SUPPLEMENTARY INFORMATION

Use of tetrameric cubane aggregates of lithium aryloxides as secondary building units in controlling network assembly

Dugald J. MacDougall, J. Jacob Morris, Bruce C. Noll, Kenneth W. Henderson*

Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556.

E-mail: khenders@nd.edu

General procedures

All experimental manipulations were performed under a dry nitrogen atmosphere in flame-dried glassware using standard Schlenk techniques. Dioxane was distilled from CaH_2 and stored over 4 Å molecular sieves prior to use. Hexane was dried by passage through columns of copper-based catalyst and alumina (Innovative Technology). BuLi was purchased from Aldrich as a 1.6 M solution in hexane and was standardized by titration against salicylaldehyde phenylhydrazone directly before use.[1] The phenols and 1-naphthol were purchased from Lancaster and dried by recrystallization from hexane or toluene prior to use.

NMR Spectroscopy

Spectra were obtained either on a Varian Unity Plus 300 MHz or on a Bruker AVANCE DPX-400 instrument. ^{1}H and ^{13}C spectra were referenced with respect to the residual solvent signal.

X-Ray Crystallography

Crystals were examined under Infineum V8512 oil. The datum crystal was affixed to a thin glass fiber mounted atop a tapered copper mounting-pin and transferred to the 100 K nitrogen stream of a Bruker APEX diffractometer equipped with an Oxford Cryosystems 700 series low-temperature apparatus. Cell parameters were determined using reflections harvested from three sets of 20 0.3° ω scans. The orientation matrix derived from this was passed to COSMO[2] to determine the optimum data collection strategy. Cell parameters were refined using reflections with $I \geq 10\sigma(I)$ harvested from the entire data collection. All data were corrected for Lorentz and polarization effects, as well as for absorption.

The structures were solved and refined using SHELXTL.[3] Structure solution was by direct methods. Non-hydrogen atoms not present in the direct methods solution were

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[1] B. E. Love, E. G. Jones, *J. Org. Chem.* **1999**, *64*, 3755-3756.
[2] J. Kaercher, *COSMO,* Bruker-Nonius AXS, Inc., Madison, Wisconsin, USA, **2003**.
[3] G. M. Sheldrick, University of Göttingen.

located by successive cycles of full-matrix least-squares refinement on F^2. All non-hydrogen atoms were refined with parameters for anisotropic thermal motion. Hydrogen atoms were placed at idealized geometries and allowed to ride on the position of the parent atom. Hydrogen thermal parameters were set to 1.2× the equivalent isotropic U of the parent atom, 1.5× for methyl hydrogens. Details on individual refinements, including descriptions of disorder, can be found in the cif files CCDC 239838, 239840 and 239844, which can be obtained online free of charge (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Phase identification was done with X-Ray powder diffraction performed on a D8 Bruker diffractometer (Cu Kα, λ = 1.54178 Å). The patterns were collected in steps of 0.02° (2θ) over the angular range 4-60° (2θ). Compound **1** used a step size of 0.02, with a step time of 20 s. Compounds **2** and **3** used a step size of 0.04, with a step time of 1 s. From the calculated crystal structures, determined by single crystal X-ray diffraction, pure powder diffraction patterns were derived using Powder Cell for Windows version 2.4.[4] The theoretical powder patterns were then compared to the actual powder patterns.

Experimental Procedures

Synthesis of $[(PhOLi)_4 \cdot 3Dioxane]_\infty$, 1

BuLi (5 mmol, 3.2 mL) was added to a stirred solution of phenol (5 mmol, 470 mg) in dioxane (7.5 mL). A white precipitate rapidly formed, which dissolved on heating. Crystalline material was obtained by slowly cooling the hot solution in a warm water bath. The product was found to lose solvent on isolation to give a dioxane:phenoxide ratio of 0.5:1, as determined by ^{1}H NMR spectroscopy. Yield: 230 mg, 31.9 %.

^{1}H NMR (300 MHz, DMSO-d_6, 25 °C): δ = 3.59 (s, 4H, OCH_2, dioxane), 6.29 (t, $^3J_{H,H}$ = 8.1 Hz, 1H, *p*-H, Ph), 6.57 (d, $^3J_{H,H}$ = 7.8 Hz, 2H, *o*-H, Ph), 6.95 (t, $^3J_{H,H}$ = 7.5 Hz, 2H, *m*-H, Ph).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6, 25 °C): δ = 66.46 (OCH_2, dioxane), 111.73 (*p*-C, Ph), 119.86 (*o*-C, Ph), 128.48 (*m*-C, Ph), 168.51 (*i*-C, Ph).

Synthesis of $[\{(4\text{-}Et\text{-}C_6H_4OLi)_4 \cdot 5/2Dioxane\} \cdot Dioxane]_\infty$, 2

BuLi (5 mmol, 3.2 mL) was added to a stirred solution of 4-isopropy1phenol (5 mmol, 621 mg) in dioxane (5 mL). On the addition of hexane (12 mL) a white precipitate formed, which dissolved on heating. Crystalline material was obtained by slowly cooling the resulting solution in a hot water bath. The product was found to lose solvent on isolation to give a dioxane:aryloxide ratio of 0.57:1, as determined by ^{1}H NMR spectroscopy. Yield: 650 mg, 72.9 %.

[4] W. Kraus, G. Nolze, Federal Institute for Materials Research and Testing, Berlin, **2000**.

^{1}H NMR (300 MHz, DMSO-d_6, 25 °C): δ = 1.13 (t, $^{3}J_{H,H}$ = 7.5 Hz, 3H, CH_3, Et), 2.44 (d, $^{3}J_{H,H}$ = 7.8 Hz, 2H, CH_2, Et), 3.59 (s, 4.6H, OCH_2, dioxane), 6.50 (d, $^{3}J_{H,H}$ = 8.1 Hz, 2H, *o*-H, Ph), 6.79 (d, $^{3}J_{H,H}$ = 8.1Hz, 2H, *m*-H, Ph).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6, 25 °C): δ = 16.86 (CH_3, Et), 27.70 (CH_2, Et), 66.46 (OCH_2, dioxane), 119.44 (*o*-C, Ph), 126.71 (*p*-C, Ph), 127.70 (*m*-C, Ph), 166.24 (*i*-C, Ph).

Synthesis of [{($C_{10}H_7OLi)_4$·2Dioxane}·3Dioxane]$_\infty$, 3

BuLi (5 mmol, 3.2 mL) was added to a stirred solution of 1-naphthol (5 mmol, 720 mg) in dioxane (5 mL). A white precipitate rapidly formed, which dissolved on dilution with dioxane (7 mL) and heating. Crystalline material was obtained by slowly cooling the resulting solution in a hot water bath. The product was found to lose solvent on isolation to give a dioxane:alkoxide ratio of 0.87:1, as determined by ^{1}H NMR spectroscopy. Yield: 730 mg, 68.5 %.

^{1}H NMR (300 MHz, DMSO-d_6, 25 °C): δ = 3.59 (s, 5.5H, OCH_2, dioxane), 6.60 (d, $^{3}J_{H,H}$ = 7.8 Hz, 1H, naphthyl-H), 6.69 (d, $^{3}J_{H,H}$ = 7.8 Hz, 1H, naphthyl-H), 7.08 (t, $^{3}J_{H,H}$ = 7.5 Hz, 1H, naphthy-H), 7.1 (t, $^{3}J_{H,H}$ = 7.8 Hz, 1H, naphthy-H), 7.24 (t, $^{3}J_{H,H}$ = 7.1 Hz, 1H, naphthy-H), 7.57 (d, $^{3}J_{H,H}$ = 8.1 Hz, 1H, naphthy-H), 8.59 (d, $^{3}J_{H,H}$ = 8.01 Hz, 1H, naphthy-H).

^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6, 25 °C): δ = 66.48 (OCH_2, dioxane), 108.17, 110.51, 120.46), 124.36, 125.74, 126.48, 128.20, 130.24, 135.90, 167.14 (naphthyl).

$[(PhOLi)_4 \cdot 3Dioxane]_\infty$, 1

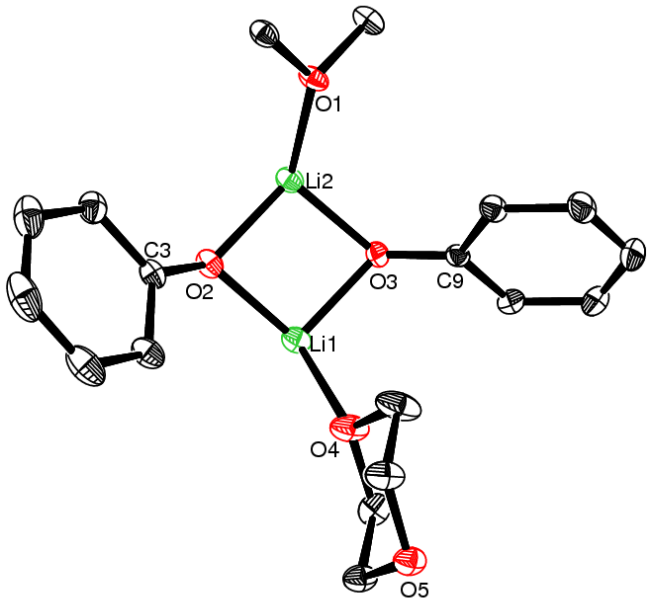


Table 1. Crystal data and structure refinement for **1**

Identification code	bcn16m	
Empirical formula	C18 H22 Li2 O5	
Formula weight	332.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 13.0937(9) Å	α= 90°.
	b = 17.7646(12) Å	β= 94.853(4)°.
	c = 15.7526(11) Å	γ = 90°.
Volume	3651.0(4) $Å^3$	
Z	8	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	1408	
Crystal size	0.36 x 0.22 x 0.17 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Bruker SMART APEX CCD area detector	
Theta range for data collection	1.94 to 33.00°	
Index ranges	-20<=h<=20, -27<=k<=24, -22<=l<=23	
Reflections collected	30134	
Independent reflections	6840 [R(int) = 0.0294]	
Observed reflections (I > 2sigma(I))	5889	
Completeness to theta = 33.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9857 and 0.9701	
Solution method	SHELXS-97 (Sheldrick, 1990)	
Refinement method	SHELXL-97 (Sheldrick, 1997)	
Data / restraints / parameters	6840 / 0 / 314	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.1170	

R indices (all data)	R1 = 0.0475, wR2 = 0.1224
Largest diff. peak and hole	0.498 and -0.229 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for **1**.

C(1)-O(1)	1.4402(8)	C(1)-C(2)#1	1.5122(10)
C(1)-H(1A)	0.974(10)	C(1)-H(1B)	0.966(12)
C(2)-O(1)	1.4330(8)	C(2)-C(1)#1	1.5122(9)
C(2)-H(2A)	0.964(11)	C(2)-H(2B)	0.960(12)
C(3)-O(2)	1.3300(8)	C(3)-C(4)	1.4085(10)
C(3)-C(8)	1.4087(10)	C(4)-C(5)	1.3959(12)
C(4)-H(4)	0.985(12)	C(5)-C(6)	1.3892(15)
C(5)-H(5)	1.022(15)	C(6)-C(7)	1.3838(15)
C(6)-H(6)	0.980(15)	C(7)-C(8)	1.3912(11)
C(7)-H(7)	0.997(15)	C(8)-H(8)	1.007(12)
C(9)-O(3)	1.3305(8)	C(9)-C(10)	1.4080(9)
C(9)-C(14)	1.4099(10)	C(10)-C(11)	1.3935(10)
C(10)-H(10)	0.983(11)	C(11)-C(12)	1.3889(13)
C(11)-H(11)	1.023(13)	C(12)-C(13)	1.3883(13)
C(12)-H(12)	0.967(13)	C(13)-C(14)	1.3947(11)
C(13)-H(13)	0.991(14)	C(14)-H(14)	0.962(12)
C(15)-O(4)	1.4403(10)	C(15)-C(16)	1.5058(11)
C(15)-H(15A)	0.984(14)	C(15)-H(15B)	1.048(14)
C(16)-O(5)	1.4205(10)	C(16)-H(16A)	1.006(12)
C(16)-H(16B)	1.014(12)	C(17)-O(5)	1.4293(9)
C(17)-C(18)	1.5036(11)	C(17)-H(17A)	0.974(11)
C(17)-H(17B)	1.002(14)	C(18)-O(4)	1.4350(10)
C(18)-H(18A)	1.003(12)	C(18)-H(18B)	1.004(13)
Li(1)-O(4)	1.9079(13)	Li(1)-O(2)#2	1.9359(13)
Li(1)-O(3)	1.9522(14)	Li(1)-O(2)	1.9645(14)
Li(1)-Li(2)#2	2.5668(17)	Li(1)-Li(2)	2.5987(18)
Li(1)-Li(1)#2	2.639(3)	Li(2)-O(2)	1.9269(13)
Li(2)-O(3)	1.9377(14)	Li(2)-O(1)	1.9403(13)
Li(2)-O(3)#2	1.9440(13)	Li(2)-Li(1)#2	2.5669(17)
Li(2)-Li(2)#2	2.673(2)	O(2)-Li(1)#2	1.9358(13)
O(3)-Li(2)#2	1.9440(13)		

O(1)-C(1)-C(2)#1	110.37(5)	O(1)-C(1)-H(1A)	107.5(6)
C(2)#1-C(1)-H(1A)	112.0(6)	O(1)-C(1)-H(1B)	106.3(7)
C(2)#1-C(1)-H(1B)	112.7(7)	H(1A)-C(1)-H(1B)	107.7(9)
O(1)-C(2)-C(1)#1	109.91(6)	O(1)-C(2)-H(2A)	107.1(7)
C(1)#1-C(2)-H(2A)	111.5(7)	O(1)-C(2)-H(2B)	106.1(7)
C(1)#1-C(2)-H(2B)	109.5(7)	H(2A)-C(2)-H(2B)	112.6(10)
O(2)-C(3)-C(4)	121.65(6)	O(2)-C(3)-C(8)	121.01(6)
C(4)-C(3)-C(8)	117.34(6)	C(5)-C(4)-C(3)	120.82(8)
C(5)-C(4)-H(4)	120.1(7)	C(3)-C(4)-H(4)	119.0(7)
C(6)-C(5)-C(4)	120.92(8)	C(6)-C(5)-H(5)	119.7(8)
C(4)-C(5)-H(5)	119.3(8)	C(7)-C(6)-C(5)	118.77(8)
C(7)-C(6)-H(6)	120.8(8)	C(5)-C(6)-H(6)	120.4(8)
C(6)-C(7)-C(8)	121.11(8)	C(6)-C(7)-H(7)	118.2(9)
C(8)-C(7)-H(7)	120.7(9)	C(7)-C(8)-C(3)	120.99(8)
C(7)-C(8)-H(8)	120.3(7)	C(3)-C(8)-H(8)	118.7(7)
O(3)-C(9)-C(10)	121.03(6)	O(3)-C(9)-C(14)	121.72(6)
C(10)-C(9)-C(14)	117.25(6)	C(11)-C(10)-C(9)	121.32(7)
C(11)-C(10)-H(10)	120.1(7)	C(9)-C(10)-H(10)	118.6(7)
C(12)-C(11)-C(10)	120.61(7)	C(12)-C(11)-H(11)	119.3(7)
C(10)-C(11)-H(11)	120.1(7)	C(13)-C(12)-C(11)	118.95(7)
C(13)-C(12)-H(12)	121.6(8)	C(11)-C(12)-H(12)	119.4(8)
C(12)-C(13)-C(14)	120.99(8)	C(12)-C(13)-H(13)	119.9(8)
C(14)-C(13)-H(13)	119.0(8)	C(13)-C(14)-C(9)	120.86(7)
C(13)-C(14)-H(14)	121.9(7)	C(9)-C(14)-H(14)	117.2(7)
O(4)-C(15)-C(16)	109.92(7)	O(4)-C(15)-H(15A)	106.5(9)
C(16)-C(15)-H(15A)	109.2(8)	O(4)-C(15)-H(15B)	107.8(8)
C(16)-C(15)-H(15B)	110.6(8)	H(15A)-C(15)-H(15B)	112.8(12)
O(5)-C(16)-C(15)	110.92(7)	O(5)-C(16)-H(16A)	108.1(7)
C(15)-C(16)-H(16A)	110.1(7)	O(5)-C(16)-H(16B)	107.4(7)
C(15)-C(16)-H(16B)	110.4(7)	H(16A)-C(16)-H(16B)	109.9(10)
O(5)-C(17)-C(18)	110.83(6)	O(5)-C(17)-H(17A)	110.0(7)
C(18)-C(17)-H(17A)	109.5(7)	O(5)-C(17)-H(17B)	108.8(8)
C(18)-C(17)-H(17B)	107.4(8)	H(17A)-C(17)-H(17B)	110.3(10)
O(4)-C(18)-C(17)	109.60(6)	O(4)-C(18)-H(18A)	107.4(7)
C(17)-C(18)-H(18A)	111.5(7)	O(4)-C(18)-H(18B)	107.7(7)
C(17)-C(18)-H(18B)	111.6(7)	H(18A)-C(18)-H(18B)	108.9(10)
O(4)-Li(1)-O(2)#2	129.52(7)	O(4)-Li(1)-O(3)	108.07(7)
O(2)#2-Li(1)-O(3)	96.81(6)	O(4)-Li(1)-O(2)	125.25(7)
O(2)#2-Li(1)-O(2)	94.13(6)	O(3)-Li(1)-O(2)	95.16(6)
O(4)-Li(1)-Li(2)#2	137.33(7)	O(2)#2-Li(1)-Li(2)#2	48.21(4)
O(3)-Li(1)-Li(2)#2	48.65(4)	O(2)-Li(1)-Li(2)#2	95.11(6)
O(4)-Li(1)-Li(2)	134.35(7)	O(2)#2-Li(1)-Li(2)	94.83(6)
O(3)-Li(1)-Li(2)	47.84(4)	O(2)-Li(1)-Li(2)	47.49(4)
Li(2)#2-Li(1)-Li(2)	62.33(6)	O(4)-Li(1)-Li(1)#2	159.45(5)
O(2)#2-Li(1)-Li(1)#2	47.87(4)	O(3)-Li(1)-Li(1)#2	92.22(4)
O(2)-Li(1)-Li(1)#2	46.96(4)	Li(2)#2-Li(1)-Li(1)#2	59.87(5)
Li(2)-Li(1)-Li(1)#2	58.68(5)	O(2)-Li(2)-O(3)	96.86(6)
O(2)-Li(2)-O(1)	122.81(7)	O(3)-Li(2)-O(1)	120.04(7)
O(2)-Li(2)-O(3)#2	97.37(6)	O(3)-Li(2)-O(3)#2	91.98(6)
O(1)-Li(2)-O(3)#2	120.94(7)	O(2)-Li(2)-Li(1)#2	48.50(4)
O(3)-Li(2)-Li(1)#2	94.81(6)	O(1)-Li(2)-Li(1)#2	145.02(7)
O(3)#2-Li(2)-Li(1)#2	48.93(4)	O(2)-Li(2)-Li(1)	48.72(4)
O(3)-Li(2)-Li(1)	48.32(4)	O(1)-Li(2)-Li(1)	145.15(7)
O(3)#2-Li(2)-Li(1)	93.66(6)	Li(1)#2-Li(2)-Li(1)	61.45(6)
O(2)-Li(2)-Li(2)#2	92.71(4)	O(3)-Li(2)-Li(2)#2	46.57(4)
O(1)-Li(2)-Li(2)#2	144.47(4)	O(3)#2-Li(2)-Li(2)#2	46.37(4)

Li(1)#2-Li(2)-Li(2)#2	59.42(5)	Li(1)-Li(2)-Li(2)#2	58.25(5)
C(2)-O(1)-C(1)	110.46(5)	C(2)-O(1)-Li(2)	130.69(6)
C(1)-O(1)-Li(2)	114.85(6)	C(3)-O(2)-Li(2)	134.52(6)
C(3)-O(2)-Li(1)#2	124.69(6)	Li(2)-O(2)-Li(1)#2	83.29(6)
C(3)-O(2)-Li(1)	128.62(6)	Li(2)-O(2)-Li(1)	83.79(6)
Li(1)#2-O(2)-Li(1)	85.17(6)	C(9)-O(3)-Li(2)	131.68(6)
C(9)-O(3)-Li(2)#2	128.22(6)	Li(2)-O(3)-Li(2)#2	87.06(6)
C(9)-O(3)-Li(1)	127.08(6)	Li(2)-O(3)-Li(1)	83.84(6)
Li(2)#2-O(3)-Li(1)	82.42(5)	C(18)-O(4)-C(15)	110.18(6)
C(18)-O(4)-Li(1)	129.67(6)	C(15)-O(4)-Li(1)	117.09(6)
C(16)-O(5)-C(17)	110.17(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+1,y,-z+1/2

[{(4-Et-$C_6H_4OLi)_4$·5/2Dioxane}·Dioxane]$_\infty$, **2**

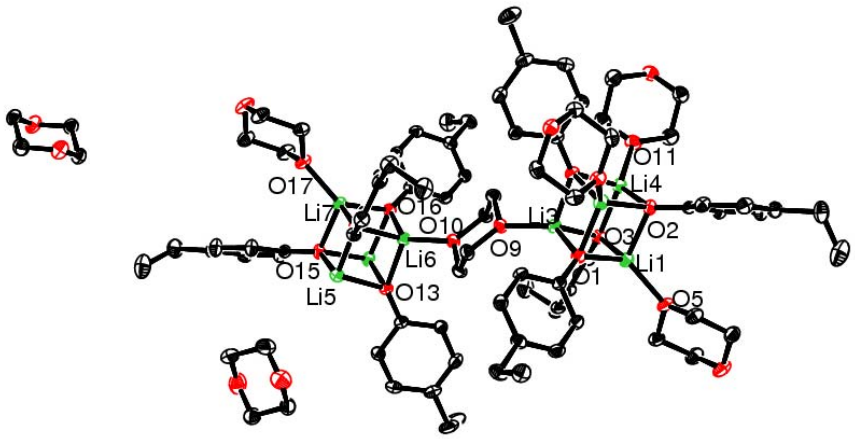


Table 3. Crystal data and structure refinement for **2**

Identification code	lw1	
Empirical formula	C92 H128 Li8 O22	
Formula weight	1641.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.3172(3) Å	α= 74.194(1)°.
	b = 15.2696(3) Å	β= 84.994(1)°.
	c = 24.5935(6) Å	γ = 62.507(1)°.
Volume	4584.39(17) Å^3	
Z	2	
Density (calculated)	1.189 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	1760	
Crystal size	0.34 x 0.30 x 0.26 mm^3	
Crystal color and habit	clear colorless cube	
Diffractometer	CCD area detector	
Theta range for data collection	0.86 to 28.28°	
Index ranges	-19<=h<=19, -20<=k<=20, -32<=l<=31	
Reflections collected	91923	
Independent reflections	22586 [R(int) = 0.0389]	
Observed reflections (I > 2sigma(I))	16431	
Completeness to theta = 28.28°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9787 and 0.9726	
Solution method	SHELXS-97 (Sheldrick, 1990)	
Refinement method	SHELXL-97 (Sheldrick, 1997)	
Data / restraints / parameters	22586 / 0 / 1107	
Goodness-of-fit on F^2	1.044	

Final R indices [I>2sigma(I)]	R1 = 0.0575, wR2 = 0.1584
R indices (all data)	R1 = 0.0810, wR2 = 0.1782
Largest diff. peak and hole	0.982 and -0.450 e.Å^{-3}

Table 4. Bond lengths [Å] and angles [°] for **2**.

Li(1)-O(3)	1.943(3)	Li(1)-O(1)	1.957(3)
Li(1)-O(2)	1.967(3)	Li(1)-O(5)	1.980(3)
Li(2)-O(2)	1.920(3)	Li(2)-O(7)	1.945(3)
Li(2)-O(1)	1.958(3)	Li(2)-O(4)	1.990(3)
Li(3)-O(4)	1.908(3)	Li(3)-O(9)	1.913(3)
Li(3)-O(1)	1.927(3)	Li(3)-O(3)	1.972(3)
Li(4)-O(3)	1.937(3)	Li(4)-O(2)	1.939(3)
Li(4)-O(4)	1.946(3)	Li(4)-O(11)	1.961(3)
Li(5)-O(13)	1.938(3)	Li(5)-O(15)	1.939(3)
Li(5)-O(14)	1.946(3)	Li(5)-O(12)#1	1.978(3)
Li(5)-Li(8)#2	2.662(4)	Li(6)-O(10)	1.907(3)
Li(6)-O(16)	1.917(3)	Li(6)-O(13)	1.918(3)
Li(6)-O(14)	1.982(3)	Li(6)-Li(8)#2	2.560(4)
Li(7)-O(14)	1.935(3)	Li(7)-O(15)	1.955(3)
Li(7)-O(16)	1.964(3)	Li(7)-O(17)	1.974(3)
Li(7)-Li(8)#2	2.617(4)	Li(8)-O(15)#3	1.914(3)
Li(8)-O(8)	1.944(3)	Li(8)-O(16)#3	1.974(3)
Li(8)-O(13)#3	1.991(3)	Li(8)-Li(6)#3	2.560(4)
Li(8)-Li(7)#3	2.617(4)	Li(8)-Li(5)#3	2.662(4)
Li(8)-C(53)#3	2.788(3)	O(1)-C(1)	1.3317(18)
O(2)-C(9)	1.3293(18)	O(3)-C(17)	1.3312(18)
O(4)-C(25)	1.3298(17)	O(5)-C(36)	1.439(2)
O(5)-C(33)	1.442(2)	O(6)-C(34)	1.428(2)
O(6)-C(35)	1.433(2)	O(7)-C(37)	1.433(2)
O(7)-C(40)	1.4383(19)	O(8)-C(38)	1.4383(19)
O(8)-C(39)	1.439(2)	O(9)-C(44)	1.4367(19)
O(9)-C(41)	1.4421(19)	O(10)-C(42)	1.4367(19)
O(10)-C(43)	1.4400(19)	O(11)-C(45)	1.436(2)
O(11)-C(48)	1.441(2)	O(12)-C(46)	1.442(2)
O(12)-C(47)	1.445(2)	O(12)-Li(5)#4	1.978(3)
O(13)-C(53)	1.3336(18)	O(13)-Li(8)#2	1.991(3)
O(14)-C(61)	1.3306(17)	O(15)-C(69)	1.3294(17)
O(15)-Li(8)#2	1.914(3)	O(16)-C(77)	1.3340(18)
O(16)-Li(8)#2	1.974(3)	O(17)-C(49)	1.436(2)
O(17)-C(52)	1.4382(19)	O(18)-C(51)	1.427(2)
O(18)-C(50)	1.430(2)	C(1)-C(6)	1.406(2)
C(1)-C(2)	1.410(2)	C(2)-C(3)	1.388(2)
C(2)-H(2)	0.9500	C(3)-C(4)	1.394(2)
C(3)-H(3)	0.9500	C(4)-C(5)	1.394(2)
C(4)-C(7)	1.515(2)	C(5)-C(6)	1.392(2)
C(5)-H(5)	0.9500	C(6)-H(6)	0.9500
C(7)-C(8)	1.520(2)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800	C(8)-H(8C)	0.9800
C(9)-C(14)	1.402(2)	C(9)-C(10)	1.402(2)
C(10)-C(11)	1.390(2)	C(10)-H(10)	0.9500
C(11)-C(12)	1.394(2)	C(11)-H(11)	0.9500
C(12)-C(13)	1.388(2)	C(12)-C(15)	1.515(2)
C(13)-C(14)	1.388(2)	C(13)-H(13)	0.9500
C(14)-H(14)	0.9500	C(15)-C(16)	1.489(3)

C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9800	C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800	C(17)-C(22)	1.401(2)
C(17)-C(18)	1.404(2)	C(18)-C(19)	1.391(2)
C(18)-H(18)	0.9500	C(19)-C(20)	1.382(3)
C(19)-H(19)	0.9500	C(20)-C(21)	1.388(3)
C(20)-C(23)	1.517(2)	C(21)-C(22)	1.387(2)
C(21)-H(21)	0.9500	C(22)-H(22)	0.9500
C(23)-C(24)	1.518(3)	C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(25)-C(26)	1.406(2)	C(25)-C(30)	1.411(2)
C(26)-C(27)	1.389(2)	C(26)-H(26)	0.9500
C(27)-C(28)	1.395(2)	C(27)-H(27)	0.9500
C(28)-C(29)	1.396(2)	C(28)-C(31)	1.514(2)
C(29)-C(30)	1.394(2)	C(29)-H(29)	0.9500
C(30)-H(30)	0.9500	C(31)-C(32)	1.525(3)
C(31)-H(31A)	0.9900	C(31)-H(31B)	0.9900
C(32)-H(32A)	0.9800	C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800	C(33)-C(34)	1.506(2)
C(33)-H(33A)	0.9900	C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900	C(34)-H(34B)	0.9900
C(35)-C(36)	1.504(2)	C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900	C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900	C(37)-C(38)	1.505(2)
C(37)-H(37A)	0.9900	C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9900	C(38)-H(38B)	0.9900
C(39)-C(40)	1.504(2)	C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900	C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900	C(41)-C(42)	1.503(2)
C(41)-H(41A)	0.9900	C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9900	C(42)-H(42B)	0.9900
C(43)-C(44)	1.502(2)	C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900	C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900	C(45)-C(46)	1.494(2)
C(45)-H(45A)	0.9900	C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9900	C(46)-H(46B)	0.9900
C(47)-C(48)	1.509(2)	C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900	C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900	C(49)-C(50)	1.507(2)
C(49)-H(49A)	0.9900	C(49)-H(49B)	0.9900
C(50)-H(50A)	0.9900	C(50)-H(50B)	0.9900
C(51)-C(52)	1.504(2)	C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900	C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900	C(53)-C(58)	1.404(2)
C(53)-C(54)	1.406(2)	C(53)-Li(8)#2	2.787(3)
C(54)-C(55)	1.391(2)	C(54)-H(54)	0.9500
C(55)-C(56)	1.387(2)	C(55)-H(55)	0.9500
C(56)-C(57)	1.394(3)	C(56)-C(59)	1.515(2)
C(57)-C(58)	1.389(2)	C(57)-H(57)	0.9500
C(58)-H(58)	0.9500	C(59)-C(60)	1.516(3)
C(59)-H(59A)	0.9900	C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9800	C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800	C(61)-C(62)	1.404(2)
C(61)-C(66)	1.407(2)	C(62)-C(63)	1.390(2)
C(62)-H(62)	0.9500	C(63)-C(64)	1.391(2)

C(63)-H(63)	0.9500	C(64)-C(65)	1.392(2)
C(64)-C(67)	1.518(2)	C(65)-C(66)	1.387(2)
C(65)-H(65)	0.9500	C(66)-H(66)	0.9500
C(67)-C(68)	1.522(2)	C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900	C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800	C(68)-H(68C)	0.9800
C(69)-C(70)	1.401(2)	C(69)-C(74)	1.404(2)
C(70)-C(71)	1.391(2)	C(70)-H(70)	0.9500
C(71)-C(72)	1.392(2)	C(71)-H(71)	0.9500
C(72)-C(73)	1.389(2)	C(72)-C(75)	1.522(2)
C(73)-C(74)	1.387(2)	C(73)-H(73)	0.9500
C(74)-H(74)	0.9500	C(75)-C(76)	1.488(3)
C(75)-H(75A)	0.9900	C(75)-H(75B)	0.9900
C(76)-H(76A)	0.9800	C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800	C(77)-C(78)	1.405(2)
C(77)-C(82)	1.407(2)	C(78)-C(79)	1.387(2)
C(78)-H(78)	0.9500	C(79)-C(80)	1.395(2)
C(79)-H(79)	0.9500	C(80)-C(81)	1.391(2)
C(80)-C(83)	1.516(2)	C(81)-C(82)	1.394(2)
C(81)-H(81)	0.9500	C(82)-H(82)	0.9500
C(83)-C(84)	1.519(3)	C(83)-H(83A)	0.9900
C(83)-H(83B)	0.9900	C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800	C(84)-H(84C)	0.9800
O(19)-C(92)	1.424(2)	O(19)-C(89)	1.425(2)
O(20)-C(91)	1.420(2)	O(20)-C(90)	1.438(2)
C(85)-O(21)	1.425(3)	C(85)-C(86)	1.511(3)
C(85)-H(85A)	0.9900	C(85)-H(85B)	0.9900
C(86)-O(22)	1.423(3)	C(86)-H(86A)	0.9900
C(86)-H(86B)	0.9900	C(87)-O(22)	1.424(2)
C(87)-C(88)	1.494(3)	C(87)-H(87A)	0.9900
C(87)-H(87B)	0.9900	C(88)-O(21)	1.409(2)
C(88)-H(88A)	0.9900	C(88)-H(88B)	0.9900
C(89)-C(90)	1.496(3)	C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900	C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900	C(91)-C(92)	1.498(2)
C(91)-H(91A)	0.9900	C(91)-H(91B)	0.9900
C(92)-H(92A)	0.9900	C(92)-H(92B)	0.9900

O(3)-Li(1)-O(1)	93.79(12)	O(3)-Li(1)-O(2)	93.69(12)
O(1)-Li(1)-O(2)	95.07(12)	O(3)-Li(1)-O(5)	125.46(14)
O(1)-Li(1)-O(5)	126.31(15)	O(2)-Li(1)-O(5)	114.51(14)
O(2)-Li(2)-O(7)	125.33(15)	O(2)-Li(2)-O(1)	96.54(12)
O(7)-Li(2)-O(1)	121.00(14)	O(2)-Li(2)-O(4)	92.77(12)
O(7)-Li(2)-O(4)	118.21(14)	O(1)-Li(2)-O(4)	95.94(12)
O(4)-Li(3)-O(9)	111.26(14)	O(4)-Li(3)-O(1)	99.78(13)
O(9)-Li(3)-O(1)	130.61(15)	O(4)-Li(3)-O(3)	93.96(12)
O(9)-Li(3)-O(3)	120.17(14)	O(1)-Li(3)-O(3)	93.80(12)
O(3)-Li(4)-O(2)	94.79(12)	O(3)-Li(4)-O(4)	93.89(12)
O(2)-Li(4)-O(4)	93.56(12)	O(3)-Li(4)-O(11)	124.43(14)
O(2)-Li(4)-O(11)	129.40(15)	O(4)-Li(4)-O(11)	111.94(14)
O(13)-Li(5)-O(15)	93.75(12)	O(13)-Li(5)-O(14)	94.38(12)
O(15)-Li(5)-O(14)	94.49(12)	O(13)-Li(5)-O(12)#1	112.44(14)
O(15)-Li(5)-O(12)#1	129.26(15)	O(14)-Li(5)-O(12)#1	124.03(14)
O(13)-Li(5)-Li(8)#2	48.20(9)	O(15)-Li(5)-Li(8)#2	45.91(8)
O(14)-Li(5)-Li(8)#2	91.79(12)	O(12)#1-Li(5)-Li(8)#2	142.74(14)

O(10)-Li(6)-O(16)	128.18(15)	O(10)-Li(6)-O(13)	112.47(14)
O(16)-Li(6)-O(13)	100.09(12)	O(10)-Li(6)-O(14)	121.08(14)
O(16)-Li(6)-O(14)	94.37(12)	O(13)-Li(6)-O(14)	93.86(12)
O(10)-Li(6)-Li(8)#2	143.52(15)	O(16)-Li(6)-Li(8)#2	49.83(9)
O(13)-Li(6)-Li(8)#2	50.34(9)	O(14)-Li(6)-Li(8)#2	94.04(12)
O(14)-Li(7)-O(15)	94.29(12)	O(14)-Li(7)-O(16)	94.35(12)
O(15)-Li(7)-O(16)	95.13(12)	O(14)-Li(7)-O(17)	126.65(15)
O(15)-Li(7)-O(17)	110.51(13)	O(16)-Li(7)-O(17)	127.56(15)
O(14)-Li(7)-Li(8)#2	93.39(12)	O(15)-Li(7)-Li(8)#2	46.77(9)
O(16)-Li(7)-Li(8)#2	48.51(9)	O(17)-Li(7)-Li(8)#2	138.02(14)
O(15)#3-Li(8)-O(8)	123.05(14)	O(15)#3-Li(8)-O(16)#3	96.15(12)
O(8)-Li(8)-O(16)#3	121.96(14)	O(15)#3-Li(8)-O(13)#3	92.85(12)
O(8)-Li(8)-O(13)#3	120.06(14)	O(16)#3-Li(8)-O(13)#3	95.70(12)
O(15)#3-Li(8)-Li(6)#3	94.52(12)	O(8)-Li(8)-Li(6)#3	142.33(14)
O(16)#3-Li(8)-Li(6)#3	47.91(9)	O(13)#3-Li(8)-Li(6)#3	47.86(9)
O(15)#3-Li(8)-Li(7)#3	48.10(9)	O(8)-Li(8)-Li(7)#3	146.60(15)
O(16)#3-Li(8)-Li(7)#3	48.20(9)	O(13)#3-Li(8)-Li(7)#3	93.34(12)
Li(6)#3-Li(8)-Li(7)#3	61.23(10)	O(15)#3-Li(8)-Li(5)#3	46.68(9)
O(8)-Li(8)-Li(5)#3	143.98(15)	O(16)#3-Li(8)-Li(5)#3	93.99(12)
O(13)#3-Li(8)-Li(5)#3	46.53(9)	Li(6)#3-Li(8)-Li(5)#3	60.76(10)
Li(7)#3-Li(8)-Li(5)#3	60.00(10)	O(15)#3-Li(8)-C(53)#3	108.40(12)
O(8)-Li(8)-C(53)#3	93.85(11)	O(16)#3-Li(8)-C(53)#3	113.82(12)
O(13)#3-Li(8)-C(53)#3	26.24(6)	Li(6)#3-Li(8)-C(53)#3	69.17(9)
Li(7)#3-Li(8)-C(53)#3	119.51(12)	Li(5)#3-Li(8)-C(53)#3	66.84(9)
C(1)-O(1)-Li(3)	125.67(12)	C(1)-O(1)-Li(1)	133.15(12)
Li(3)-O(1)-Li(1)	86.13(12)	C(1)-O(1)-Li(2)	129.01(12)
Li(3)-O(1)-Li(2)	82.24(12)	Li(1)-O(1)-Li(2)	83.70(12)
C(9)-O(2)-Li(2)	131.17(12)	C(9)-O(2)-Li(4)	134.59(12)
Li(2)-O(2)-Li(4)	87.48(12)	C(9)-O(2)-Li(1)	116.63(12)
Li(2)-O(2)-Li(1)	84.45(12)	Li(4)-O(2)-Li(1)	85.36(12)
C(17)-O(3)-Li(4)	139.20(13)	C(17)-O(3)-Li(1)	128.04(12)
Li(4)-O(3)-Li(1)	86.06(12)	C(17)-O(3)-Li(3)	115.75(12)
Li(4)-O(3)-Li(3)	85.00(12)	Li(1)-O(3)-Li(3)	85.26(12)
C(25)-O(4)-Li(3)	139.07(12)	C(25)-O(4)-Li(4)	130.50(12)
Li(3)-O(4)-Li(4)	86.53(12)	C(25)-O(4)-Li(2)	113.54(12)
Li(3)-O(4)-Li(2)	81.90(12)	Li(4)-O(4)-Li(2)	85.34(12)
C(36)-O(5)-C(33)	110.45(12)	C(36)-O(5)-Li(1)	124.60(12)
C(33)-O(5)-Li(1)	119.87(13)	C(34)-O(6)-C(35)	109.29(13)
C(37)-O(7)-C(40)	109.52(11)	C(37)-O(7)-Li(2)	124.15(13)
C(40)-O(7)-Li(2)	125.53(13)	C(38)-O(8)-C(39)	109.40(11)
C(38)-O(8)-Li(8)	126.06(12)	C(39)-O(8)-Li(8)	124.00(12)
C(44)-O(9)-C(41)	110.55(11)	C(44)-O(9)-Li(3)	134.11(12)
C(41)-O(9)-Li(3)	114.64(12)	C(42)-O(10)-C(43)	110.78(11)
C(42)-O(10)-Li(6)	130.89(12)	C(43)-O(10)-Li(6)	117.94(12)
C(45)-O(11)-C(48)	109.16(13)	C(45)-O(11)-Li(4)	126.80(13)
C(48)-O(11)-Li(4)	121.00(12)	C(46)-O(12)-C(47)	109.80(12)
C(46)-O(12)-Li(5)#4	115.01(12)	C(47)-O(12)-Li(5)#4	131.68(13)
C(53)-O(13)-Li(6)	137.82(12)	C(53)-O(13)-Li(5)	132.38(12)
Li(6)-O(13)-Li(5)	86.50(12)	C(53)-O(13)-Li(8)#2	112.45(12)
Li(6)-O(13)-Li(8)#2	81.79(12)	Li(5)-O(13)-Li(8)#2	85.27(11)
C(61)-O(14)-Li(7)	134.09(12)	C(61)-O(14)-Li(5)	136.36(12)
Li(7)-O(14)-Li(5)	85.72(12)	C(61)-O(14)-Li(6)	111.81(12)
Li(7)-O(14)-Li(6)	84.63(11)	Li(5)-O(14)-Li(6)	84.56(12)
C(69)-O(15)-Li(8)#2	133.19(12)	C(69)-O(15)-Li(5)	130.08(12)
Li(8)#2-O(15)-Li(5)	87.40(12)	C(69)-O(15)-Li(7)	119.79(12)
Li(8)#2-O(15)-Li(7)	85.13(12)	Li(5)-O(15)-Li(7)	85.36(12)

C(77)-O(16)-Li(6)	130.69(12)	C(77)-O(16)-Li(7)	132.86(12)
Li(6)-O(16)-Li(7)	85.58(12)	C(77)-O(16)-Li(8)#2	124.63(12)
Li(6)-O(16)-Li(8)#2	82.25(12)	Li(7)-O(16)-Li(8)#2	83.29(12)
C(49)-O(17)-C(52)	110.71(12)	C(49)-O(17)-Li(7)	125.24(12)
C(52)-O(17)-Li(7)	120.91(12)	C(51)-O(18)-C(50)	108.94(13)
O(1)-C(1)-C(6)	121.63(13)	O(1)-C(1)-C(2)	121.60(14)
C(6)-C(1)-C(2)	116.76(14)	C(3)-C(2)-C(1)	121.09(15)
C(3)-C(2)-H(2)	119.5	C(1)-C(2)-H(2)	119.5
C(2)-C(3)-C(4)	121.93(15)	C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0	C(3)-C(4)-C(5)	117.17(14)
C(3)-C(4)-C(7)	120.90(15)	C(5)-C(4)-C(7)	121.88(15)
C(6)-C(5)-C(4)	121.61(15)	C(6)-C(5)-H(5)	119.2
C(4)-C(5)-H(5)	119.2	C(5)-C(6)-C(1)	121.32(14)
C(5)-C(6)-H(6)	119.3	C(1)-C(6)-H(6)	119.3
C(4)-C(7)-C(8)	112.31(14)	C(4)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1	C(4)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1	H(7A)-C(7)-H(7B)	107.9
C(7)-C(8)-H(8A)	109.5	C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(8B)-C(8)-H(8C)	109.5
O(2)-C(9)-C(14)	121.52(14)	O(2)-C(9)-C(10)	121.44(13)
C(14)-C(9)-C(10)	117.02(14)	C(11)-C(10)-C(9)	121.17(14)
C(11)-C(10)-H(10)	119.4	C(9)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	121.51(15)	C(10)-C(11)-H(11)	119.2
C(12)-C(11)-H(11)	119.2	C(13)-C(12)-C(11)	117.36(15)
C(13)-C(12)-C(15)	121.25(16)	C(11)-C(12)-C(15)	121.38(16)
C(14)-C(13)-C(12)	121.73(15)	C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1	C(13)-C(14)-C(9)	121.21(15)
C(13)-C(14)-H(14)	119.4	C(9)-C(14)-H(14)	119.4
C(16)-C(15)-C(12)	112.98(17)	C(16)-C(15)-H(15A)	109.0
C(12)-C(15)-H(15A)	109.0	C(16)-C(15)-H(15B)	109.0
C(12)-C(15)-H(15B)	109.0	H(15A)-C(15)-H(15B)	107.8
C(15)-C(16)-H(16A)	109.5	C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5	C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(16B)-C(16)-H(16C)	109.5
O(3)-C(17)-C(22)	121.65(14)	O(3)-C(17)-C(18)	121.48(14)
C(22)-C(17)-C(18)	116.86(14)	C(19)-C(18)-C(17)	121.42(15)
C(19)-C(18)-H(18)	119.3	C(17)-C(18)-H(18)	119.3
C(20)-C(19)-C(18)	121.51(16)	C(20)-C(19)-H(19)	119.2
C(18)-C(19)-H(19)	119.2	C(19)-C(20)-C(21)	117.18(15)
C(19)-C(20)-C(23)	122.23(17)	C(21)-C(20)-C(23)	120.55(17)
C(22)-C(21)-C(20)	122.36(16)	C(22)-C(21)-H(21)	118.8
C(20)-C(21)-H(21)	118.8	C(21)-C(22)-C(17)	120.65(16)
C(21)-C(22)-H(22)	119.7	C(17)-C(22)-H(22)	119.7
C(20)-C(23)-C(24)	112.45(15)	C(20)-C(23)-H(23A)	109.1
C(24)-C(23)-H(23A)	109.1	C(20)-C(23)-H(23B)	109.1
C(24)-C(23)-H(23B)	109.1	H(23A)-C(23)-H(23B)	107.8
C(23)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
O(4)-C(25)-C(26)	121.29(14)	O(4)-C(25)-C(30)	121.73(14)
C(26)-C(25)-C(30)	116.97(14)	C(27)-C(26)-C(25)	121.42(15)
C(27)-C(26)-H(26)	119.3	C(25)-C(26)-H(26)	119.3
C(26)-C(27)-C(28)	121.57(15)	C(26)-C(27)-H(27)	119.2
C(28)-C(27)-H(27)	119.2	C(27)-C(28)-C(29)	117.40(15)
C(27)-C(28)-C(31)	120.90(16)	C(29)-C(28)-C(31)	121.59(16)

C(30)-C(29)-C(28)	121.70(15)	C(30)-C(29)-H(29)	119.1
C(28)-C(29)-H(29)	119.1	C(29)-C(30)-C(25)	120.90(15)
C(29)-C(30)-H(30)	119.6	C(25)-C(30)-H(30)	119.6
C(28)-C(31)-C(32)	111.91(14)	C(28)-C(31)-H(31A)	109.2
C(32)-C(31)-H(31A)	109.2	C(28)-C(31)-H(31B)	109.2
C(32)-C(31)-H(31B)	109.2	H(31A)-C(31)-H(31B)	107.9
C(31)-C(32)-H(32A)	109.5	C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5	C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(32B)-C(32)-H(32C)	109.5
O(5)-C(33)-C(34)	110.58(14)	O(5)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33A)	109.5	O(5)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33B)	109.5	H(33A)-C(33)-H(33B)	108.1
O(6)-C(34)-C(33)	110.63(14)	O(6)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34A)	109.5	O(6)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34B)	109.5	H(34A)-C(34)-H(34B)	108.1
O(6)-C(35)-C(36)	111.13(14)	O(6)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35A)	109.4	O(6)-C(35)-H(35B)	109.4
C(36)-C(35)-H(35B)	109.4	H(35A)-C(35)-H(35B)	108.0
O(5)-C(36)-C(35)	110.84(14)	O(5)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36A)	109.5	O(5)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36B)	109.5	H(36A)-C(36)-H(36B)	108.1
O(7)-C(37)-C(38)	110.70(13)	O(7)-C(37)-H(37A)	109.5
C(38)-C(37)-H(37A)	109.5	O(7)-C(37)-H(37B)	109.5
C(38)-C(37)-H(37B)	109.5	H(37A)-C(37)-H(37B)	108.1
O(8)-C(38)-C(37)	110.12(13)	O(8)-C(38)-H(38A)	109.6
C(37)-C(38)-H(38A)	109.6	O(8)-C(38)-H(38B)	109.6
C(37)-C(38)-H(38B)	109.6	H(38A)-C(38)-H(38B)	108.2
O(8)-C(39)-C(40)	109.89(13)	O(8)-C(39)-H(39A)	109.7
C(40)-C(39)-H(39A)	109.7	O(8)-C(39)-H(39B)	109.7
C(40)-C(39)-H(39B)	109.7	H(39A)-C(39)-H(39B)	108.2
O(7)-C(40)-C(39)	110.10(13)	O(7)-C(40)-H(40A)	109.6
C(39)-C(40)-H(40A)	109.6	O(7)-C(40)-H(40B)	109.6
C(39)-C(40)-H(40B)	109.6	H(40A)-C(40)-H(40B)	108.2
O(9)-C(41)-C(42)	110.10(13)	O(9)-C(41)-H(41A)	109.6
C(42)-C(41)-H(41A)	109.6	O(9)-C(41)-H(41B)	109.6
C(42)-C(41)-H(41B)	109.6	H(41A)-C(41)-H(41B)	108.2
O(10)-C(42)-C(41)	110.04(13)	O(10)-C(42)-H(42A)	109.7
C(41)-C(42)-H(42A)	109.7	O(10)-C(42)-H(42B)	109.7
C(41)-C(42)-H(42B)	109.7	H(42A)-C(42)-H(42B)	108.2
O(10)-C(43)-C(44)	110.26(13)	O(10)-C(43)-H(43A)	109.6
C(44)-C(43)-H(43A)	109.6	O(10)-C(43)-H(43B)	109.6
C(44)-C(43)-H(43B)	109.6	H(43A)-C(43)-H(43B)	108.1
O(9)-C(44)-C(43)	110.16(13)	O(9)-C(44)-H(44A)	109.6
C(43)-C(44)-H(44A)	109.6	O(9)-C(44)-H(44B)	109.6
C(43)-C(44)-H(44B)	109.6	H(44A)-C(44)-H(44B)	108.1
O(11)-C(45)-C(46)	110.77(14)	O(11)-C(45)-H(45A)	109.5
C(46)-C(45)-H(45A)	109.5	O(11)-C(45)-H(45B)	109.5
C(46)-C(45)-H(45B)	109.5	H(45A)-C(45)-H(45B)	108.1
O(12)-C(46)-C(45)	110.05(14)	O(12)-C(46)-H(46A)	109.7
C(45)-C(46)-H(46A)	109.6	O(12)-C(46)-H(46B)	109.7
C(45)-C(46)-H(46B)	109.7	H(46A)-C(46)-H(46B)	108.2
O(12)-C(47)-C(48)	110.17(14)	O(12)-C(47)-H(47A)	109.6
C(48)-C(47)-H(47A)	109.6	O(12)-C(47)-H(47B)	109.6
C(48)-C(47)-H(47B)	109.6	H(47A)-C(47)-H(47B)	108.1
O(11)-C(48)-C(47)	110.75(14)	O(11)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48A)	109.5	O(11)-C(48)-H(48B)	109.5

C(47)-C(48)-H(48B)	109.5	H(48A)-C(48)-H(48B)	108.1
O(17)-C(49)-C(50)	110.56(14)	O(17)-C(49)-H(49A)	109.5
C(50)-C(49)-H(49A)	109.5	O(17)-C(49)-H(49B)	109.5
C(50)-C(49)-H(49B)	109.5	H(49A)-C(49)-H(49B)	108.1
O(18)-C(50)-C(49)	110.51(15)	O(18)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50A)	109.5	O(18)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50B)	109.5	H(50A)-C(50)-H(50B)	108.1
O(18)-C(51)-C(52)	111.12(14)	O(18)-C(51)-H(51A)	109.4
C(52)-C(51)-H(51A)	109.4	O(18)-C(51)-H(51B)	109.4
C(52)-C(51)-H(51B)	109.4	H(51A)-C(51)-H(51B)	108.0
O(17)-C(52)-C(51)	110.80(14)	O(17)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52A)	109.5	O(17)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52B)	109.5	H(52A)-C(52)-H(52B)	108.1
O(13)-C(53)-C(58)	121.18(14)	O(13)-C(53)-C(54)	121.57(14)
C(58)-C(53)-C(54)	117.24(14)	O(13)-C(53)-Li(8)#2	41.31(8)
C(58)-C(53)-Li(8)#2	107.26(11)	C(54)-C(53)-Li(8)#2	118.24(11)
C(55)-C(54)-C(53)	120.74(15)	C(55)-C(54)-H(54)	119.6
C(53)-C(54)-H(54)	119.6	C(56)-C(55)-C(54)	122.02(15)
C(56)-C(55)-H(55)	119.0	C(54)-C(55)-H(55)	119.0
C(55)-C(56)-C(57)	117.20(15)	C(55)-C(56)-C(59)	121.51(17)
C(57)-C(56)-C(59)	121.18(16)	C(58)-C(57)-C(56)	121.82(15)
C(58)-C(57)-H(57)	119.1	C(56)-C(57)-H(57)	119.1
C(57)-C(58)-C(53)	120.94(15)	C(57)-C(58)-H(58)	119.5
C(53)-C(58)-H(58)	119.5	C(56)-C(59)-C(60)	112.12(16)
C(56)-C(59)-H(59A)	109.2	C(60)-C(59)-H(59A)	109.2
C(56)-C(59)-H(59B)	109.2	C(60)-C(59)-H(59B)	109.2
H(59A)-C(59)-H(59B)	107.9	C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5	H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5	H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5	O(14)-C(61)-C(62)	121.89(13)
O(14)-C(61)-C(66)	121.47(14)	C(62)-C(61)-C(66)	116.64(14)
C(63)-C(62)-C(61)	121.43(14)	C(63)-C(62)-H(62)	119.3
C(61)-C(62)-H(62)	119.3	C(62)-C(63)-C(64)	121.63(15)
C(62)-C(63)-H(63)	119.2	C(64)-C(63)-H(63)	119.2
C(63)-C(64)-C(65)	117.23(14)	C(63)-C(64)-C(67)	121.89(15)
C(65)-C(64)-C(67)	120.87(15)	C(66)-C(65)-C(64)	121.80(14)
C(66)-C(65)-H(65)	119.1	C(64)-C(65)-H(65)	119.1
C(65)-C(66)-C(61)	121.27(14)	C(65)-C(66)-H(66)	119.4
C(61)-C(66)-H(66)	119.4	C(64)-C(67)-C(68)	113.17(14)
C(64)-C(67)-H(67A)	108.9	C(68)-C(67)-H(67A)	108.9
C(64)-C(67)-H(67B)	108.9	C(68)-C(67)-H(67B)	108.9
H(67A)-C(67)-H(67B)	107.8	C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5	H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5	H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5	O(15)-C(69)-C(70)	121.27(14)
O(15)-C(69)-C(74)	121.83(14)	C(70)-C(69)-C(74)	116.90(14)
C(71)-C(70)-C(69)	121.40(15)	C(71)-C(70)-H(70)	119.3
C(69)-C(70)-H(70)	119.3	C(70)-C(71)-C(72)	121.50(16)
C(70)-C(71)-H(71)	119.3	C(72)-C(71)-H(71)	119.3
C(73)-C(72)-C(71)	117.05(15)	C(73)-C(72)-C(75)	120.65(16)
C(71)-C(72)-C(75)	122.27(16)	C(74)-C(73)-C(72)	122.21(15)
C(74)-C(73)-H(73)	118.9	C(72)-C(73)-H(73)	118.9
C(73)-C(74)-C(69)	120.92(15)	C(73)-C(74)-H(74)	119.5
C(69)-C(74)-H(74)	119.5	C(76)-C(75)-C(72)	115.89(17)
C(76)-C(75)-H(75A)	108.3	C(72)-C(75)-H(75A)	108.3
C(76)-C(75)-H(75B)	108.3	C(72)-C(75)-H(75B)	108.3

H(75A)-C(75)-H(75B)	107.4	C(75)-C(76)-H(76A)	109.5
C(75)-C(76)-H(76B)	109.5	H(76A)-C(76)-H(76B)	109.5
C(75)-C(76)-H(76C)	109.5	H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5	O(16)-C(77)-C(78)	121.55(13)
O(16)-C(77)-C(82)	121.82(13)	C(78)-C(77)-C(82)	116.62(13)
C(79)-C(78)-C(77)	121.32(14)	C(79)-C(78)-H(78)	119.3
C(77)-C(78)-H(78)	119.3	C(78)-C(79)-C(80)	121.91(14)
C(78)-C(79)-H(79)	119.0	C(80)-C(79)-H(79)	119.0
C(81)-C(80)-C(79)	117.04(14)	C(81)-C(80)-C(83)	121.85(15)
C(79)-C(80)-C(83)	121.06(15)	C(80)-C(81)-C(82)	121.71(14)
C(80)-C(81)-H(81)	119.1	C(82)-C(81)-H(81)	119.1
C(81)-C(82)-C(77)	121.23(14)	C(81)-C(82)-H(82)	119.4
C(77)-C(82)-H(82)	119.4	C(80)-C(83)-C(84)	112.90(14)
C(80)-C(83)-H(83A)	109.0	C(84)-C(83)-H(83A)	109.0
C(80)-C(83)-H(83B)	109.0	C(84)-C(83)-H(83B)	109.0
H(83A)-C(83)-H(83B)	107.8	C(83)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84B)	109.5	H(84A)-C(84)-H(84B)	109.5
C(83)-C(84)-H(84C)	109.5	H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5	C(92)-O(19)-C(89)	108.80(13)
C(91)-O(20)-C(90)	109.37(14)	O(21)-C(85)-C(86)	110.81(17)
O(21)-C(85)-H(85A)	109.5	C(86)-C(85)-H(85A)	109.5
O(21)-C(85)-H(85B)	109.5	C(86)-C(85)-H(85B)	109.5
H(85A)-C(85)-H(85B)	108.1	O(22)-C(86)-C(85)	109.77(19)
O(22)-C(86)-H(86A)	109.7	C(85)-C(86)-H(86A)	109.7
O(22)-C(86)-H(86B)	109.7	C(85)-C(86)-H(86B)	109.7
H(86A)-C(86)-H(86B)	108.2	O(22)-C(87)-C(88)	109.51(16)
O(22)-C(87)-H(87A)	109.8	C(88)-C(87)-H(87A)	109.8
O(22)-C(87)-H(87B)	109.8	C(88)-C(87)-H(87B)	109.8
H(87A)-C(87)-H(87B)	108.2	O(21)-C(88)-C(87)	111.05(16)
O(21)-C(88)-H(88A)	109.4	C(87)-C(88)-H(88A)	109.4
O(21)-C(88)-H(88B)	109.4	C(87)-C(88)-H(88B)	109.4
H(88A)-C(88)-H(88B)	108.0	C(88)-O(21)-C(85)	108.30(16)
C(86)-O(22)-C(87)	109.19(16)	O(19)-C(89)-C(90)	110.33(15)
O(19)-C(89)-H(89A)	109.6	C(90)-C(89)-H(89A)	109.6
O(19)-C(89)-H(89B)	109.6	C(90)-C(89)-H(89B)	109.6
H(89A)-C(89)-H(89B)	108.1	O(20)-C(90)-C(89)	110.58(15)
O(20)-C(90)-H(90A)	109.5	C(89)-C(90)-H(90A)	109.5
O(20)-C(90)-H(90B)	109.5	C(89)-C(90)-H(90B)	109.5
H(90A)-C(90)-H(90B)	108.1	O(20)-C(91)-C(92)	110.31(15)
O(20)-C(91)-H(91A)	109.6	C(92)-C(91)-H(91A)	109.6
O(20)-C(91)-H(91B)	109.6	C(92)-C(91)-H(91B)	109.6
H(91A)-C(91)-H(91B)	108.1	O(19)-C(92)-C(91)	110.38(15)
O(19)-C(92)-H(92A)	109.6	C(91)-C(92)-H(92A)	109.6
O(19)-C(92)-H(92B)	109.6	C(91)-C(92)-H(92B)	109.6
H(92A)-C(92)-H(92B)	108.1		

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 x,y-1,z #3 x,y+1,z #4 x+1,y,z

$[\{(C_{10}H_7OLi)_4 \cdot 2Dioxane\} \cdot 3Dioxane]_\infty$, 3

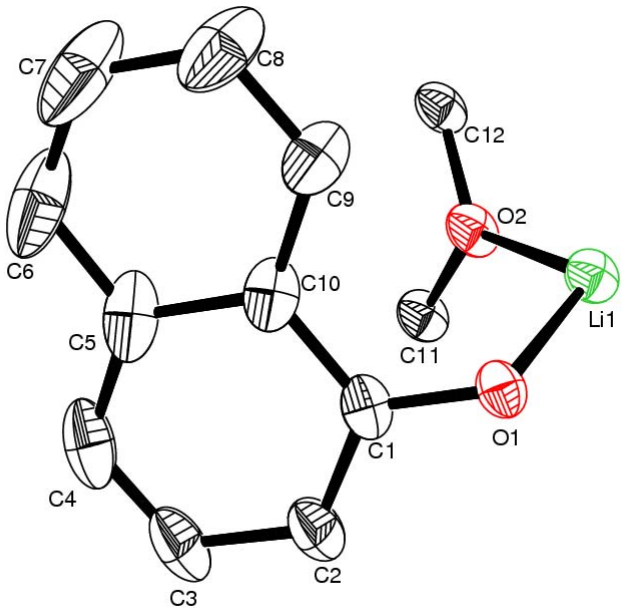


Table 5. Crystal data and structure refinement for **3**

Identification code	dmd14sq	
Empirical formula	C15 H17 Li O3.50	
Formula weight	260.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	tetragonal	
Space group	I4(1)/a	
Unit cell dimensions	a = 15.0031(1) Å	α= 90°.
	b = 15.0031(1) Å	β= 90°.
	c = 24.7185(4) Å	γ = 90°.
Volume	5563.96(10) $Å^3$	
Z	16	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	2208	
Crystal size	0.32 x 0.32 x 0.32 mm^3	
Crystal color and habit	clear colorless octahedron	
Diffractometer	Bruker SMART APEX CCD area detector	
Theta range for data collection	1.59 to 30.51°	
Index ranges	-16<=h<=20, -21<=k<=9, -34<=l<=23	
Reflections collected	18864	
Independent reflections	4247 [R(int) = 0.0234]	
Observed reflections (I > 2sigma(I))	3158	
Completeness to theta = 30.51°	99.8 %	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.9730 and 0.8112	
Solution method	SHELXS-97 (Sheldrick, 1990)	
Refinement method	SHELXL-97 (Sheldrick, 1997)	
Data / restraints / parameters	4247 / 0 / 136	

Goodness-of-fit on F^2	1.161
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1319
R indices (all data)	R1 = 0.0583, wR2 = 0.1360
Largest diff. peak and hole	0.272 and -0.206 e.Å^{-3}

Table 6. Bond lengths [Å] and angles [°] for **3**.

Li(1)-O(2)	1.9349(16)	Li(1)-O(1)#1	1.9490(16)
Li(1)-O(1)	1.9519(16)	Li(1)-O(1)#2	1.9531(17)
Li(1)-Li(1)#2	2.605(3)	Li(1)-Li(1)#1	2.658(3)
Li(1)-Li(1)#3	2.658(3)	O(1)-C(1)	1.3285(10)
O(1)-Li(1)#3	1.9490(16)	O(1)-Li(1)#2	1.9531(17)
O(2)-C(12)	1.4370(11)	O(2)-C(11)	1.4377(11)
C(1)-C(2)	1.3824(14)	C(1)-C(10)	1.4402(14)
C(2)-C(3)	1.4092(14)	C(2)-H(2)	0.9500
C(3)-C(4)	1.3572(18)	C(3)-H(3)	0.9500
C(4)-C(5)	1.4163(18)	C(4)-H(4)	0.9500
C(5)-C(6)	1.4220(18)	C(5)-C(10)	1.4245(14)
C(6)-C(7)	1.356(2)	C(6)-H(6)	0.9500
C(7)-C(8)	1.399(2)	C(7)-H(7)	0.9500
C(8)-C(9)	1.3682(16)	C(8)-H(8)	0.9500
C(9)-C(10)	1.4153(15)	C(9)-H(9)	0.9500
C(11)-C(12)#4	1.5065(13)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	C(12)-C(11)#4	1.5065(13)
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900

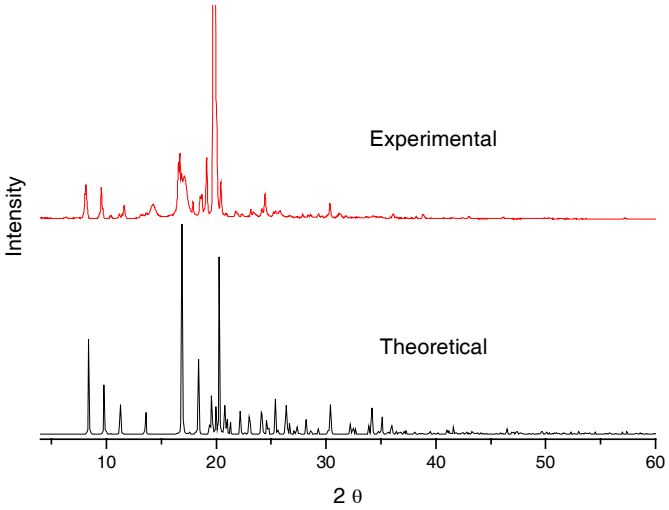
O(2)-Li(1)-O(1)#1	126.94(9)	O(2)-Li(1)-O(1)	110.28(8)
O(1)#1-Li(1)-O(1)	93.78(7)	O(2)-Li(1)-O(1)#2	127.58(8)
O(1)#1-Li(1)-O(1)#2	93.74(7)	O(1)-Li(1)-O(1)#2	96.28(7)
O(2)-Li(1)-Li(1)#2	136.93(5)	O(1)#1-Li(1)-Li(1)#2	94.46(5)
O(1)-Li(1)-Li(1)#2	48.17(5)	O(1)#2-Li(1)-Li(1)#2	48.13(6)
O(2)-Li(1)-Li(1)#1	156.93(9)	O(1)#1-Li(1)-Li(1)#1	47.09(6)
O(1)-Li(1)-Li(1)#1	92.77(5)	O(1)#2-Li(1)-Li(1)#1	47.00(4)
Li(1)#2-Li(1)-Li(1)#1	60.65(3)	O(2)-Li(1)-Li(1)#3	138.34(9)
O(1)#1-Li(1)-Li(1)#3	47.13(6)	O(1)-Li(1)-Li(1)#3	47.00(4)
O(1)#2-Li(1)-Li(1)#3	92.74(5)	Li(1)#2-Li(1)-Li(1)#3	60.65(3)
Li(1)#1-Li(1)-Li(1)#3	58.69(7)	C(1)-O(1)-Li(1)#3	129.90(7)
C(1)-O(1)-Li(1)	117.34(7)	Li(1)#3-O(1)-Li(1)	85.91(7)
C(1)-O(1)-Li(1)#2	136.88(7)	Li(1)#3-O(1)-Li(1)#2	85.87(7)
Li(1)-O(1)-Li(1)#2	83.70(7)	C(12)-O(2)-C(11)	110.14(6)
C(12)-O(2)-Li(1)	125.44(7)	C(11)-O(2)-Li(1)	124.05(7)
O(1)-C(1)-C(2)	121.74(9)	O(1)-C(1)-C(10)	119.99(9)
C(2)-C(1)-C(10)	118.27(8)	C(1)-C(2)-C(3)	121.34(10)
C(1)-C(2)-H(2)	119.3	C(3)-C(2)-H(2)	119.3
C(4)-C(3)-C(2)	121.29(11)	C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4	C(3)-C(4)-C(5)	119.99(9)
C(3)-C(4)-H(4)	120.0	C(5)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	122.52(11)	C(4)-C(5)-C(10)	119.55(10)
C(6)-C(5)-C(10)	117.93(12)	C(7)-C(6)-C(5)	121.77(12)
C(7)-C(6)-H(6)	119.1	C(5)-C(6)-H(6)	119.1
C(6)-C(7)-C(8)	120.16(12)	C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9	C(9)-C(8)-C(7)	120.33(14)
C(9)-C(8)-H(8)	119.8	C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(10)	121.07(11)	C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5	C(9)-C(10)-C(5)	118.72(10)

C(9)-C(10)-C(1)	121.73(9)	C(5)-C(10)-C(1)	119.54(10)
O(2)-C(11)-C(12)#4	110.59(8)	O(2)-C(11)-H(11A)	109.5
C(12)#4-C(11)-H(11A)	109.5	O(2)-C(11)-H(11B)	109.5
C(12)#4-C(11)-H(11B)	109.5	H(11A)-C(11)-H(11B)	108.1
O(2)-C(12)-C(11)#4	110.58(7)	O(2)-C(12)-H(12A)	109.5
C(11)#4-C(12)-H(12A)	109.5	O(2)-C(12)-H(12B)	109.5
C(11)#4-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12B)	108.1

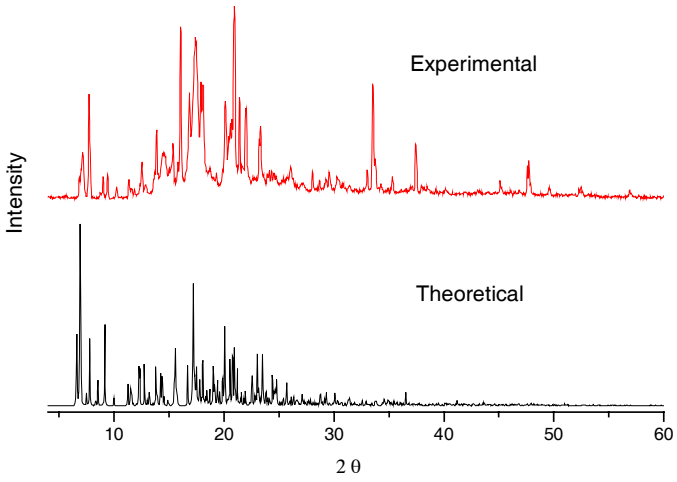
Symmetry transformations used to generate equivalent atoms:

#1 y-1/4,-x+5/4,-z+1/4 #2 -x+1,-y+3/2,z+0 #3 -y+5/4,x+1/4,-z+1/4
#4 -x+1,-y+1,-z

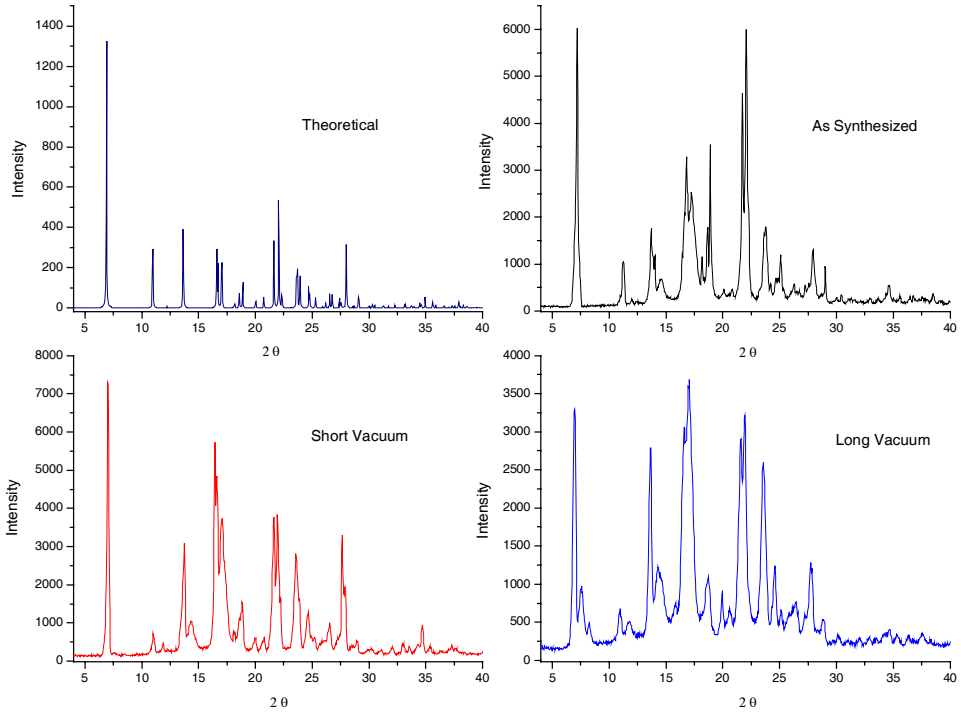
Powder diffraction patterns for $[(PhOLi)_4 \cdot 3Dioxane]_\infty$, 1



Powder diffraction patterns for $[\{(4\text{-}Et\text{-}C_6H_4OLi)_4 \cdot 5/2Dioxane\} \cdot Dioxane]_\infty$, 2



Powder diffraction patterns for $[\{(C_{10}H_7OLi)_4 \cdot 2Dioxane\} \cdot 3Dioxane]_\infty$, 3



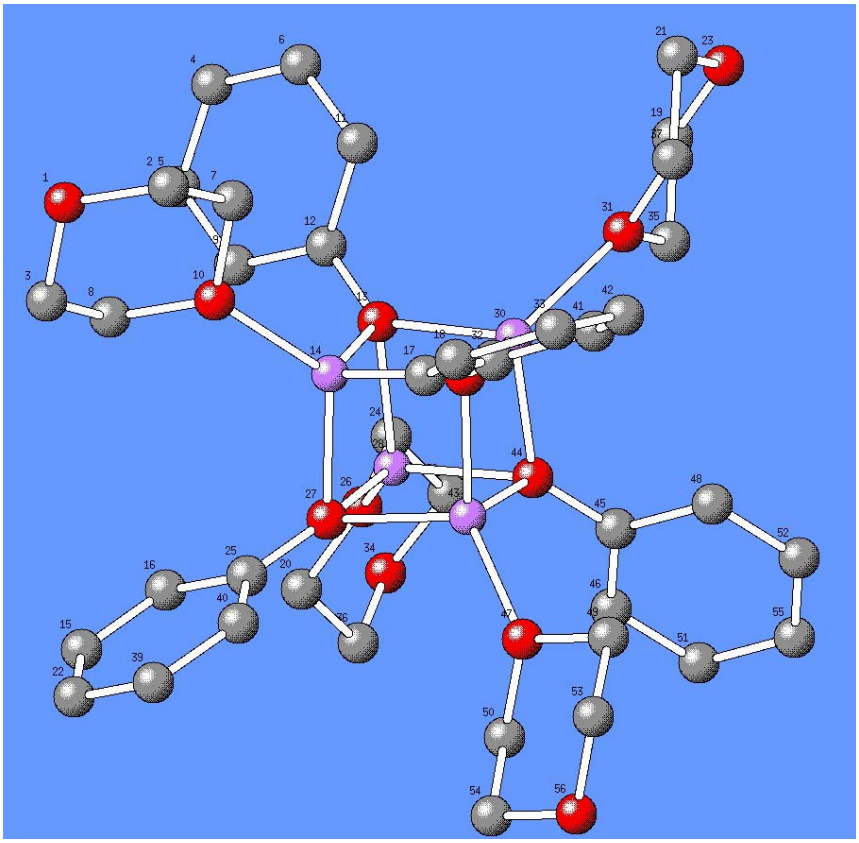
Calculations

Tables of atomic coordinates and associated energies for the calculated geometries of [(PhOLi)$_4$·4Dioxane] (**I**), [{(PhOLi)$_4$}$_2$·7Dioxane] (**II**), and 1,4-dioxane (**III**) are provided. Geometry optimizations were performed at the HF/6-31G* level and single point energies recalculated at the B3LYP/6311G** level.

[(PhOLi)$_4$·4Dioxane] (I)

Optimization HF/6-31G*: -4641.2757 h

Single Point B3LYP/6-311G**: -4671.0704 h



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.617329	-5.176931	0.330208
2	6	0	-3.293324	-4.545783	-0.877871
3	6	0	-3.624156	-4.282027	1.408674
4	6	0	2.674432	-5.148334	1.010944
5	6	0	2.217223	-4.340862	2.041396
6	6	0	2.573427	-4.677130	-0.289056
7	6	0	-1.942542	-3.864804	-0.774445

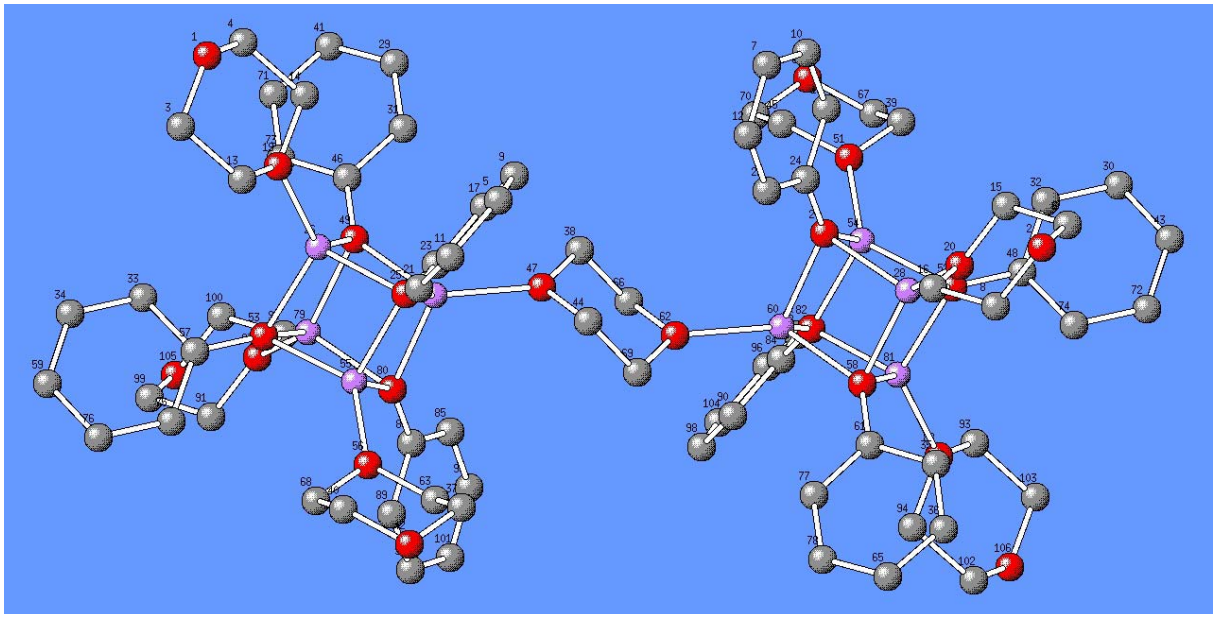
8	6	0	-2.275752	-3.602517	1.540166
9	6	0	1.676185	-3.092596	1.784729
10	8	0	-1.947599	-2.962733	0.318402
11	6	0	2.034263	-3.430555	-0.558013
12	6	0	1.575172	-2.600489	0.474531
13	8	0	1.055604	-1.415511	0.226321
14	3	0	-0.904531	-1.277826	0.182707
15	6	0	-2.499986	-0.327962	4.725180
16	6	0	-1.558589	-0.285129	3.709848
17	6	0	-3.219768	-0.581123	-2.220910
18	6	0	-4.151047	-0.531354	-3.243581
19	6	0	4.652286	-1.009287	-2.928798
20	6	0	2.144010	0.833269	4.133063
21	6	0	3.191465	-1.862922	-4.521089
22	6	0	-3.804797	0.085130	4.507740
23	8	0	4.476338	-1.366569	-4.273342
24	6	0	3.630730	-0.044617	2.532501
25	6	0	-1.891624	0.182567	2.430416
26	8	0	2.323233	0.440739	2.786150
27	8	0	-1.001633	0.220924	1.459666
28	3	0	0.954027	0.215988	1.309573
29	8	0	-1.001611	-0.219418	-1.459992
30	3	0	0.954002	-0.217336	-1.309325
31	8	0	2.323560	-0.444550	-2.785287
32	6	0	-1.891418	-0.179592	-2.430853
33	6	0	-3.804188	-0.078978	-4.508392
34	8	0	4.477100	1.359657	4.274558
35	6	0	3.631789	0.038495	-2.531031
36	6	0	3.192994	1.858272	4.521721
37	6	0	2.144086	-0.836294	-4.132387
38	6	0	4.652873	1.001585	2.930207
39	6	0	-4.150709	0.538266	3.242942
40	6	0	-3.219233	0.586489	2.220377
41	6	0	-1.557408	0.287359	-3.710300
42	6	0	-2.498617	0.331757	-4.725738
43	3	0	-0.902629	1.279157	-0.183017
44	8	0	1.057584	1.414082	-0.226066
45	6	0	1.579517	2.597996	-0.474378
46	6	0	2.040302	3.427218	0.558083
47	8	0	-1.942976	2.965797	-0.318921
48	6	0	1.681466	3.089805	-1.784621
49	6	0	-2.270014	3.606076	-1.540720
50	6	0	-1.936316	3.867927	0.773865
51	6	0	2.581973	4.672684	0.289009
52	6	0	2.225011	4.336954	-2.041404
53	6	0	-3.617223	4.287960	-1.409262
54	6	0	-3.285896	4.551292	0.877263
55	6	0	2.683890	5.143579	-1.011028
56	8	0	-3.608808	5.182923	-0.330857
57	1	0	-3.275871	-5.309673	-1.644214
58	1	0	-4.056590	-3.813990	-1.134972
59	1	0	-3.850111	-4.854443	2.298726
60	1	0	-4.402772	-3.533960	1.270135
61	1	0	3.093868	-6.116850	1.214822
62	1	0	2.279150	-4.686476	3.059480
63	1	0	2.916760	-5.288012	-1.106888

64	1	0	-1.155196	-4.596326	-0.625339
65	1	0	-1.728866	-3.286157	-1.661381
66	1	0	-1.504303	-4.328541	1.775717
67	1	0	-2.293406	-2.839782	2.304089
68	1	0	1.318535	-2.479742	2.594131
69	1	0	1.955259	-3.078496	-1.570775
70	1	0	-2.208724	-0.692769	5.695656
71	1	0	-0.553661	-0.625962	3.888348
72	1	0	-3.504768	-0.927598	-1.242891
73	1	0	-5.161518	-0.847769	-3.047635
74	1	0	4.555348	-1.885763	-2.291980
75	1	0	5.656161	-0.617458	-2.831137
76	1	0	2.224024	-0.042170	4.771800
77	1	0	1.146456	1.239563	4.216611
78	1	0	3.033092	-2.785292	-3.965818
79	1	0	3.129739	-2.083555	-5.578712
80	1	0	-4.532356	0.050786	5.298303
81	1	0	3.785596	-0.958879	3.095569
82	1	0	3.682255	-0.273046	1.478112
83	1	0	-4.531597	-0.043428	-5.299039
84	1	0	3.683362	0.266410	-1.476532
85	1	0	3.788385	0.952718	-3.093680
86	1	0	3.131300	2.079391	5.579245
87	1	0	3.036354	2.780710	3.966070
88	1	0	1.145886	-1.240914	-4.216372
89	1	0	2.225738	0.039234	-4.770795
90	1	0	5.656113	0.608015	2.833002
91	1	0	4.557626	1.877986	2.293032
92	1	0	-5.160593	0.856504	3.046922
93	1	0	-3.503509	0.933581	1.242368
94	1	0	-0.551855	0.626378	-3.888733
95	1	0	-2.206598	0.695929	-5.696224
96	1	0	1.960600	3.075409	1.570875
97	1	0	1.322540	2.477616	-2.593963
98	1	0	-2.288998	2.843327	-2.304599
99	1	0	-1.497300	4.330741	-1.776319
100	1	0	-1.723649	3.288962	1.660836
101	1	0	-1.147683	4.598052	0.624706
102	1	0	2.926558	5.282938	1.106784
103	1	0	2.287589	4.682370	-3.059515
104	1	0	-4.397149	3.541270	-1.270660
105	1	0	-3.842185	4.860712	-2.299349
106	1	0	-4.050445	3.820863	1.134428
107	1	0	-3.267086	5.315206	1.643550
108	1	0	3.105272	6.111230	-1.214995

[{(PhOLi)$_4$}$_2$·7Dioxane] (II)

Optimization HF/6-31G*: -2473.5505 h

Single Point B3LYP/6-311G**: -2489.4056 h



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-8.850182	3.194014	-2.466345
4	6	0	-7.450689	2.715570	-4.260995
5	6	0	-3.468667	5.684131	-0.387732
6	6	0	7.604123	5.077945	-0.330191
7	6	0	2.284196	3.919257	-3.676189
8	6	0	6.052188	5.378088	1.375323
9	6	0	-2.876163	4.702783	-1.167972
10	6	0	3.271552	3.086602	-4.180541
11	6	0	-4.351337	5.291113	0.606643
12	6	0	1.884024	3.744241	-2.360018
13	6	0	-7.693773	3.018993	-1.501285
14	6	0	-6.277600	2.539281	-3.317769
15	6	0	6.704557	4.049790	-0.986857
16	6	0	5.135582	4.351741	0.738863
17	6	0	-3.150952	3.361666	-0.960493
18	6	0	3.842201	2.097135	-3.398050
19	8	0	-6.750520	2.115024	-2.049685
20	8	0	5.906542	3.419488	0.001212
21	6	0	-4.634414	3.953017	0.823143
22	6	0	2.447564	2.757874	-1.568461
23	6	0	-4.035653	2.949970	0.047558
24	6	0	3.438235	1.899778	-2.069594

25	8	0	-4.304512	1.674874	0.245025
26	3	0	-5.737788	0.891229	-0.857157
27	8	0	3.977399	0.962462	-1.318089
28	3	0	5.401970	1.499854	-0.071178
29	6	0	-3.650225	-0.831012	-4.992659
30	6	0	9.678396	0.936236	-2.373789
31	6	0	-3.627360	-0.512102	-3.644910
32	6	0	8.347959	0.635718	-2.131436
33	6	0	-8.842092	-0.370224	-0.195806
34	6	0	-10.168130	-0.673796	0.059222
35	6	0	5.710533	1.659990	3.348058
36	6	0	5.721703	1.973436	4.696275
37	6	0	-3.790076	2.960659	4.773361
38	6	0	-0.400796	-0.360678	-1.289081
39	6	0	6.263001	-1.750741	-4.335440
40	6	0	-6.101491	3.138810	4.917843
41	6	0	-4.692957	-1.564828	-5.535960
42	8	0	-4.884990	3.244641	5.601800
43	6	0	10.605624	0.954301	-1.344130
44	6	0	-0.689489	1.094198	0.531287
45	6	0	3.919450	-1.563135	-4.204563
46	6	0	-4.654962	-0.924674	-2.784695
47	8	0	-1.318855	0.214126	-0.379929
48	6	0	7.895669	0.333378	-0.838735
49	8	0	-4.642355	-0.619575	-1.502921
50	3	0	-3.329511	0.047059	-0.221703
51	8	0	5.152179	-1.430414	-3.519052
52	8	0	6.630790	0.049441	-0.603170
53	8	0	-6.630600	-0.050578	0.603571
54	3	0	5.111412	-0.600477	-1.660661
55	3	0	-5.111266	0.599243	1.661190
56	8	0	-5.151695	1.427766	3.520238
57	6	0	-7.895255	-0.335389	0.839287
58	8	0	4.642284	0.621314	1.502274
59	6	0	-10.604722	-0.958181	1.345000
60	3	0	3.329425	-0.045681	0.221278
61	6	0	4.654788	0.927534	2.783782
62	8	0	1.318651	-0.211549	0.378939
63	6	0	-3.918629	1.561084	4.205027
64	8	0	4.885154	-3.248781	-5.599268
65	6	0	4.692551	1.570097	5.534490
66	6	0	0.689293	-1.091637	-0.532275
67	6	0	6.101305	-3.143511	-4.914600
68	6	0	-6.262272	1.746373	4.337632
69	6	0	0.400590	0.363228	1.288095
70	6	0	3.789960	-2.963071	-4.771795
71	6	0	-5.721874	-1.969190	-4.697948
72	6	0	10.168483	0.671231	-0.058249
73	6	0	-5.710588	-1.656927	-3.349456
74	6	0	8.842204	0.368580	0.196622
75	6	0	-8.346982	-0.639061	2.131873
76	6	0	-9.677184	-0.940490	2.374386
77	6	0	3.626949	0.515997	3.644209
78	6	0	3.649702	0.836086	4.991682
79	3	0	-5.401164	-1.499881	0.069955
80	8	0	-3.976548	-0.962801	1.316939

81	3	0	5.737050	-0.890657	0.858099
82	8	0	4.303663	-1.674436	-0.243810
83	6	0	-3.436554	-1.900510	2.067355
84	6	0	4.033850	-2.949175	-0.045346
85	6	0	-2.446177	-2.758097	1.564770
86	6	0	4.631982	-3.953288	-0.820037
87	8	0	-5.904904	-3.419679	-0.003913
88	8	0	6.748840	-2.114053	2.051832
89	6	0	-3.839294	-2.098817	3.396039
90	6	0	3.148713	-3.359409	0.962918
91	6	0	-6.702082	-4.051191	0.984060
92	6	0	-5.134118	-4.350976	-0.742950
93	6	0	7.691605	-3.019046	1.504283
94	6	0	6.275458	-2.537015	3.320176
95	6	0	-1.881734	-3.744879	2.355165
96	6	0	4.347905	-5.291003	-0.602486
97	6	0	-3.267754	-3.088693	4.177365
98	6	0	2.872927	-4.700158	1.171458
99	6	0	-7.601744	-5.078997	0.326977
100	6	0	-6.050806	-5.376994	-1.379822
101	6	0	-2.280692	-3.920828	3.671582
102	6	0	7.448292	-2.713312	4.263718
103	6	0	8.847755	-3.194047	2.469658
104	6	0	3.464823	-5.682571	0.392094
105	8	0	-6.839455	-6.000294	-0.404264
106	8	0	8.380488	-3.609600	3.722911
107	1	0	-9.531874	3.954542	-2.108510
108	1	0	-9.395779	2.257129	-2.562563
109	1	0	-7.120861	3.128859	-5.205014
110	1	0	-7.921219	1.752208	-4.449154
111	1	0	-3.252334	6.724101	-0.552512
112	1	0	8.152592	5.636047	-1.077562
113	1	0	8.317194	4.579582	0.323894
114	1	0	1.844947	4.686116	-4.288109
115	1	0	5.474839	6.152640	1.863011
116	1	0	6.684899	4.896962	2.118782
117	1	0	-2.193352	4.982140	-1.952501
118	1	0	3.606302	3.209536	-5.196657
119	1	0	-4.829294	6.034983	1.221537
120	1	0	1.127007	4.385260	-1.940341
121	1	0	-7.205047	3.969298	-1.313779
122	1	0	-8.027969	2.598448	-0.563857
123	1	0	-5.739945	3.474180	-3.197861
124	1	0	-5.598212	1.780104	-3.674728
125	1	0	6.054086	4.521334	-1.716724
126	1	0	7.283023	3.277003	-1.469854
127	1	0	4.430194	4.833621	0.069833
128	1	0	4.593871	3.793769	1.488347
129	1	0	-2.689252	2.612551	-1.580158
130	1	0	4.615099	1.465583	-3.799994
131	1	0	-5.327331	3.660448	1.591556
132	1	0	2.139326	2.641798	-0.544207
133	1	0	-2.844796	-0.496684	-5.624381
134	1	0	9.990401	1.163125	-3.379232
135	1	0	-2.820914	0.075257	-3.241224
136	1	0	7.634605	0.645931	-2.937364

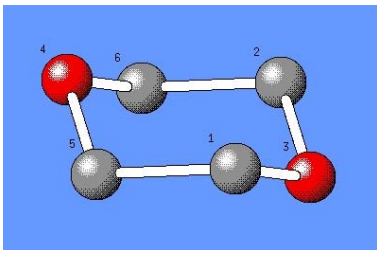
137	1	0	-8.516020	-0.160278	-1.199548
138	1	0	-10.868227	-0.690986	-0.758755
139	1	0	6.519754	1.971787	2.710517
140	1	0	6.547096	2.537585	5.096231
141	1	0	-3.730002	3.687264	3.966816
142	1	0	-2.899097	3.041842	5.382004
143	1	0	0.026811	0.422002	-1.907530
144	1	0	-0.956964	-1.044366	-1.914323
145	1	0	6.336492	-1.020202	-5.136590
146	1	0	7.144111	-1.682438	-3.714723
147	1	0	-6.150520	3.881162	4.123727
148	1	0	-6.890308	3.344274	5.629526
149	1	0	-4.706673	-1.810455	-6.582360
150	1	0	11.637235	1.187625	-1.535946
151	1	0	-0.279313	1.935931	-0.014158
152	1	0	-1.453943	1.454249	1.203443
153	1	0	3.875310	-0.828493	-5.002257
154	1	0	3.137980	-1.349139	-3.490091
155	1	0	-11.636148	-1.192215	1.536939
156	1	0	-3.137442	1.348444	3.489838
157	1	0	-3.873246	0.825807	5.002067
158	1	0	4.706179	1.816642	6.580676
159	1	0	1.453753	-1.451646	-1.204449
160	1	0	0.279154	-1.933372	0.013177
161	1	0	6.890397	-3.350299	-5.625595
162	1	0	6.149122	-3.885251	-4.119838
163	1	0	-7.143729	1.677772	3.717441
164	1	0	-6.334550	1.015097	5.138220
165	1	0	0.956745	1.046913	1.913351
166	1	0	-0.027027	-0.419467	1.906519
167	1	0	2.899307	-3.043938	-5.380958
168	1	0	3.728675	-3.688934	-3.964672
169	1	0	-6.547170	-2.533215	-5.098278
170	1	0	10.868336	0.688736	0.759930
171	1	0	-6.519628	-1.969507	-2.712068
172	1	0	8.515709	0.159650	1.200439
173	1	0	-7.633371	-0.649585	2.937569
174	1	0	-9.988756	-1.168394	3.379734
175	1	0	2.820411	-0.071510	3.240924
176	1	0	2.844090	0.502529	5.623580
177	1	0	-2.138896	-2.641304	0.540308
178	1	0	5.325208	-3.661846	-1.588598
179	1	0	-4.611954	-1.467681	3.799089
180	1	0	2.687458	-2.609460	1.581903
181	1	0	-7.280488	-3.279058	1.468173
182	1	0	-6.050991	-4.523230	1.713052
183	1	0	-4.593052	-3.792113	-1.492235
184	1	0	-4.428162	-4.833284	-0.074829
185	1	0	8.026213	-2.599440	0.566581
186	1	0	7.202306	-3.969187	1.317440
187	1	0	5.596500	-1.777125	3.676435
188	1	0	5.737225	-3.471665	3.200920
189	1	0	-1.124969	-4.385469	1.934382
190	1	0	4.825400	-6.035719	-1.216713
191	1	0	-3.601569	-3.212360	5.193699
192	1	0	2.189816	-4.978370	1.956133

193	1	0	-8.315394	-4.580227	-0.326165
194	1	0	-8.149553	-5.637998	1.074160
195	1	0	-6.684145	-4.895347	-2.122409
196	1	0	-5.473524	-6.150890	-1.868631
197	1	0	-1.840754	-4.688006	4.282605
198	1	0	7.919408	-1.750103	4.451196
199	1	0	7.118058	-3.125653	5.208010
200	1	0	9.393930	-2.257434	2.565228
201	1	0	9.529018	-3.955287	2.112522
202	1	0	3.247719	-6.722250	0.557694

Dioxane (III)

Optimization HF/6-31G*: -305.8253 h

Single Point B3LYP/6-311G**: -307.74074 h



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.163875	0.734832	-0.187585
2	6	0	1.162912	0.736247	-0.187608
3	8	0	-0.000864	1.355297	0.290141
4	8	0	0.000864	-1.355297	-0.290141
5	6	0	-1.162912	-0.736247	0.187608
6	6	0	1.163875	-0.734831	0.187585
7	1	0	-1.223379	0.838150	-1.269983
8	1	0	-2.005920	1.250570	0.255919
9	1	0	1.222295	0.839664	-1.269989
10	1	0	2.004256	1.253003	0.255986
11	1	0	-2.004256	-1.253003	-0.255986
12	1	0	-1.222295	-0.839664	1.269988
13	1	0	2.005920	-1.250570	-0.255917
14	1	0	1.223378	-0.838149	1.269984
