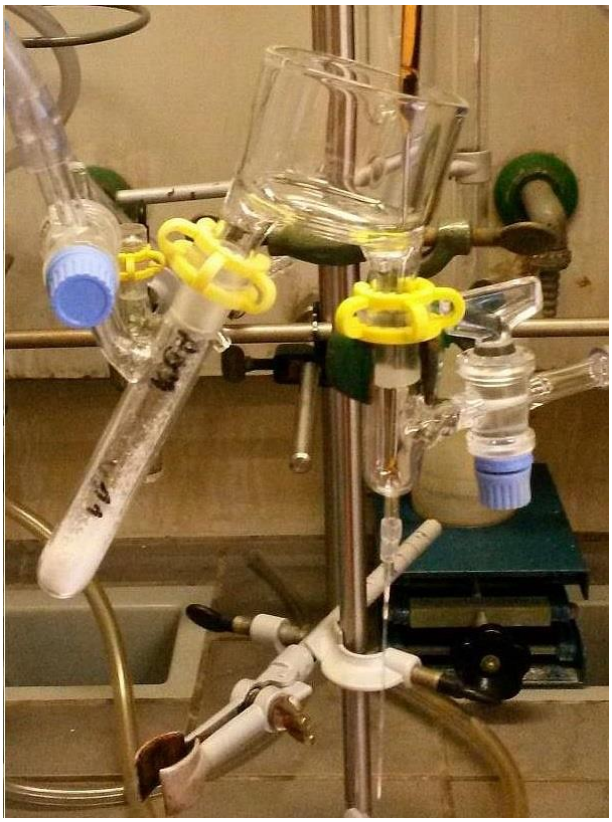

Fig S7. Picture of the glass trousers and the capillary station for transfer of sample from a Schlenk tube to capillary.

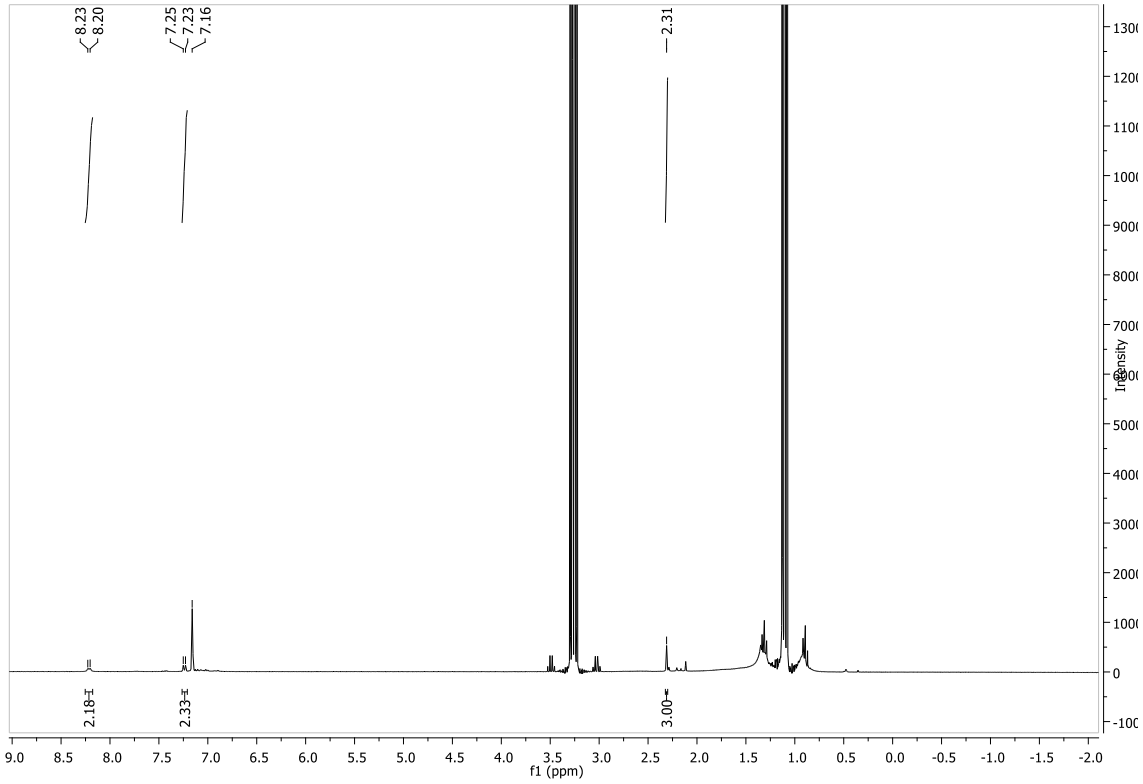

Fig. S8. ^{1}H NMR spectrum of *p*-TolLi Et_2O adduct in C_6D_6 with excess Et_2O.

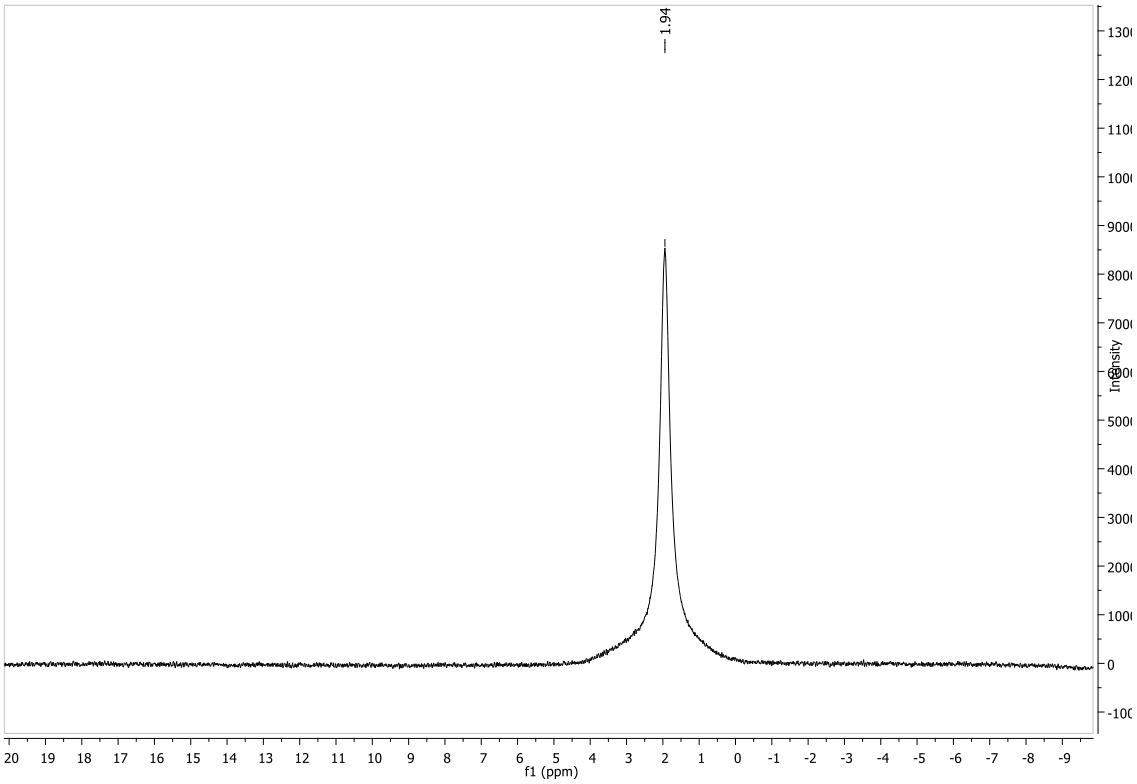

Fig. S9. ^{7}Li NMR spectrum of *p*-TolLi Et_2O adduct in C_6D_6 with excess Et_2O.

Table S2. Crystal data and structure refinement for s84.

Identification code	s84	
Empirical formula	C39 H63 Br Li4 O3	
Formula weight	687.56	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	P a -3	
Unit cell dimensions	a = 20.5485(6) Å	α= 90°.
	b = 20.5485(6) Å	β= 90°.
	c = 20.5485(6) Å	γ = 90°.
Volume	8676.4(8) $Å^3$	
Z	8	
Density (calculated)	1.053 Mg/m^3	
Absorption coefficient	0.977 mm^{-1}	
F(000)	2944	
Crystal size	0.150 x 0.150 x 0.150 mm^3	
Theta range for data collection	2.216 to 25.018°.	
Index ranges	-24<=h<=24, -24<=k<=24, -24<=l<=24	
Reflections collected	124239	
Independent reflections	2569 [R(int) = 0.1024]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.402	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2569 / 0 / 144
Goodness-of-fit on F^2	1.462
Final R indices [I>2sigma(I)]	R1 = 0.0883, wR2 = 0.1394
R indices (all data)	R1 = 0.0930, wR2 = 0.1412
Extinction coefficient	n/a
Largest diff. peak and hole	0.231 and -0.255 e.$Å^{-3}$

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s84. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	8086(1)	3086(1)	1914(1)	52(1)
Li(1)	9115(3)	4115(3)	885(3)	44(3)
Li(2)	8242(3)	4324(3)	1667(3)	48(2)
C(1)	9438(2)	3166(2)	667(2)	45(1)
C(2)	9881(2)	3411(2)	209(2)	44(1)
C(3)	10296(2)	3044(2)	-172(2)	50(1)
C(4)	10272(2)	2378(2)	-100(2)	65(1)
C(5)	9840(3)	2082(2)	333(2)	65(1)
C(6)	9445(2)	2484(2)	706(2)	53(1)
C(7)	10749(2)	3364(3)	-656(2)	66(1)
C(8)	9804(4)	1345(3)	405(4)	121(3)
O(1)	7622(2)	4889(1)	2124(2)	60(1)
C(10)	7602(2)	5601(2)	2121(2)	59(1)
C(11)	6966(3)	5834(3)	1820(4)	115(3)
C(12)	7680(4)	5852(3)	2804(3)	109(2)
C(13)	8163(2)	5809(2)	1699(3)	73(2)
C(14)	7109(4)	4573(3)	2452(4)	153(4)

Table S4. Bond lengths [Å] and angles [°] for s84.

Br(1)-Li(2)#1	2.613(7)
Br(1)-Li(2)#2	2.613(7)
Br(1)-Li(2)	2.614(7)
Li(1)-C(1)	2.109(5)
Li(1)-C(1)#2	2.109(5)
Li(1)-C(1)#1	2.109(5)
Li(1)-Li(2)	2.447(10)
Li(1)-Li(2)#1	2.447(10)
Li(1)-Li(2)#2	2.447(10)
Li(1)-C(2)#2	2.549(5)
Li(1)-C(2)	2.549(5)
Li(1)-C(2)#1	2.549(5)
Li(2)-O(1)	1.962(7)
Li(2)-C(1)#1	2.276(8)
Li(2)-C(1)#2	2.279(7)
Li(2)-C(6)#1	2.767(8)
Li(2)-C(6)#2	2.788(8)
Li(2)-Li(2)#1	3.020(12)
Li(2)-Li(2)#2	3.020(12)
C(1)-C(6)	1.403(6)
C(1)-C(2)	1.404(5)
C(1)-Li(2)#2	2.276(8)
C(1)-Li(2)#1	2.279(7)
C(2)-C(3)	1.383(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.376(6)
C(3)-C(7)	1.512(6)
C(4)-C(5)	1.397(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(6)
C(5)-C(8)	1.522(7)
C(6)-Li(2)#2	2.767(8)
C(6)-Li(2)#1	2.788(8)
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
O(1)-C(14)	1.411(6)
O(1)-C(10)	1.464(5)
C(10)-C(12)	1.504(7)
C(10)-C(13)	1.505(6)
C(10)-C(11)	1.522(8)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800

C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

Li(2)#1-Br(1)-Li(2)#2	70.6(2)
Li(2)#1-Br(1)-Li(2)	70.6(2)
Li(2)#2-Br(1)-Li(2)	70.6(2)
C(1)-Li(1)-C(1)#2	114.9(2)
C(1)-Li(1)-C(1)#1	114.9(2)
C(1)#2-Li(1)-C(1)#1	114.9(2)
C(1)-Li(1)-Li(2)	122.1(5)
C(1)#2-Li(1)-Li(2)	59.5(3)
C(1)#1-Li(1)-Li(2)	59.4(3)
C(1)-Li(1)-Li(2)#1	59.5(3)
C(1)#2-Li(1)-Li(2)#1	59.4(3)
C(1)#1-Li(1)-Li(2)#1	122.1(5)
Li(2)-Li(1)-Li(2)#1	76.2(4)
C(1)-Li(1)-Li(2)#2	59.4(3)
C(1)#2-Li(1)-Li(2)#2	122.1(5)
C(1)#1-Li(1)-Li(2)#2	59.5(3)
Li(2)-Li(1)-Li(2)#2	76.2(4)
Li(2)#1-Li(1)-Li(2)#2	76.2(4)
C(1)-Li(1)-C(2)#2	121.34(15)
C(1)#2-Li(1)-C(2)#2	33.41(15)
C(1)#1-Li(1)-C(2)#2	123.49(15)
Li(2)-Li(1)-C(2)#2	85.3(2)
Li(2)#1-Li(1)-C(2)#2	83.9(2)
Li(2)#2-Li(1)-C(2)#2	155.5(5)
C(1)-Li(1)-C(2)	33.42(15)
C(1)#2-Li(1)-C(2)	123.49(15)
C(1)#1-Li(1)-C(2)	121.34(15)
Li(2)-Li(1)-C(2)	155.5(5)
Li(2)#1-Li(1)-C(2)	85.3(2)
Li(2)#2-Li(1)-C(2)	83.9(2)
C(2)#2-Li(1)-C(2)	108.9(3)
C(1)-Li(1)-C(2)#1	123.49(15)
C(1)#2-Li(1)-C(2)#1	121.34(15)
C(1)#1-Li(1)-C(2)#1	33.41(15)
Li(2)-Li(1)-C(2)#1	83.9(2)
Li(2)#1-Li(1)-C(2)#1	155.5(5)
Li(2)#2-Li(1)-C(2)#1	85.3(2)
C(2)#2-Li(1)-C(2)#1	108.9(3)
C(2)-Li(1)-C(2)#1	108.9(3)
O(1)-Li(2)-C(1)#1	115.3(3)

O(1)-Li(2)-C(1)#2	120.4(4)
C(1)#1-Li(2)-C(1)#2	102.5(3)
O(1)-Li(2)-Li(1)	153.3(4)
C(1)#1-Li(2)-Li(1)	52.88(18)
C(1)#2-Li(2)-Li(1)	52.85(17)
O(1)-Li(2)-Br(1)	113.8(3)
C(1)#1-Li(2)-Br(1)	101.1(3)
C(1)#2-Li(2)-Br(1)	101.1(3)
Li(1)-Li(2)-Br(1)	92.7(3)
O(1)-Li(2)-C(6)#1	92.4(3)
C(1)#1-Li(2)-C(6)#1	30.35(16)
C(1)#2-Li(2)-C(6)#1	132.9(3)
Li(1)-Li(2)-C(6)#1	82.3(2)
Br(1)-Li(2)-C(6)#1	94.0(2)
O(1)-Li(2)-C(6)#2	98.7(3)
C(1)#1-Li(2)-C(6)#2	132.6(3)
C(1)#2-Li(2)-C(6)#2	30.06(15)
Li(1)-Li(2)-C(6)#2	81.9(2)
Br(1)-Li(2)-C(6)#2	93.5(2)
C(6)#1-Li(2)-C(6)#2	162.8(3)
O(1)-Li(2)-Li(2)#1	147.9(4)
C(1)#1-Li(2)-Li(2)#1	96.8(2)
C(1)#2-Li(2)-Li(2)#1	48.4(3)
Li(1)-Li(2)-Li(2)#1	51.90(19)
Br(1)-Li(2)-Li(2)#1	54.70(11)
C(6)#1-Li(2)-Li(2)#1	116.8(3)
C(6)#2-Li(2)-Li(2)#1	56.7(3)
O(1)-Li(2)-Li(2)#2	142.9(4)
C(1)#1-Li(2)-Li(2)#2	48.5(3)
C(1)#2-Li(2)-Li(2)#2	96.7(2)
Li(1)-Li(2)-Li(2)#2	51.90(19)
Br(1)-Li(2)-Li(2)#2	54.70(11)
C(6)#1-Li(2)-Li(2)#2	57.4(3)
C(6)#2-Li(2)-Li(2)#2	116.1(3)
Li(2)#1-Li(2)-Li(2)#2	60.000(1)
C(6)-C(1)-C(2)	112.9(4)
C(6)-C(1)-Li(1)	156.3(4)
C(2)-C(1)-Li(1)	90.8(4)
C(6)-C(1)-Li(2)#2	94.6(3)
C(2)-C(1)-Li(2)#2	128.9(3)
Li(1)-C(1)-Li(2)#2	67.7(3)
C(6)-C(1)-Li(2)#1	95.5(3)
C(2)-C(1)-Li(2)#1	132.2(3)
Li(1)-C(1)-Li(2)#1	67.7(3)
Li(2)#2-C(1)-Li(2)#1	83.1(4)
C(3)-C(2)-C(1)	125.7(4)
C(3)-C(2)-Li(1)	178.3(4)
C(1)-C(2)-Li(1)	55.8(3)
C(3)-C(2)-H(2)	117.1
C(1)-C(2)-H(2)	117.1

Li(1)-C(2)-H(2)	61.3
C(4)-C(3)-C(2)	117.4(4)
C(4)-C(3)-C(7)	121.7(4)
C(2)-C(3)-C(7)	121.0(4)
C(3)-C(4)-C(5)	121.7(4)
C(3)-C(4)-H(4)	119.2
C(5)-C(4)-H(4)	119.2
C(6)-C(5)-C(4)	117.5(4)
C(6)-C(5)-C(8)	120.7(5)
C(4)-C(5)-C(8)	121.7(5)
C(5)-C(6)-C(1)	124.8(4)
C(5)-C(6)-Li(2)#2	143.7(4)
C(1)-C(6)-Li(2)#2	55.1(3)
C(5)-C(6)-Li(2)#1	148.5(4)
C(1)-C(6)-Li(2)#1	54.5(3)
Li(2)#2-C(6)-Li(2)#1	65.9(3)
C(5)-C(6)-H(6)	117.6
C(1)-C(6)-H(6)	117.6
Li(2)#2-C(6)-H(6)	75.4
Li(2)#1-C(6)-H(6)	73.0
C(3)-C(7)-H(7A)	109.5
C(3)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(3)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(14)-O(1)-C(10)	116.1(4)
C(14)-O(1)-Li(2)	116.2(4)
C(10)-O(1)-Li(2)	127.5(3)
O(1)-C(10)-C(12)	109.6(4)
O(1)-C(10)-C(13)	105.2(3)
C(12)-C(10)-C(13)	111.0(4)
O(1)-C(10)-C(11)	109.9(4)
C(12)-C(10)-C(11)	111.3(5)
C(13)-C(10)-C(11)	109.5(5)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5

C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(1)-C(14)-H(14A)	109.5
O(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
O(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 y+1/2,-z+1/2,-x+1 #2 -z+1,x-1/2,-y+1/2

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s84. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	52(1)	52(1)	52(1)	9(1)	9(1)	-9(1)
Li(1)	44(3)	44(3)	44(3)	1(3)	1(3)	-1(3)
Li(2)	40(4)	53(4)	50(4)	0(3)	7(3)	-3(3)
C(1)	46(2)	43(2)	45(2)	1(2)	3(2)	2(2)
C(2)	47(2)	47(2)	39(2)	0(2)	-3(2)	-3(2)
C(3)	42(2)	69(3)	39(2)	-3(2)	-1(2)	1(2)
C(4)	67(3)	72(3)	57(3)	-4(2)	14(2)	25(3)
C(5)	80(3)	51(3)	63(3)	5(2)	14(3)	16(2)
C(6)	57(3)	57(3)	44(2)	8(2)	8(2)	7(2)
C(7)	51(3)	95(4)	50(3)	-3(2)	10(2)	-7(3)
C(8)	164(7)	56(4)	143(6)	14(4)	63(5)	32(4)
O(1)	60(2)	52(2)	68(2)	-5(2)	32(2)	-8(1)
C(10)	55(3)	53(3)	69(3)	-11(2)	25(2)	0(2)
C(11)	84(4)	96(5)	165(7)	25(5)	27(5)	12(4)
C(12)	136(6)	103(5)	89(4)	-41(4)	41(4)	-32(4)
C(13)	75(3)	51(3)	93(4)	-6(2)	42(3)	-9(2)
C(14)	157(7)	75(4)	226(9)	3(5)	148(7)	-25(4)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s84.

	x	y	z	U(eq)
H(2)	9897	3870	156	53
H(4)	10557	2114	-351	78
H(6)	9160	2283	1009	63
H(7A)	11088	3055	-785	98
H(7B)	10950	3747	-457	98
H(7C)	10501	3497	-1042	98
H(8A)	10104	1204	747	181
H(8B)	9925	1140	-8	181
H(8C)	9359	1218	521	181
H(11A)	6956	6311	1820	172
H(11B)	6935	5675	1372	172
H(11C)	6599	5667	2075	172
H(12A)	7666	6328	2801	164
H(12B)	7326	5684	3077	164
H(12C)	8099	5706	2980	164
H(13A)	8177	6285	1677	109
H(13B)	8571	5646	1885	109
H(13C)	8106	5630	1260	109
H(14A)	7169	4101	2424	229
H(14B)	7107	4706	2910	229
H(14C)	6694	4692	2249	229

Table S7. Torsion angles [°] for s84.

C(6)-C(1)-C(2)-C(3)	-0.6(6)
Li(1)-C(1)-C(2)-C(3)	-179.0(4)
Li(2)#2-C(1)-C(2)-C(3)	-117.4(5)
Li(2)#1-C(1)-C(2)-C(3)	121.1(5)
C(6)-C(1)-C(2)-Li(1)	178.4(4)
Li(2)#2-C(1)-C(2)-Li(1)	61.6(3)
Li(2)#1-C(1)-C(2)-Li(1)	-59.9(4)
C(1)-C(2)-C(3)-C(4)	0.3(6)
C(1)-C(2)-C(3)-C(7)	179.3(4)
C(2)-C(3)-C(4)-C(5)	1.0(7)
C(7)-C(3)-C(4)-C(5)	-178.1(4)
C(3)-C(4)-C(5)-C(6)	-1.9(7)
C(3)-C(4)-C(5)-C(8)	178.8(5)
C(4)-C(5)-C(6)-C(1)	1.7(7)
C(8)-C(5)-C(6)-C(1)	-179.0(5)
C(4)-C(5)-C(6)-Li(2)#2	78.2(8)
C(8)-C(5)-C(6)-Li(2)#2	-102.5(7)
C(4)-C(5)-C(6)-Li(2)#1	-75.5(8)
C(8)-C(5)-C(6)-Li(2)#1	103.8(8)
C(2)-C(1)-C(6)-C(5)	-0.5(6)
Li(1)-C(1)-C(6)-C(5)	175.6(6)
Li(2)#2-C(1)-C(6)-C(5)	135.4(5)
Li(2)#1-C(1)-C(6)-C(5)	-141.2(5)
C(2)-C(1)-C(6)-Li(2)#2	-135.8(4)
Li(1)-C(1)-C(6)-Li(2)#2	40.3(7)
Li(2)#1-C(1)-C(6)-Li(2)#2	83.4(4)
C(2)-C(1)-C(6)-Li(2)#1	140.7(4)
Li(1)-C(1)-C(6)-Li(2)#1	-43.2(7)
Li(2)#2-C(1)-C(6)-Li(2)#1	-83.4(4)
C(14)-O(1)-C(10)-C(12)	65.1(7)
Li(2)-O(1)-C(10)-C(12)	-120.1(5)
C(14)-O(1)-C(10)-C(13)	-175.4(6)
Li(2)-O(1)-C(10)-C(13)	-0.6(6)
C(14)-O(1)-C(10)-C(11)	-57.6(7)
Li(2)-O(1)-C(10)-C(11)	117.2(5)

Symmetry transformations used to generate equivalent atoms:
#1 y+1/2,-z+1/2,-x+1 #2 -z+1,x-1/2,-y+1/2

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