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Structural Diversity in Lithium Aryloxides, Part 1. Structurally characterized $[Li(OAr)(THF)_x]_n$ where OAr = OC_6H_5, OC_6H_4(2-Me), OC_6H_3(2,6-Me)$_2$, OC_6H_4(2-Pr^i), OC_6H_3(2,6-Pr^i)$_2$, OC_6H_4(2-Bu^t), OC_6H_3(2,6-Bu^t)$_2$.

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Abstract. A series of aryl alcohols [H-OAr where OAr = OC_6H_5 (OPh), OC_6H_4(2-Me) (oMP), OC_6H_3(2,6-Me)$_2$ (DMP), OC_6H_4(2-Pr^i) (oPP), OC_6H_3(2,6-Pr^i)$_2$ (DIP), OC_6H_4(2-Bu^t) (oBP), OC_6H_3(2,6-Bu^t)$_2$ (DBP); Me = CH_3, Pr^i = $CHMe_2$, and Bu^t = CMe_3] were reacted with $LiN(SiMe_3)_2$ in tetrahydrofuran (THF) to generate the appropriate "Li(OAr)($\bar{T}$HF)$_x$". The OPh was previously identified as the hexagonal prismatic complex $[Li(OPh)(THF)]_6$; however, the structure isolated from the above route proved to be the tetranuclear species $[Li(OPh)(THF)]_4$ (**1**). The other "Li(OAr)(THF)$_x$" products were characterized by single crystal X-ray diffraction as $[Li(oMP)(THF)]_4$ (**2**), $[Li(DMP)(THF)]_4$ (**3**), $[Li(oPP)(THF)]_4$ (**4**), $[Li(DIP)(THF)]_3$ (**5**), $[Li(oBP)(THF)_2]_2$, (**6**), and $[Li(DBP)(THF)]_2$, (**7**). The tetranuclear species (**1** - **4**) consist of symmetric cubes of alternating tetrahedral Li and pyramidal O atoms, with terminal THF solvent molecules bound to each metal center. The trinuclear species of **5** consists of a 6-membered ring of alternating trigonal planar Li and bridging O atoms, with one THF solvent molecule bound to each metal center. Compound **6** possesses two Li atoms which adopt tetrahedral geometries involving two bridging oBP and two terminal THF ligands. The structure of **7** was identical to the previously reported structure of $[Li(DBP)(THF)]_2$ but different unit cell parameters were observed. Compound **7** varies from **6** in that only one solvent molecule is bound to each Li metal center of **7** due to the steric bulk of the DBP ligand. Multinuclear (^{7}Li and ^{13}C) solid state MAS NMR spectroscopic studies indicate that the bulk powder is consistent with the crystalline material. Solution NMR studies indicate that "transitional" compounds display multiple structures in solution.

DISCLAIMER

Introduction

Metal alkoxides have been extensively used with a great deal of success as precursors to ceramic materials. In order to generate higher quality materials with controlled stoichiometries, mixed metal alkoxides are desired. These "single-source" precursors can be generated through the introduction of a metathesizable cations such as alkali metals (eqs 1 and 2).[1-6] Unfortunately, the reaction does not always proceed as written and retention of the alkali metal or halide atoms is often observed. To understand this phenomenon, we have previously characterized the mixed metal precursors, $[ATi(OR)_5]_n$ where A = Li, Na, K and OR = $OCHMe_2$ or OCH_2CMe_3 and n = 2 or ∞.[5,6] It was thought that the alkali metal cation and "$Ti(OR)_5^-$" anion were tight ion pairs in solution which did not allow for successful removal of the alkali metal. For the reactions shown in eq 1, only the $Ti(OR)_4$ precursors have been extensively characterized. However, the "simplistically" written A(OR) precursors are often more complex than is typically written.[7-22]

In order to fully exploit and understand the reactivity of the A(OR) precursors, it is necessary to identify the structures of these compounds. Therefore, our studies have focused on the lithium adducts of aryl alcohols [H-OAr where OAr = OC_6H_5, OPh; OC_6H_4(2-Me), oMP; OC_6H_3(2,6-Me)$_2$, DMP; OC_6H_4(2-Pr^i), oPP; OC_6H_3(2,6-Pr^i)$_2$, DIP; OC_6H_4(2-Bu^t), oBP; OC_6H_3(2,6-Bu^t)$_2$, DBP; Me = CH_3, Pr^i = $CHMe_2$, and Bu^t = CMe_3] due to the systematic variations of ring substituents that are readily available. The *ortho*-substituted OAr were chosen for this investigation since the steric bulk in this position would have the greatest influence over the final structure adopted for the various Li(OAr) species.

We have synthesized a series of Li(OAr) compounds in different solvents. Part 1 details the "Li(OAr)(THF)$_x$" adducts that were synthesized through the amide alcohol exchange reaction shown in eq 3. The unhindered OPh was previously reported as [Li(OPh)(THF)]$_6$ (THF = tetrahydrofuran)[8] and the sterically hindered DBP was found to adopt a dinuclear arrangement, [Li(DBP)(THF)]$_2$[15]. Our investigation of sterically varied Li(OAr) in THF led to the isolation of: [Li(OPh)(THF)]$_4$ (**1**), [Li(oMP)(THF)]$_4$ (**2**), [Li(DMP)(THF)]$_4$ (**3**), [Li(oPP)(THF)]$_4$ (**4**), [Li(DIP)(THF)]$_3$ (**5**), [Li(oBP)(THF)$_2$]$_2$ (**6**), and [Li(DBP)(THF)]$_2$ (**7**). Solid and solution state multi-nuclear NMR spectroscopy were used to determine the properties and structural aspects of the THF adducts of Li(OAr) complexes. Part 2[23] of this study details the synthesis and characterization of the structural diversity observed for the Li(OAr) isolated from pyridine solutions as [Li(OAr)(py)$_x$]$_2$ (x = 2 for OAr = oMP, DMP, oPP, DIP, oBP; x = 1 for OAr = DBP). Details of the syntheses and characterizations of these compounds are presented below.

Experimental

All compounds described below were handled with rigorous exclusion of air and water using standard Schlenk line and glove box techniques. All solvents were freshly distilled from the appropriate drying agent immediately prior to use.[24]The following chemicals were used as received (Aldrich), stored, and handled under an argon atmosphere: H-OPh, H-oMP, H-DMP, H-oPP, H-DIP, H-oBP, H-DBP, and LiN(SiMe$_3$)$_2$.

All solid state NMR spectra were obtained on an AMX-400 at 100.6, 155.5 and 58.9 MHz for ^{13}C, ^{7}Li and ^{6}Li, respectively. A 4 mm broadband MAS probe, spinning at 10 - 12.5 kHz, was used for all experiments. For ^{13}C, 12.5 kHz was used to reduce the overlap between the spinning sidebands of the aromatic resonances with other peaks of interest. The ^{13}C Cross Polarization

(CP) MAS spectra were obtained using high power ^{1}H decoupling, 1 ms contact time and 64 - 256 scan averages. The ^{13}C spectra were referenced against the carbonyl resonance of external glycine (δ 176.0 ppm with respect to TMS). The $^{6,7}Li$ MAS NMR spectra were obtained using single pulse Bloch decay with high power ^{1}H decoupling, 64 - 256 scans and referenced to either 1 M LiCl(aq) or 1 M $^{6}LiCl$(aq) (δ = 0.0 ppm). FT-IR data were obtained on a Bruker Vector 22 spectrometer using KBr pellets under an atmosphere of flowing nitrogen. Elemental analysis was performed on a Perkin-Elmer 2400 CHN-S/O Elemental Analyzer.

General Synthesis. To a solution of $LiN(SiMe_3)_2$ in THF, the appropriate alcohol was added with stirring. After 12 h., the volatile portion of the reaction mixture was removed by rotary evaporation to drastically reduce the volume of the solution. The reaction mixture was allowed to sit for several hours until X-ray quality crystals formed which were used for all analyses. Bulk powder yields were quantitative but crystalline yields were not optimized.

$[Li(OPh)(THF)]_4$ (1). Used $LiN(SiMe_3)_2$ (1.00 g, 5.98 mmol), H-OPh (0.84 g, 8.97 mmol), THF (~10 mL). FT-IR (KBR pellet, cm^{-1}) 3063(m), 3030(m), 2980(s), 2880(s), 2546(w), 2490(w), 1592(s), 1482.31(s), 1295(br, s), 1163(m), 1047(s), 991(m), 878(m), 826(m), 763(s), 700(s), 620(w), 565(s), 500(s). ^{1}H NMR (400.1 MHz, THF-d_8) δ 6.95(2H, t, OC_6H_5, J_{H-H} = 7.2Hz), 6.58 (2H, d, OC_6H_5, J_{H-H} = 3.6Hz), 6.43(1H, t, OC_6H_5, J_{H-H} = 7.2Hz), 3.56(mult., THF), 1.73(mult., THF). $^{13}C\{^{1}H\}$ NMR (100.6 MHz, THF-d_8) δ 165.1, 129.8, 118.8, 116.2 (OC_6H_5), 67.8(mult., THF), 25.5(mult., THF). ^{7}Li (155.5 MHz, THF-d_8) δ 1.26. Elemental analysis for $C_{10}H_{13}LiO_2$: Calc'd 69.77 %C, 7.61 %H; Found 68.62 %C, 7.23 %H.

$[Li(oMP)(THF)]_4$ (2). Used $LiN(SiMe_3)_2$ (0.44 g, 2.63 mmol), H-oMP (0.43g, 3.95 mmol), THF (5 mL). FT-IR (KBR pellet, cm^{-1}) 3058(w), 1593(s), 1562(sh,w), 1482(s), 1440(s), 1286(s), 1152(w), 1110(w), 1069(m), 1035(w), 1001(w), 922(w), 863(s), 752(s), 718(sh,w), 701(s).

620(m), 598(m), 555(m), 477(m), 422(s). ^{1}H NMR (400.1 MHz, THF-d_8) δ 7.72 (0.6H, d, OC_6H_5Me, J_{H-H} = 8.0Hz), 7.64 (0.9H, t, OC_6H_5Me, J_{H-H} = 7.6Hz), 7.45 (0.8H, (br)d, OC_6H_5Me, J_{H-H} = 8.0Hz), 7.15 (0.9H, t, OC_6H_5Me, J_{H-H} = 7.6Hz), 4.45 (mult., THF), 3.02 (3.0H, s, C_6H_5Me), 2.62 (mult., THF). ^{13}C NMR (100.6 MHz, THF-d_8) δ 168.2, 131.0, 127.5, 126.8, 119.2, 114.8(OC_6H_5Me), 67.6, 25.5 (mult., THF), 18.4 (OC_6H_5Me). ^{7}Li (155.5 MHz, THF-d_8) δ 1.15 (s). Elemental analysis for $C_{11}H_{15}LiO_2$: Calc'd 70.96 %C, 8.12 %H; Found 70.82 %C, 7.97 %H.

[Li(DMP)(THF)]$_4$ (3). Used $LiN(SiMe_3)_2$ (0.44 g, 2.63 mmol), H-DMP (0.48 g, 3.95 mmol), THF (5 mL). FT-IR (KBR pellet, cm-1) 2952(br,s), 2860(sh,w), 1587(m), 1428(s), 1341(s), 1269(s), 1202(m), 1149(w), 1103(m), 1036(s), 917(sh,w), 884(m), 844(s), 758(s), 678(s), 612(s), 499(m), 420(m). 1H NMR (400.1 MHz, THF-d8) δ 6.71 (1.9H, (br)s, $OC_6H_3(Me)_2$), 6.10 (1.0H, (br)s, $OC_6H_3(Me)_2$), 3.61 (mult., THF), 2.15(8.4H, s, $OC_6H_3(Me)_2$), 1.79 (mult., THF). ^{13}C NMR (100.6 MHz, THF-d_8) δ 166.4, 128.4, 125.4, 112.1 ($OC_6H_3(Me)_2$), 67.8, 25.5 (mult., THF), 18.6($OC_6H_3(Me)_2$). ^{7}Li (155.5 MHz, THF-d_8) δ 0.64. Elemental analysis for $C_{12}H_{17}LiO_2$: Calc'd 71.99 %C, 8.56 %H; Found 72.51 %C, 8.80 %H.

[Li(oPP)(THF)]$_4$ (4). Used $LiN(SiMe_3)_2$ (0.44 g, 2.63 mmol), H-oPP (0.48 g, 3.94 mmol), THF (5 mL). FT-IR (KBR pellet, cm^{-1}) 2961(s), 1591(m), 1482(s), 1443(s), 1360(w), 1297(s), 1268(s), 1145(m), 1082(w), 1046(s), 893(m), 846.70(s), 762(sh,m), 742(m), 601(m), 552(m), 442(m), 420(m). ^{1}H NMR (400.1 MHz, THF-d_8) δ 7.03 (1.0H, d, $OC_6H_4(CHMe_2)$, J_{H-H} = 7.6Hz), 6.84(1.0H, t, 4H, $OC_6H_4(CHMe_2)$, J_{H-H} = 6.8Hz), 6.62(1.0H, d, $OC_6H_4(CHMe_2)$, J_{H-H} = 6.4Hz,), 6.54(1.0H, t, $OC_6H_4(CHMe_2)$, J_{H-H} = 6.8Hz), 3.65(mult., THF), 3.44(0.8H, (br)s, $OC_6H_4(CHMe_2)$), 1.79(mult., THF), 1.20 (7.5H, d, $OC_6H_4(CHMe_2)$, J_{H-H} = 8.0Hz). ^{13}C NMR (100.6 MHz, THF-d_8) δ 159.5, 136.3, 126.9, 126.3, 117.1 ($OC_6H_4(CHMe_2)$), 67.8(mult., THF), 27.3 ($OC_6H_4(CHMe_2)$), 25.5(mult., THF), 23.7($OC_6H_4(CHMe_2)$). ^{7}Li (155.5 MHz, THF-d_8) δ

1.65(1.34). Elemental analysis for $C_{13}H_{19}LiO_2$: Calc'd 72.88 %C, 8.94 %H; Found 73.35 %C, 8.18 %H.

[Li(DIP)(THF)]$_3$ (5). Used $LiN(SiMe_3)_2$ (0.44 g, 2.63 mmol), H-DIP (0.57 g, 3.95 mmol), THF (5 mL). FT-IR (KBR pellet, cm^{-1}) 2946(sh,w), 2866(br,s), 1580(sh,w), 1421(m), 1381(s), 1328(s), 1269(s), 1209(m), 1156(w), 1103(m), 1043(s), 917(sh,w), 871(m), 844(s), 758(s), 678(s), 599(s), 506(m), 420(m). ^{1}H NMR (400.1 MHz, THF-d_8) δ 6.81 (2.0H, d, $OC_6H_3(CHMe_2)_2$, J_{H-H} = 8.0 Hz), 6.36 (0.9H, t, $OC_6H_3(CHMe_2)_2$, J_{H-H} = 8.0Hz), 3.64 (mult., THF), 3.53 (2.25H, sept., $OC_6H_3(CHMe_2)_2$), 1.79(mult., THF), 1.17(16.0H, d, $OC_6H_3(CHMe_2)_2$), J_{H-H} = 8.0Hz). ^{13}C NMR (100.6 MHz, THF-d_8) δ 161.8, 136.4, 123.0, 114.2 ($OC_6H_3(CHMe_2)_2$), 67.8(mult., THF) 27.2 ($OC_6H_3(CHMe_2)_2$), 25.5(mult., THF), 24.4($OC_6H_3(CHMe_2)_2$). ^{7}Li (155.5 MHz, THF-d_8) δ 0.70. Elemental analysis for $C_{16}H_{25}LiO_2$: Calc'd 74.98 %C, 9.83 %H; Found 74.91 %C 9.80 %H.

[Li(oBP)(THF)$_2$]$_2$ (6). Used $LiN(SiMe_3)_2$ (1.00 g, 5.98 mmol), H-oBP(1.34 g, 8.96 mmol), THF (10 mL). FT-IR (KBR pellet, cm^{-1}) 3561(w), 3504(w), 3053(w), 2957(s), 2872(m), 2853(m), 1590(m), 1562(m), 1479(s), 1436(s), 1389(w), 1361(w), 1298(s), 1256(s), 1201(w), 1128(w), 1086(s), 1045(m), 864(m), 818(m), 747(s), 647(m), 600(w), 542(m), 516(w), 433(m). ^{1}H NMR (400.1 MHz, THF-d_8) δ 6.94(1H, dd, ($OC_6H_4(CMe_3)$)), 6.71(1H, dt, ($OC_6H_4(CMe_3)$)), 6.48(1H, dd, ($OC_6H_4(CMe_3)$), 6.16(1H, dt, ($OC_6H_3(CMe_3)_2$)), 3.57, 1.72 (THF), 1.42 (9H, s, $OC_6H_3(CMe_3)_2$). ^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8) δ 169.0, 137.6, 127.0, 126.2, 122.0, 112.4 ($OC_6H_4(CMe_3)$), 67.4(mult., THF), 35.6 ($OC_6H_4(CMe_3)$), 30.5 ($OC_6H_4(CMe_3)$), 25.6(mult., THF). ^{7}Li (155.5 MHz, THF-d_8) δ 0.35. Elemental analysis for $C_{18}H_{29}LiO_3$: Calc'd: 71.98, %C; 9.73, %H. Found: 75.02, %C; 8.94, % H.

[Li(DBP)(THF)]$_2$ (7). Used LiN(SiMe$_3$)$_2$ (1.00 g, 5.98 mmol), H-DBP(1.85g, 8.96mmol), THF (10 mL). FT-IR (KBR pellet, cm^{-1}) 3050(sh, w), 2956(br, s), 1583(m), 1456(m), 1412(s), 1381(m), 1348(w), 1275(s), 1199(m), 1149(w), 1104(s), 1041(s), 918(m), 893(m), 859(s), 816(m), 816(s), 651(m), 551(m), 478(m). ^{1}H NMR (400.1 MHz, THF-d_8) δ 6.80 (2H, bs, OC$_6$*H*$_3$(CMe$_3$)$_2$), 5.99 (0.8H, bs, OC$_6$*H*$_3$(CMe$_3$)$_2$), 0.74(mult., THF), 1.70(mult., THF), 1.34 (18.2H, s, OC$_6$H$_3$(CMe$_3$)$_2$). ^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8) δ 137.6, 124.6, 113.9 (*O*C$_6$H$_3$(CMe$_3$)$_2$), 67.8(mult., THF), 35.9 (OC$_6$H$_3$(*C*Me$_3$)$_2$), 31.4 (OC$_6$H$_3$(C*Me*$_3$)$_2$), 25.5(mult., THF). ^{7}Li (155.5 MHz, THF-d_8) δ 0.90. Elemental analysis for C$_{18}$H$_{29}$LiO$_2$: Calc'd: 76.03, %C; 10.27, %H. Found: 75.35, %C; 9.96, % H.

X-ray Crystal Structures. Table 1 lists the data collection parameters for **1** - **7**. Metrical data are presented in Tables 2 and 3 for **1** - **4** and **5** - **7**, respectively. All crystals were mounted onto a thin glass fiber from a pool of Fluorolube™ and immediately placed under a liquid N$_2$ stream, on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ = 0.7107 Å). The lattice parameters were optimized from a least-squares calculation on carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software.[25] Data reduction was performed using SAINT Version 6.01 software.[25] The structure refinement was performed using XSHELL 3.0 software.[25] The data were not corrected for absorption due to the low absorption coefficient.

Each structure was solved using direct methods which yielded the Li and O atoms, along with a number of the C atoms. Subsequent Fourier synthesis yielded the remaining C atom positions. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software.[25] These idealized hydrogen atoms had their isotropic temperature factors

fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement of each compound included anisotropic thermal parameters on all non-hydrogen atoms. Additional information concerning the data collection and final structural solutions of **1** - **7** can be found in the supplemental information.

Results and Discussion.

The crystal structures of several lithium alkoxide (OR) and aryloxide (OAr) species have been reported in the literature, including $[Li(OMe)]_\infty$,[13,19] $[Li(OCMe_2Ph)]_6$,[11] $[Li(OCBu^t_3)(THF)]_2$,[17] $[Li(OCBu^t_3)]_2$,[12] $[Li(OC(Me)=CMe_3]_6$,[14] $[Li(OCBu^t=CH_2)(THF)]_4$,[22] $[Li(OCMe_2\text{-}C\equiv C\text{-}H)]_6$,[7] $Li(OC(Me)(c\text{-}CHCH_2CH_2)_2]_6$,[9] and OAr = $[Li(OC_6H_5)(THF)]_6$,[8] $[Li(OC_6H_2(2,4,6\text{-}Me)_3)]_4(THF)_3$,[21] $[Li(OC_6H_2(4\text{-}Me)(2,6\text{-}Bu^t)_2(OEt_2)]_2$,[18] $[Li(OC_6H_3(2,6\text{-}Bu^t)_2(solv)]_2$ (solv = OEt_2,[10] and THF[15]). While a number of Li(OR) have been structurally characterized, little systematic investigation concerning the solid state structure of these compounds has been forthcoming. Due to the continued interest in Li(OR) for use as metathesizable reagents and the variability of steric bulk readily available with the OAr ligands, we synthesized and characterized a series of Li(OAr) with increased steric bulk in the *ortho* position. The results of these studies in THF are detailed below. Part 2[23] of this study details the structural aspects of the same set of "Li(OAr)" species isolated from py.

Synthesis.

Upon addition of the desired H-OAr to a solution of $LiN(SiMe_3)_2$ dissolved in THF, an amide-alcohol exchange reaction rapidly occurred to yield the respective "$Li(OAr)(THF)_x$" (eq 3). Each product of the individual H-OAr used in eq 3 remained soluble. Upon drastic reduction

of the volatile fraction of the reaction mixture and allowing it to sit at glovebox temperatures, crystals suitable for X-ray analysis of **1 - 7** were isolated . Several acceptable elemental analyses were collected for **1 - 7** when rigorous exclusion of air was undertaken; however, it is of note that we collected a wide range of results for each sample. This deviation was attributed to several factors including, excess "trapped' solvent, the volatility of the bound solvent, the volatility of the Li ion upon combustion, and the incomplete decomposition forming Li_2CO_3 instead of the presumed Li_2O. The formation of Li_2CO_3 was verified by the XRD analyses of thermally treated material under an atmosphere of oxygen. The FT-IR spectra of **1 - 7** all possess stretches and bends consistent with THF and the appropriate parent alcohol with the notable absence of the OH stretch (3400-3500 cm^{-1}). Stretches of THF and the parent alcohol overlap, thereby making it difficult to identify the Li-(μ_x-O) stretches.

To insure the identity of the bulk powders of the Li(OAr) compounds, alternative analyses were undertaken. Due to the limited analytical data that were available for the previously identified Li(OAr), $[Li(OPh)(THF)]_6$[8] and $[Li(DBP)(THF)]_2$,[15] it was necessary to synthesize each of these compounds from the reaction mixture of eq 3 and re-solve the structures. The structures adopted for $[Li(OPh)(THF)]_6$ and that found for **1** were not the same (*vide infra*); however, for **7**, and the literature DBP complex, identical structures were recorded but different unit cell parameters were recorded.

Solid State

Crystal structure. Table 1 lists the collection data parameters for **1 - 7**. Tables 2 and 3 list the metrical data for **1 - 4** and **5 - 7**, respectively. The thermal ellipsoid plots of **1 - 7** are shown in Figures 1 - 7, respectively. Compounds **2 - 7** were all solved in the P2(1)/n or c space group.

Additional information pertaining to the structural studies presented here is available in the Supplementary Information.

The structure of the least sterically hindered aryloxide, OPh, was previously determined to be a tetranuclear cube in solution but only the hexagonal prismatic structure $[Li(OPh)(THF)]_6$ could be characterized crystallographically.[8] Using the synthetic route described in eq 3, we isolated **1** in a tetranuclear geometry. Due to this difference and the lack of significant structural data available concerning Li(OAr), the other sterically varied Li(OAr) were characterized. A series of H-OAr which demonstrated a stepwise addition of methyl, propyl, and *t*-butyl pendant hydrocarbon chains in the *ortho* position of the phenol ring were investigated (eq 3).

Compounds **1** - **4**, the least sterically hindered OAr ligands investigated were each found to adopt a cubane structure, $[Li(OAr)(THF)]_4$. Each Li atom adopts a distorted tetrahedral geometry with central core angles distorted from the ideal 90 °, Li-(μ_3-O)-Li (82.2 ° to 87.1 °) and (μ_3-O)-Li-(μ_3O) (92.9 ° to 97.2 °). Additional disorder was noted for the pendant hydrocarbon chains of the alkoxide ligand and the bound solvent. The *ortho* and *para* substituted $OC_6H_2(2,4,6\text{-}Me)_3$ derivatives were also reported to adopt a cubane structure, however, one of the Li atoms did not have a bound THF molecule.[21] The Li-(μ_3-O) distances of **1** - **4** (av. Li-(μ_3-O) = 1.93 Å, **1**; 1.95 Å; **2**; 2.00 Å, **3**; 1.95 Å, **4**) are within statistical agreement with each other and the Li-(μ_3-O) distance of the literature compound $[Li(OPh)(THF)]_6$ (1.99 Å).[8] The longer Li-(μ_3-O) distances noted for **3**, are also reflected in longer Li-O_{THF} distances (2.08 Å). For comparison, the average Li-O_{THF} distances were on average 1.92 Å for **1**, 1.94 Å for **2**, 1.95Å for **4**, and 1.96 Å for $[Li(OPh)(THF)]_6$.[8] The longer distances noted for **3** must be a reflection of the increased steric bulk in both *ortho* positions which does not allow the ligand to bind as tightly as noted for the other cube structures. This is the first step in the deconstruction

of the ubiquitous cube observed for Li(OAr) compounds. For **4**, the Pr^i group is more sterically demanding than the Me groups of **3**. However, due to the asymmetric substitution of the phenoxide ring, **4** adopts an arrangement where the Pr^i group is pointed away from the center of the cube and thus steric interactions are minimized.

Increasing the bulk of the *ortho* substituents to iso-propyl groups, **5**, introduces too much steric bulk to allow a cube to form and a 6-membered $[Li\text{-}O]_3$ ring was isolated. This is the one dimension representation of the hexagonal prismatic structure observed for **1**. The central core of **5** is nearly planar which forces the Li---Li distance of **5** (av. 3.09 Å) to be greater than what was recorded for the cubane compounds (av. 2.62 Å, **2**; av. 2.70 Å, **3**; 2.64 Å, **4**). The Li-(μ-O) distances of av. 1.83 Å for **5** are significantly shorter than those of the Li-(μ_3-O) cubes or the hexagonal prism (*vide infra*). The terminal $Li\text{-}O_{THF}$ distances of **5** (av. 1.94 Å) are consistent with those observed for the cubane compounds. The standard trend where the M-O distances increase with increased bonding agrees with the distances observed for **1** - **5**. The regularity of the six membered ring is reflected in the approximate ideal bond angles of 120 °C noted for **5** (av. 119.8 °; range 112.1 ° to 128.7 °). The trigonal planar arrangement of the Li atoms also allows the terminal THF ligands to adopt angles approaching 120 ° (av. 117.8 °; range 114.7 ° to 120.8 °).

The introduction of a single Bu^t group on the phenoxide ring is too much steric bulk to maintain the ring structure and a dinuclear compound was isolated for the oBP ligated compound, **6**. The structure of **6** can be thought of as a 1 dimensional representation of the cube. The lithium metal of **6** coordinates two terminal THF molecules which leads to a tetrahedral arrangement for both Li ions. Substituting both *ortho* positions with Bu^t groups also leads to a dinuclear complex; however, for **7** only one solvent molecule can bind to the Li metal center. It

was necessary to re-solve the structure of **7** due to the absence of analytical data previously presented in the initial report and the isolation of crystalline material with an alternative unit cell and space group than previously reported.[15] The Li-(μ-O) and Li---Li distances of **6** (1.91 Å and 2.53 Å, respectively) and **7** (1.82 Å and 2.39 Å, respectively) are significantly shorter than those noted for **1 – 5** but within agreement with the literature structure. The steric bulk of the Bu^t group limits the amount of electron density available to the Li metal center, thus a stronger interaction between the Li and O atoms occurs resulting in shorter Li-O distances. Compound **7**, which has only one coordinated THF molecule, displays even shorter Li-O distances than **6**, due to the reduction in electron donation by the coordinated solvents. Other reported structures of OAr ligands with substitutions in the *para* position, such as $[Li(OC_6H_2(2,6Bu^t)_2(4\text{-}Me)(OEt_2)]_2$,[18] did not further decrease the nuclearity of the observed products.

Solid State NMR. For each sample of **1 - 7**, a ^{13}C MAS NMR spectrum was collected and the chemical shifts tabulated in Table 4. For each sample, one set of ^{13}C resonances was observed for the respective ligands. The splitting observed for a number of these resonances was attributed to packing inequivalancies, hindered rotation of the ligands, and the disorder noted in the crystal structure for various Li(OAr) compounds.

As the substituent increases in size and the nuclearity of the molecule decreases, the chemical shift of the methyl moiety of the various substituents is shifted further down field (**2**, 17.2; **3**, 18.4; **4**, 22.1; **5**, 21.8; **6**, 30.0, **7**, 31.5 ppm). The compounds with larger substituents yield smaller nuclearity species which requires increased electron donation by the phenoxide rings, thus shifting the substituents to higher resonances. The solid state structures of **1 - 7** are symmetric and thus it is not possible from the respective ^{13}C MAS NMR spectra to determine

nuclearity of the bulk powder. Therefore, alternative nuclei were used to further confirm the identity of the bulk powder.

The ^{6}Li MAS NMR spectra for compounds **1** - **7** are shown in Figure 8. In the solid state the ^{6}Li shift is equal to the true isotropic chemical shift (since the second order quadrupolar shift is negligible for ^{6}Li) and will be used to discuss changes in structure. Compound **3** displayed two distinct ^{6}Li resonances, whereas, the remainder of the samples revealed only one resonance which would be consistent with the symmetric solid state structures. The spectra of **1**, **2**, and **6** are very broad with overlapping peaks. The overlapping peaks of ^{6}Li and the multiple resonances observed in the ^{13}C MAS of **1** are most likely an indication of packing inequivalencies coupled with the multiple structural types (cube and hexagonal prism) observed for this compound. Compounds **2** and **6** show shoulders on the main resonance but these are not well defined. Based on the data collected in this report, the ^{6}Li resonances of compound **3** are consistent with a cube or ring structure (δ 0.47) [cube structures are expected to appear around 0.6 ppm with the ring structure appearing at a slightly upfield shift at 0.4 ppm]; however, the resonance at 2.02 ppm observed for **2** is further downfield than that of any of the other observed resonances and remains unassigned. The chemical shifts of the expected decomposition products, Li_2O (δ 2.8, 1.3, 0.31) or Li_2CO_3(δ 0.02) do not correspond to this additional resonance. The similarity of the ^{6}Li chemical shifts for **1** - **5**, **7** demonstrates that these lithiums are in very similar environments. The shift of the dinuclear compound **6** is significantly varied from all of the other samples, displaying negative shifts. Structurally, **6** is the only compound with 2 THF ligands bound to the metal center in the solid state.

Interestingly, the compounds that display multiple Li environments (**1** and **3**) may be on the verge of changing from one structure to another geometry (or structural transition ligated

species). For **1**, the hexagonal prismatic to cube arrangement has already been reported. Therefore, the change from a cube to a ring arrangement should also be observable. While the two Me substituents of **3** impose some very large steric constraints, as evidenced by the metrical data, it was found to adopt the cube structure. However, it is quite possible that both a ring and cube arrangement are present, explaining the observed spectra, but only the cube structure was crystallographically isolated.

The ^{7}Li (spin 3/2) MAS spectra for **1** - **7** are shown in Figure 9 and are dominated by the central ±1/2 to ±1/2 transition, but a manifold of spinning sidebands for the ±3/2 to ±1/2 transition is also clearly evident. The extent of this side-band manifold provides a measure of the quadrupolar coupling constant. For **5** and **7**, the large quadrupolar coupling observed (~ 1000 ppm) implies that a very asymmetric Li environment exists for these compounds in contrast to **1** - **4**, **6**. The increased symmetry observed for the other compounds may reflect a highly symmetric bonding environment or partial averaging of the quadrupolar interaction due to dynamics of the Li. Comparison of the shifts observed in the ^{6}Li and ^{7}Li MAS experiments can also provide a measure of the quadrupolar interaction but the absence of any significant shift (within experimental error) indicates that the quadrupolar interaction is rather small for most of these compounds.

The quadrupolar coupling constant (also known as SOQE or QSC) is defined by $P_Q = C_Q(1+(\eta_Q)^2/3)^{1/2}$, where $C_Q = e^2qQ/h$ is the quadrupolar coupling constant and η_Q is the quadrupolar electrical field gradient asymmetry parameter. The experiments and analysis described here do not allow for C_Q and η_Q to be separated, since $0 \leq \eta_Q \leq 1$, C_Q and P_Q differ at most by 15%. The quadrupolar values derived from the spinning side-band manifold for ^{7}Li MAS are listed in Table 5. The P_Q value is used an indication of asymmetry around the Li

cations (i.e., large P_Q values indicate less symmetry around the Li cation). As can be discerned from the data, there are two distinct regions of P_Q values which directly correlate to the coordination number of the Li atom. The values below 150 kHz are consistent with tetra-coordinated Li metal centers and those values above 250 kHz are consistent with tri-coordinated metal centers. Jackmann et al. reported a solid state P_Q value of only 73 kHz for $[Li(OPh)(THF)]_6$.[8] While we have described our sample of **1** as a mixture of both the tetra- and hexanuclear species, several other experimental variables may also contribute to the differences in the observed ^7Li line shape (i.e., the size of P_Q), including our use of MAS, high spinning speeds and high power excitation pulses to obtain a larger excitation band width. It may also be possible that the 73 kHz value reported by Jackmann et al. represents a P_Q that has been partially motionally averaged (a smaller QSC indicates higher dynamical averaging). The QSC values noted for $LiPO_3$, which also have tetra-coordinate Li, were found to be 110 kHz[26] which is consistent with the values reported for the Li(OAr) compounds in Table 5.

Solution State. Previously, Jackman and co-workers have reported on a series of elegant investigations regarding the solution nuclearity of Li(OAr) in a variety of solvents,[8,16,20] one of which was THF at -60 °C. The conclusions reached on the THF derivatives that overlap with this investigation indicated that, in solution, the OPh molecule was a mixture of tetranuclear/hexanuclear[16], the oMP derivative was a tetranuclear[20], and the oBP analog was dinuclear[20]. This is consistent with the solid state structures observed in this study.

For this study, all samples were prepared using crystalline material dissolved in THF at saturated concentrations at room temperature. It is difficult to judge the number of solvent molecules as they relate to the solid state structure, due to the use of deuterated parent solvent to

maximize solubility and minimize exchange. For each sample, the solution ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra obtained revealed that the species in solution possessed a high degree of symmetry in solution. The sharpness of the peaks indicated a lack of dynamic behavior; however, this did not lead to any conclusions concerning the nuclearity of the precursor in solution. Therefore, an alternative nucleus was necessary to study solution behavior of these compounds.

^{7}Li NMR is a very sensitive method for determining the environment of the Li cation and in solution the quadrupolar interactions are effectively averaged to zero. The solution spectra are shown in Figure 10. The shifts of these compounds are quite varied from the solid state structures and reflect changes in the local bonding environment of the Li atom. For **1**, two peaks are present which are consistent with the hexagonal prismatic and cube structures previously reported.[8] The resonance consistent with the cube was also observed as the only peak for **2** but as a minor peak for **4**. Compound **4** also displays a peak that correlates with the hexagonal prismatic resonance observed for **1**. For the di-substituted species (**3**, **5**, and **7**), each has a ^{7}Li NMR resonance around 0.6 ppm. This may be a reflection of the solid state structures converting into the smallest component (i.e., a dinuclear arrangement) upon dissolution in the presence of an excess amount of THF.[20] The free rotation of the ortho substitutents may allow for the smaller nuclearity compounds form in solution but once crystallization is initiated, the free rotation is halted and the larger species are isolated in the solid state. For **6**, the shift is at 0.35 ppm and may be at the low end of the range of shifts noted for dinuclear species.

Summary and Conclusion

A number of sterically varied Li(OAr) precursors have been identified by single crystal X-ray diffraction and $^{6,7}Li$ NMR spectroscopy. The structures of the THF adducts of the various

Li(OAr) oscillate between 6 and 4-membered rings of Li-O atoms of various dimensions (hexagonal prism to a cube to a hexagon to a square) as the steric bulk of the *ortho* substituent is increased. Solid state ^{6}Li MAS NMR reveals multiple peaks for **1** and **3** which are "structural transition" ligated species; however, only single peaks are observed for the ^{7}Li MAS NMR spectra. As the nuclearity decreases, the shifts move further downfield which is reflected in the metrical data. In solution, the ^{7}Li NMR shifts are consistent with the solid state chemical shifts but **1** and **4** display multiple resonances. Compound **4** should also be considered a transitional ligated species which indicates that multiple solid state structure types could be observed under the proper conditions. In solution, the transition from one structural unit to another is based on the total substitution of the ring not merely the size of the substituent. Due to the fluctionality in structural arrangements, it should be possible to use the steric bulk of the substituent to control the solution and solid state structures resulting in a fine tuning the Li-O bond strength and thus the ultimate reactivity of the Li(OAr) in methathical processes.

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Supporting Information Available. X-ray crystallographic files in CIF format for the structures of $[Li(OAr)(THF)_x]_n$ (**1** - **7**) are available, free of charge, via the Internet at http://pubs.acs.org.

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List of Tables

Table 1. Data collection parameters for **1- 7.**

Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**
chemical formula	$C_{20}H_{26}Li_2O_4$	$C_{44}H_{60}Li_4O_8$	$C_{48}H_{68}Li_4O_8$	$C_{52}H_{76}Li_4O_8$	$C_{48}H_{75}Li_3O_6$	$C_{18}H_{29}LiO_3$	$C_{36}H_{58}Li_2O_4$
formula weight	344.29	744.68	800.78	856.89	768.90	300.35	568.70
temp (K)	168	168	168	293	168	168	168
space group	monoclinic C2/c	monoclinic P2(1)/c	monoclinic P2(1)/n	monoclinic P2(1)/c	monoclinic P2(1)/n	monoclinic P2(1)/n	monoclinic P2(1)/n
a (Å)	26.890(3)	16.187(7)	12.562(1)	12.946(2)	13.316(2)	9.1510(7)	12.483(3)
b (Å)	9.2373(9)	14.941(7)	20.819(3)	15.119(2)	16.148(3)	14.4287(12)	14.693(4)
c (Å)	19.761(2)	18.920(10)	17.135(2)	27.015(4)	22.427(3)	14.1346(12)	20.207(5)
β (deg)	124.81(1)	108.43(1)	91.77(1)	101.01(1)	90.00(1)	105.32(1)	107.993(4)
V (Å^3)	4030(1)	4341(4)	4479(1)	5190(1)	4822(1)	1800(1)	3525(1)
Z	8	4	4	4	4	4	4
D_{calcd}(Mg/m^3)	1.135	1.139	1.187	1.097	1.059	1.108	1.072
μ,(Mo, Kα) (mm^{-1})	0.076	0.075	0.077	0.070	0.066	0.072	0.066
R1[a] ([I>2σ(I)], %)	5.41	8.64	9.01	8.59	6.26	5.27	5.76
wR2[b] ([I>2σ(I)], %)	12.52	27.60	24.80	23.24	15.66	14.71	12.89
R1[a] (all data, %)	15.70	19.00	11.12	17.93	26.20	9.16	17.14
wR2[b] (all data, %)	15.82	30.87	27.68	29.24	21.79	17.24	16.73

[a]**R1** = $\Sigma \; | \; |F_o|-|F_c| \; | \; / \; \Sigma \; |F_o| \times 100$

[b]**wR2** = $[\Sigma \; w \; (\; F_o^2-F_c^2 \;)^2 \; / \; \Sigma \; (w \; |F_o|^2)^2]^{1/2} \times 100$

Table 2. Select bond distances (Å) and angles (deg) for **1** - **4**.

Distance (Å)	1		2		3		4	
Li---Li	Li(1)---Li(2)	2.656(6)	Li(1)---Li(2)	2.606(10)	Li(1)---Li(2)	2.690(10)	Li(1)---Li(2)	2.676(7)
	Li(1)---Li(1a)	2.631(8)	Li(1)---Li(3)	2.606(1)	Li(1)---Li(3)	2.711(10)	Li(1)---Li(3)	2.563(7)
	Li(1)---Li(2a)	2.589(5)	Li(1)---Li(4)	2.599(10)	Li(1)---Li(4)	2.656(10)	Li(1)---Li(4)	2.636(7)
	Li(2)---Li(1a)	2.589(5)	Li(2)---Li(3)	2.644(10)	Li(2)---Li(3)	2.718(10)	Li(2)---Li(3)	2.648(7)
	Li(2)---Li(2a)	2.585(7)	Li(2)---Li(4)	2.599(10)	Li(2)---Li(4)	2.708(10)	Li(2)---Li(4)	2.640(7)
			Li(3)---Li(4)	2.637(11)	Li(3)---Li(4)	2.716(10)	Li(3)---Li(4)	2.659(7)
Li-(μ_3-O)	Li(1)-O(1)	1.933(4)	Li(1)-O(1)	1.974(8)	Li(1)-O(2)	1.977(7)	Li(1)-O(1)	1.967(5)
	Li(1)-O(2)	1.984(5)	Li(2)-O(1)	1.933(7)	Li(2)-O(2)	1.971(7)	Li(2)-O(1)	1.990(5)
	Li(1)-O(1a)	1.912(4)	Li(4)-O(1)	1.947(8)	Li(4)-O(2)	2.018(7)	Li(4)-O(1)	1.990(5)
	Li(2)-O(1)	1.990(4)	Li(1)-O(2)	1.947(7)	Li(2)-O(4)	1.994(7)	Li(1)-O(2)	1.979(5)
	Li(2)-O(2)	1.922(4)	Li(2)-O(2)	1.979(8)	Li(3)-O(4)	2.046(8)	Li(3)-O(2)	1.902(5)
	Li(2)-O(2a)	1.907(4)	Li(3)-O(2)	1.950(8)	Li(4)-O(4)	1.992(7)	Li(2)-O(2)	1.980(6)
	Li(1a)-O(1)	1.912(4)	Li(2)-O(3)	1.958(7)	Li(1)-O(5)	1.989(7)	Li(2)-O(3)	1.965(5)
	Li(2a)-O(2)	1.907(4)	Li(3)-O(3)	1.972(8)	Li(2)-O(5)	2.033(7)	Li(3)-O(3)	2.019(6)
			Li(4)-O(3)	1.935(7)	Li(3)-O(5)	1.996(8)	Li(4)-O(3)	1.915(5)
			Li(1)-O(4)	1.926(8)	Li(1)-O(7)	2.013(7)	Li(1)-O(4)	1.921(5)
			Li(3)-O(4)	1.953(8)	Li(3)-O(7)	1.970(7)	Li(3)-O(4)	1.979(5)
			Li(4)-O(4)	1.982(8)	Li(4)-O(7)	1.971(7)	Li(4)-O(4)	1.969(6)
Li-O_{THF}	Li(1)-O(4)	1.925(4)	Li(1)-O(5)	1.958(7)	Li(1)-O(1)	2.018(7)	Li(1)-O(7)	1.948(5)
	Li(2)-O(3)	1.912(4)	Li(2)-O(6)	1.933(7)	Li(2)-O(3)	2.082(8)	Li(2)-O(8)	1.960(5)
			Li(3)-O(7)	1.930(8)	Li(3)-O(6)	2.183(8)	Li(3)-O(6)	1.948(6)
			Li(4)-O(8)	1.928(8)	Li(4)-O(8)	2.027(7)	Li(4)-O(9)	1.955(5)

Angles (Å)	1	2	3	4
Li-(μ_3-O)-Li	Li(1)-O(1)-Li(1a) 86.33(18)	Li(1)-O(1)-Li(2) 83.4(3)	Li(1)-O(2)-Li(2) 85.9(3)	Li(1)-O(1)-Li(2) 85.1(2)
	Li(1)-O(1)-Li(2) 85.21(18)	Li(1)-O(1)-Li(4) 83.0(3)	Li(1)-O(2)-Li(4) 83.3(3)	Li(1)-O(1)-Li(4) 83.5(2)
	Li(1)-O(2)-Li(2) 85.66(17)	Li(2)-O(1)-Li(4) 83.8(3)	Li(1)-O(5)-Li(2) 83.9(3)	Li(1)-O(2)-Li(2) 85.0(2)
	Li(1)-O(2)-Li(2a) 83.37(16)	Li(1)-O(2)-Li(2) 83.2(3)	Li(1)-O(5)-Li(3) 85.8(3)	Li(1)-O(2)-Li(3) 82.6(2)
	Li((2)-O(1)-Li(1a) 83.09(17)	Li(1)-O(2)-Li(3) 83.9(3)	Li(1)-O(7)-Li(3) 85.8(3)	Li(1)-O(4)-Li(3) 82.2(2)
	Li(2)-O(2)-Li(2a) 84.90(17)	Li(2)-O(2)-Li(3) 84.6(3)	Li(1)-O(7)-Li(4) 83.6(3)	Li(1)-O(4)-Li(4) 85.3(2)
		Li(2)-O(3)-Li(3) 84.6(3)	Li(2)-O(2)-Li(4) 85.5(3)	Li(2)-O(1)-Li(4) 83.1(2)
		Li(2)-O(3)-Li(4) 83.8(3)	Li(2)-O(4)-Li(3) 84.5(3)	Li(2)-O(2)-Li(3) 86.0(2)
		Li(3)-O(3)-Li(4) 84.9(3)	Li(2)-O(4)-Li(4) 85.6(3)	Li(2)-O(3)-Li(3) 83.3(2)
		Li(1)-O(4)-Li(3) 84.4(3)	Li(2)-O(5)-Li(3) 84.9(3)	Li(2)-O(3)-Li(4) 85.7(2)
		Li(1)-O(4)-Li(4) 83.4(3)	Li(3)-O(4)-Li(4) 84.5(3)	Li(3)-O(3)-Li(4) 85.0(2)
		Li(3)-O(4)-Li(4) 84.2(3)	Li(3)-O(7)-Li(4) 87.1(3)	Li(3)-O(4)-Li(4) 84.7(2)
(μ_3-O)-Li-(μ_3-O)	O(1)-Li(1)-O(1a) 93.21(18)	O(1)-Li(1)-O(2) 96.4(3)	O(2)-Li(1)-O(5) 95.4(3)	O(1)-Li(1)-O(2) 94.9(2)
	O(1)-Li(1)-O(2) 94.12(18)	O(1)-Li(1)-O(4) 97.0(4)	O(2)-Li(1)-O(7) 96.5(3)	O(1)-Li(1)-O(4) 96.2(2)
	O(1)-Li(2)-O(2a) 96.73(17)	O(1)-Li(2)-O(3) 95.6(3)	O(2)-Li(2)-O(4) 94.8(3)	O(1)-Li(2)-O(2) 94.1(2)
	O(1)-Li(2)-O(2) 94.27(18)	O(1)-Li(4)-O(3) 96.2(3)	O(2)-Li(2)-O(5) 94.2(3)	O(1)-Li(2)-O(3) 94.6(2)
	O(2)-Li(1)-O(1a) 96.76(18)	O(1)-Li(4)-O(4) 96.0(3)	O(2)-Li(4)-O(4) 93.4(3)	O(1)-Li(4)-O(3) 96.2(2)
	O(2)-Li(2)-O(2a) 94.68(17)	O(2)-Li(2)-O(1) 96.4(3)	O(2)-Li(4)-O(7) 96.5(3)	O(1)-Li(4)-O(4) 94.0(2)
		O(2)-Li(2)-O(3) 94.9(3)	O(4)-Li(2)-O(5) 95.4(3)	O(2)-Li(1)-O(4) 97.2(2)
		O(2)-Li(1)-O(4) 96.0(3)	O(4)-Li(3)-O(5) 95.0(3)	O(2)-Li(2)-O(3) 94.8(2)
		O(2)-Li(3)-O(3) 95.4(3)	O(4)-Li(3)-O(7) 93.1(3)	O(2)-Li(3)-O(3) 95.5(2)
		O(2)-Li(3)-O(4) 95.0(3)	O(4)-Li(4)-O(7) 94.8(3)	O(2)-Li(3)-O(4) 97.8(2)
		O(3)-Li(3)-O(4) 95.1(4)	O(5)-Li(1)-O(7) 93.4(3)	O(3)-Li(3)-O(4) 92.9(2)
		O(3)-Li(4)-O(4) 95.3(3)	O(5)-Li(3)-O(7) 94.5(3)	O(3)-Li(4)-O(4) 96.6(2)

O_{THF}-Li-(μ_3-O)	O(3)-Li(2)-O(1)	125.3(2)	O(5)-Li(1)-O(1)	123.7(4)	O(1)-Li(1)-O(2)	101.8(3)	O(6)-Li(3)-O(2)	123.0(3)
	O(3)-Li(2)-O(2a)	119.9(2)	O(5)-Li(1)-O(2)	122.5(4)	O(1)-Li(1)-O(5)	122.1(4)	O(6)-Li(3)-O(3)	131.7(3)
	O(3)-Li(2)-O(3)	119.0(2)	O(5)-Li(1)-O(4)	115.2(4)	O(1)-Li(1)-O(7)	137.7(4)	O(6)-Li(3)-O(4)	107.6(2)
	O(4)-Li(1)-O(1)	120.1(2)	O(6)-Li(2)-O(1)	115.2(4)	O(3)-Li(2)-O(2)	112.8(3)	O(7)-Li(1)-O(1)	123.5(3)
	O(4)-Li(1)-O(1a)	120.7(2)	O(6)-Li(2)-O(2)	126.1(4)	O(3)-Li(2)-O(4)	107.3(3)	O(7)-Li(1)-O(2)	109.6(2)
	O(4)-Li(1)-O(2)	124.6(2)	O(6)-Li(2)-O(3)	122.0(4)	O(3)-Li(2)-O(5)	142.4(4)	O(7)-Li(1)-O(4)	128.1(3)
			O(7)-Li(3)-O(2)	118.1(4)	O(6)-Li(3)-O(4)	140.6(4)	O(8)-Li(2)-O(1)	135.7(3)
			O(7)-Li(3)-O(3)	124.5(4)	O(6)-Li(3)-O(5)	108.4(3)	O(8)-Li(2)-O(2)	117.5(3)
			O(7)-Li(3)-O(4)	121.9(4)	O(6)-Li(3)-O(7)	115.4(3)	O(8)-Li(2)-O(3)	111.4(3)
			O(8)-Li(4)-O(1)	122.4(4)	O(8)-Li(4)-O(2)	138.2(4)	O(9)-Li(4)-O(1)	112.9(3)
			O(8)-Li(4)-O(3)	115.5(4)	O(8)-Li(4)-O(4)	122.3(4)	O(9)-Li(4)-O(3)	132.4(3)
			O(8)-Li(4)-O(4)	124.9(4)	O(8)-Li(4)-O(7)	101.0(3)	O(9)-Li(4)-O(4)	116.9(3)

Table 3. Select bond distances (Å) and angles (deg) for **5 - 7**.

Distance (Å)	**5**		**6**		**7**	
Li---Li	Li(1)---Li(2)	3.162(8)	Li(1)---Li(1a)	2.527(6)	Li(1)---Li(1a)	2.382(9)
	Li(1)---Li(3)	3.048(8)			Li(2)----Li(2a)	2.399(8)
	Li(2)---Li(3)	3.060(8)				
Li-(μ_x-O)	Li(1)-O(1)	1.830(6)	Li(1)-O(1)	1.907(3)	Li(1)-O(1)	1.822(4)
	Li(1)-O(3)	1.844(6)	Li(1)-O(1a)	1.911(3)	Li(2)-O(2)	1.816(4)
	Li(2)-O(1)	1.822(6)	Li(1a)-O(1)	1.911(3)		
	Li(2)-O(2)	1.807(6)				
	Li(3)-O(2)	1.846(6)				
	Li(3)-O(3)	1.829(6)				
Li-O_{THF}	Li(1)-O(4)	1.937(6)	Li(1)-O(2)	2.002(3)	Li(1)-O(4)	1.891(5)
	Li(2)-O(5)	1.958(6)	Li(1)-O(3)	2.014(3)	Li(2)-O(3)	1.883(4)
	Li(3)-O(6)	1.920(6)				
Angles (Å)	**5**		**6**		**7**	
Li-(μ_x-O)-Li	Li(1)-O(1)-Li(2)	119.9(3)	Li(1)-O(1)-Li(1a)	82.90(13)	Li(1)-O(1)-Li(1a)	80.5(2)
	Li(2)-O(2)-Li(3)	113.8(3)			Li(2)-O(2)-Li(2a)	81.1(2)
	Li(3)-O(3)-Li(1)	112.1(3)				
(μ_x-O)-Li-(μ_x-O)	O(1)-Li(1)-O(3)	122.5(3)	O(1)-Li(1)-O(1a)	97.10(13)	O(1)-Li(1)-O(1a)	99.5(1)
	O(1)-Li(2)-O(2)	121.8(3)			O(2)-Li(2)-O(2a)	98.9(2)
	O(2)-Li(3)-O(3)	128.7(3)				
O_{THF}-Li-(μ_x-O)	O(1)-Li(1)-O(4)	116.7(3)			O(1)-Li(1)-O(4)	130.2(2)
	O(1)-Li(2)-O(5)	118.9(3)			O(1a)-Li(1)-O(4)	130.2(2)
	O(2)-Li(2)-O(5)	119.3(3)			O(2)-Li(2)-O(3)	136.1(2)
	O(2)-Li(3)-O(6)	116.1(3)			O(2a)-Li(2)-O(3)	125.0(2)
	O(3)-Li(1)-O(4)	120.8(3)				
	O(3)-Li(3)-O(6)	114.7(3)				

Table 4. Solid state MAS and solution NMR data for **1** - **7**.

Compound	δ ^{7}Li [a] tol.-d_8	δ ^{13}C{^{1}H} MAS	δ ^{6}Li MAS	δ ^{7}Li[a] MAS	^{7}Li P_Q (kHz)[e]	MC[c]	CN[d]	Li-O (av.)	Ref
1	1.26(1)	167.0,162.9, 128.9, 119.5,118.5, 114.3, 57.0(THF), 24.6(THF)	0.58(5), -0.11(5)	0.2(1)	120	4	4	1.93	f
						6	4	1.96	8
2	1.15(1)	165.3, 129.9, 127.3, 118.8, 114.3, 67.6 (THF), 25.0 (THF), 17.2	0.62(5)	0.8(2)	50	4	4	1.95	f
3	0.64(1)	163.4, 129.4, 126.9, 123.7, 113.4, 68.5(THF), 26.1, 25.0(THF), 18.4	0.56(5) (2.02(5))	0.7(1)	70	4	4	2.00	f
4	1.65(1) (1.34(1))	163.7, 162.6, 161.2, 135.9, 135.0, 127.7, 125.3, 118.9, 116.3, 67.3(THF), 25.3(THF), 22.1	0.55(5)	0.6(1)	50	4	4	1.95	f
5	0.70(1)	161.3, 136.0, 123.5, 122.4, 116.5, 114.7, 68.0(THF), 25.5(THF), 21.8	0.41(5)	0.5(1)	275	4	3	1.83	f
6	0.35(1)	168.7, 164.4, 136.9, 125.2, 115.3, 111.5, 67.9(THF), 34.5, 30.0, 26.1(THF)	-0.25(5)	-0.1(1)	140	2	4	1.91	f
7	0.90(1)	165.1, 138.2, 136.8, 125.1, 112.9, 112.0, 100.1, 68.2(THF), 35.4, 31.5, 25.2(THF).	0.51(5)	0.1(1)	260	2	3	1.82	f
						2	3	1.85	15

[a] Solution NMR. [b] Peak maximum, not corrected for quadrupolar shift effects. [c]MC = Molecular complexity from this work
[d]CN = Coordination Number from this work. [e]Quadrupolar coupling product was estimated from the width of the spinning side band manifold and has an error of ~ ± 10 kHz. [f]This work.

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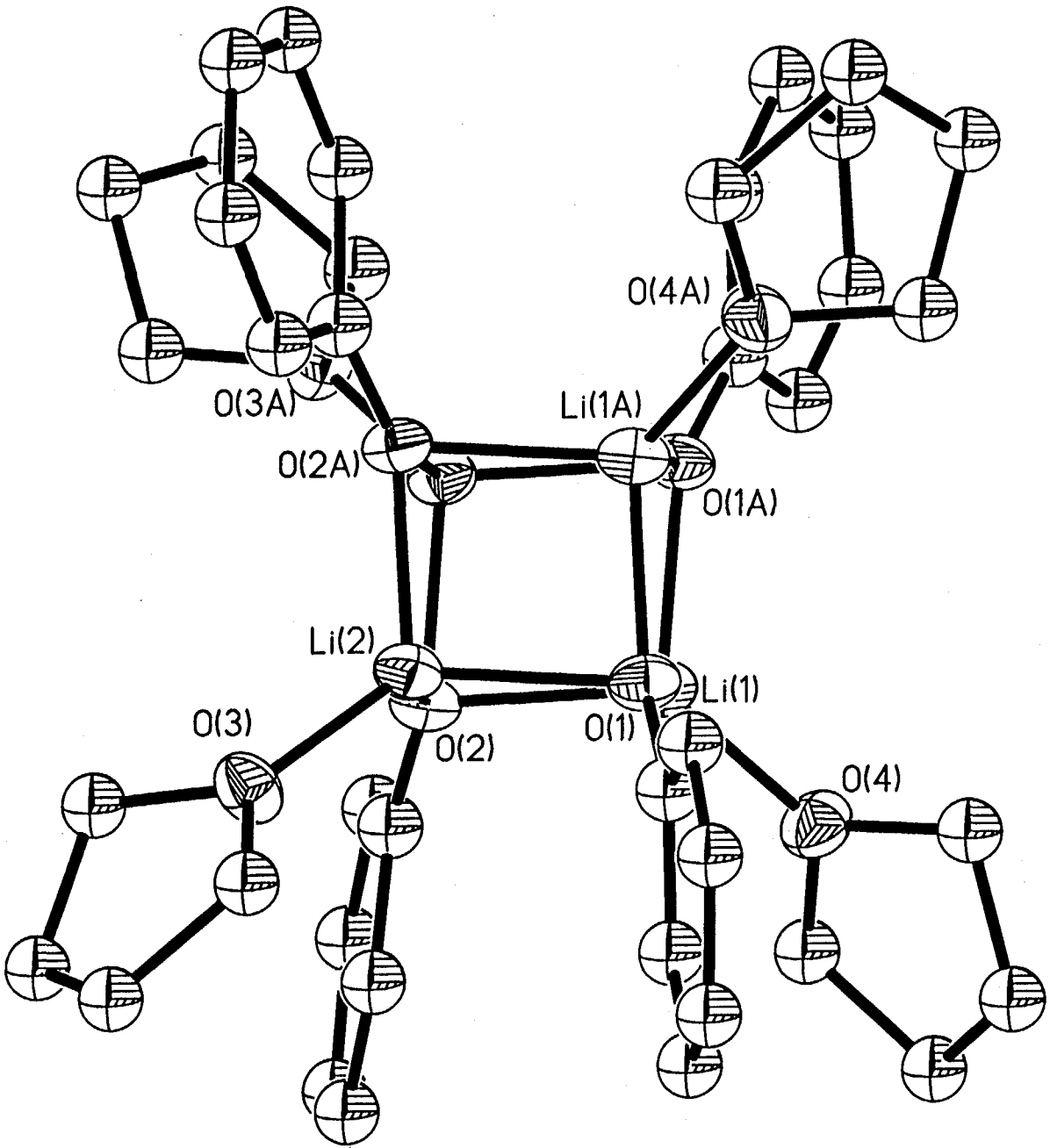
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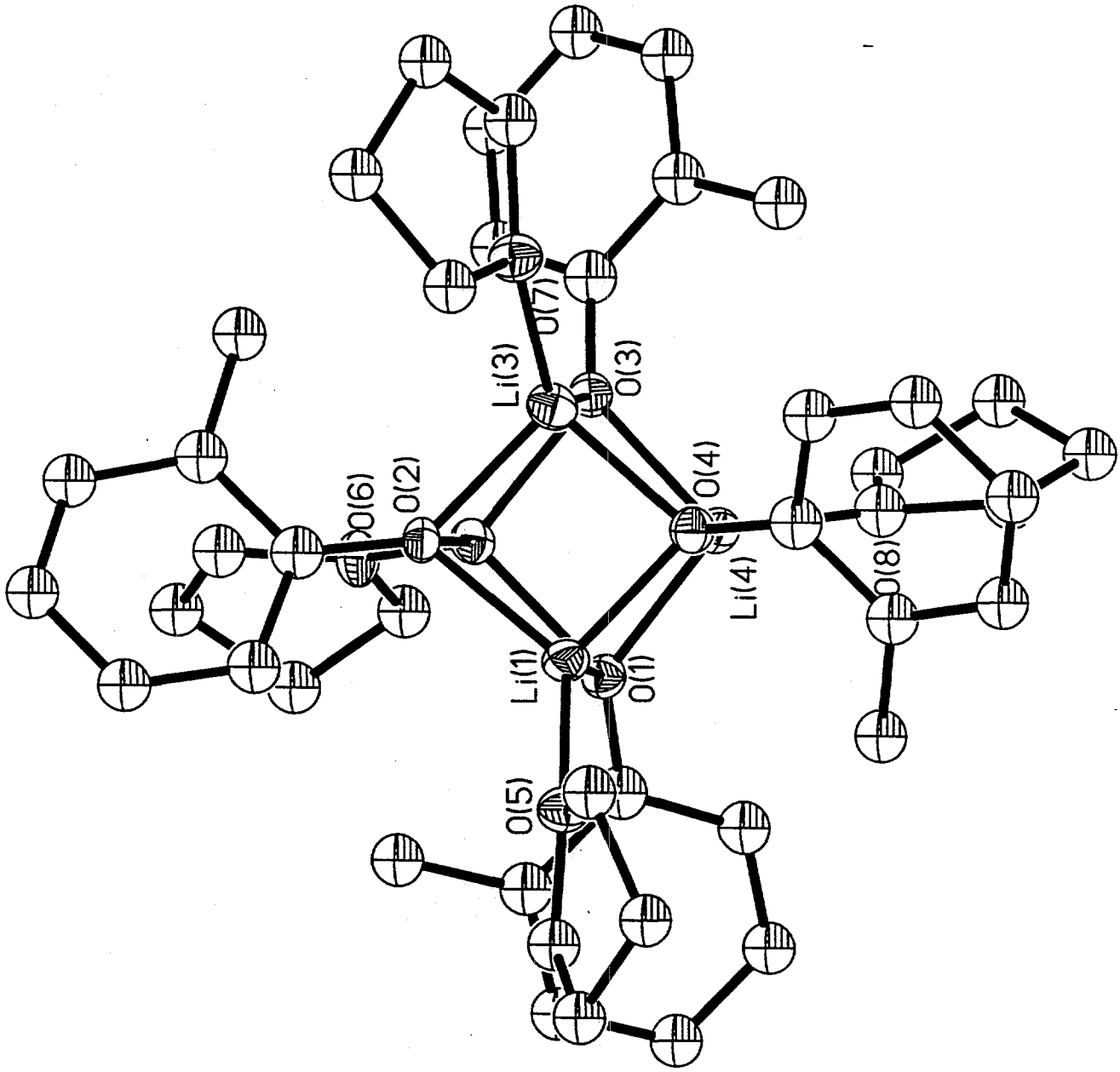
Li(1A)
O(2A)
O(1A)
Li(2)
Li(1)
O(3)
O(2)
O(1)
O(4)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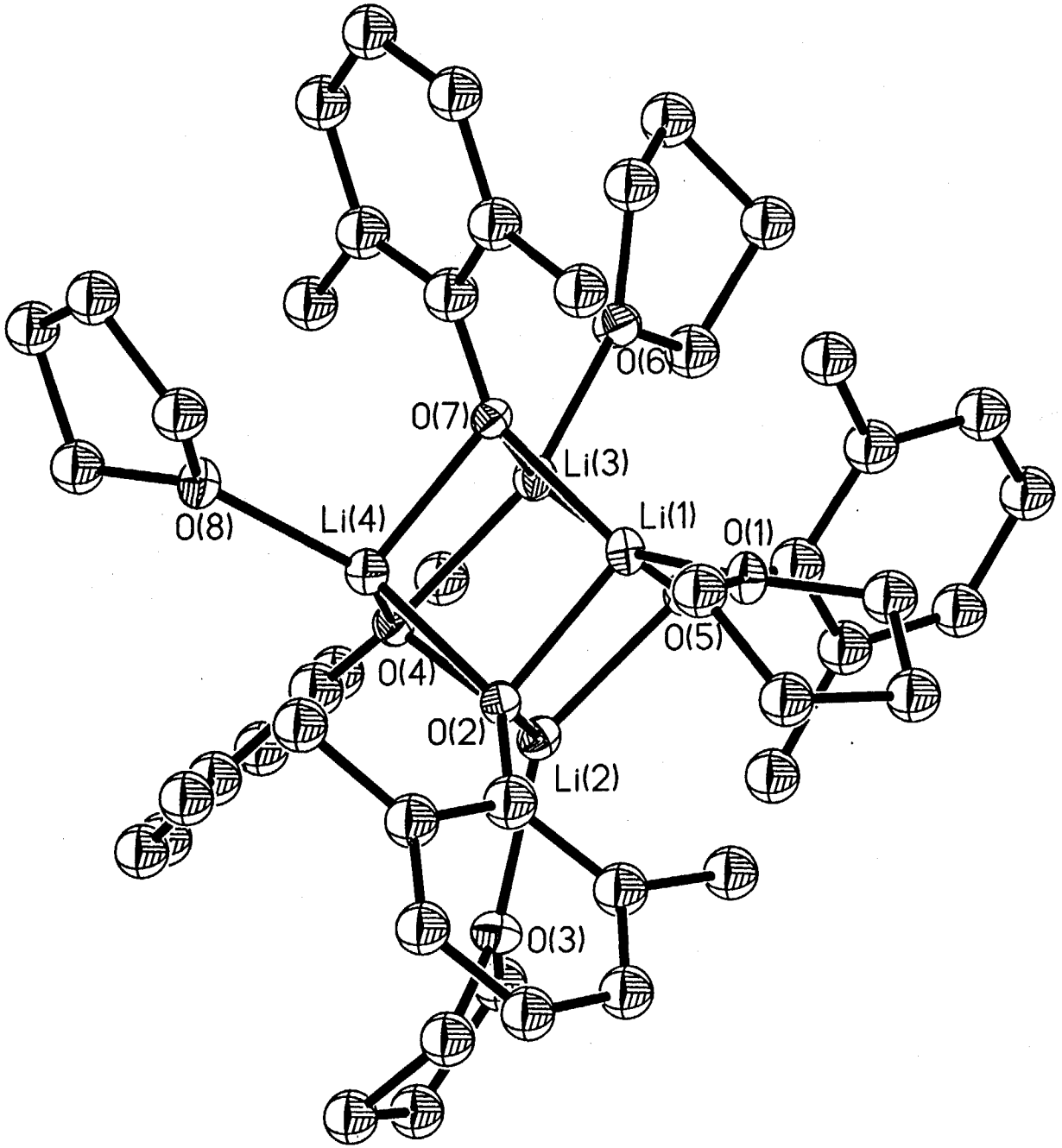
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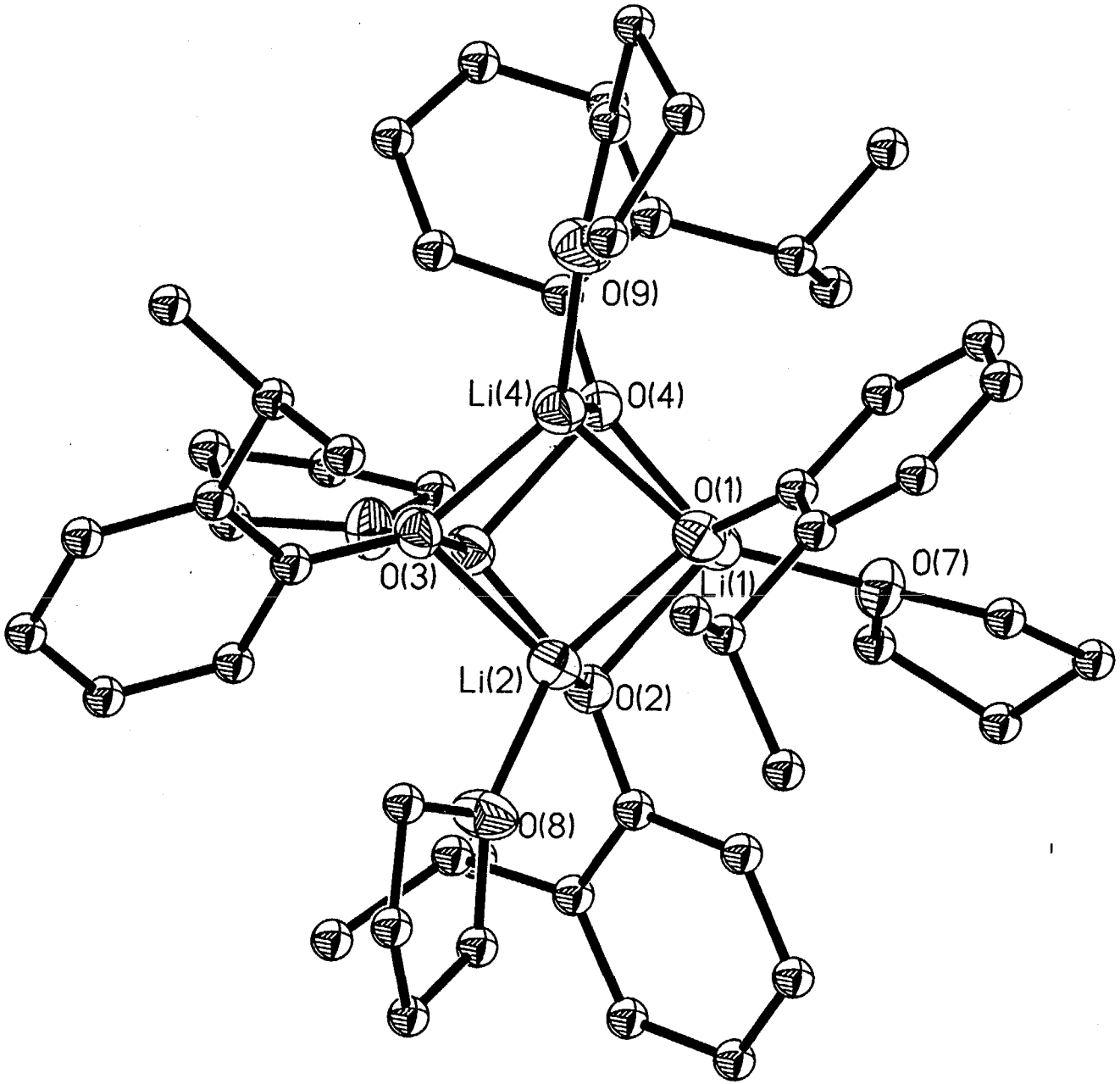
Li(2)
O(3)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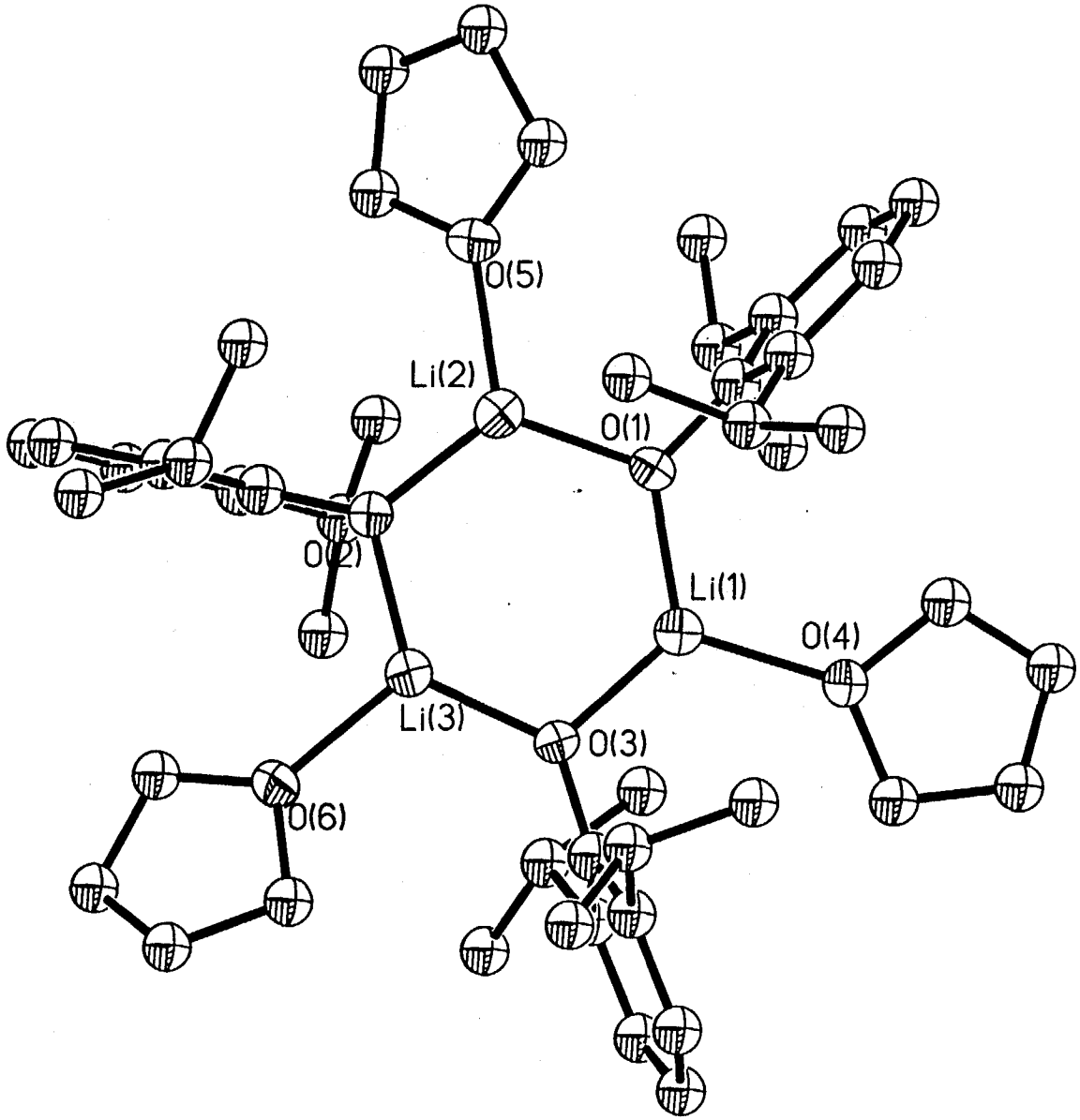
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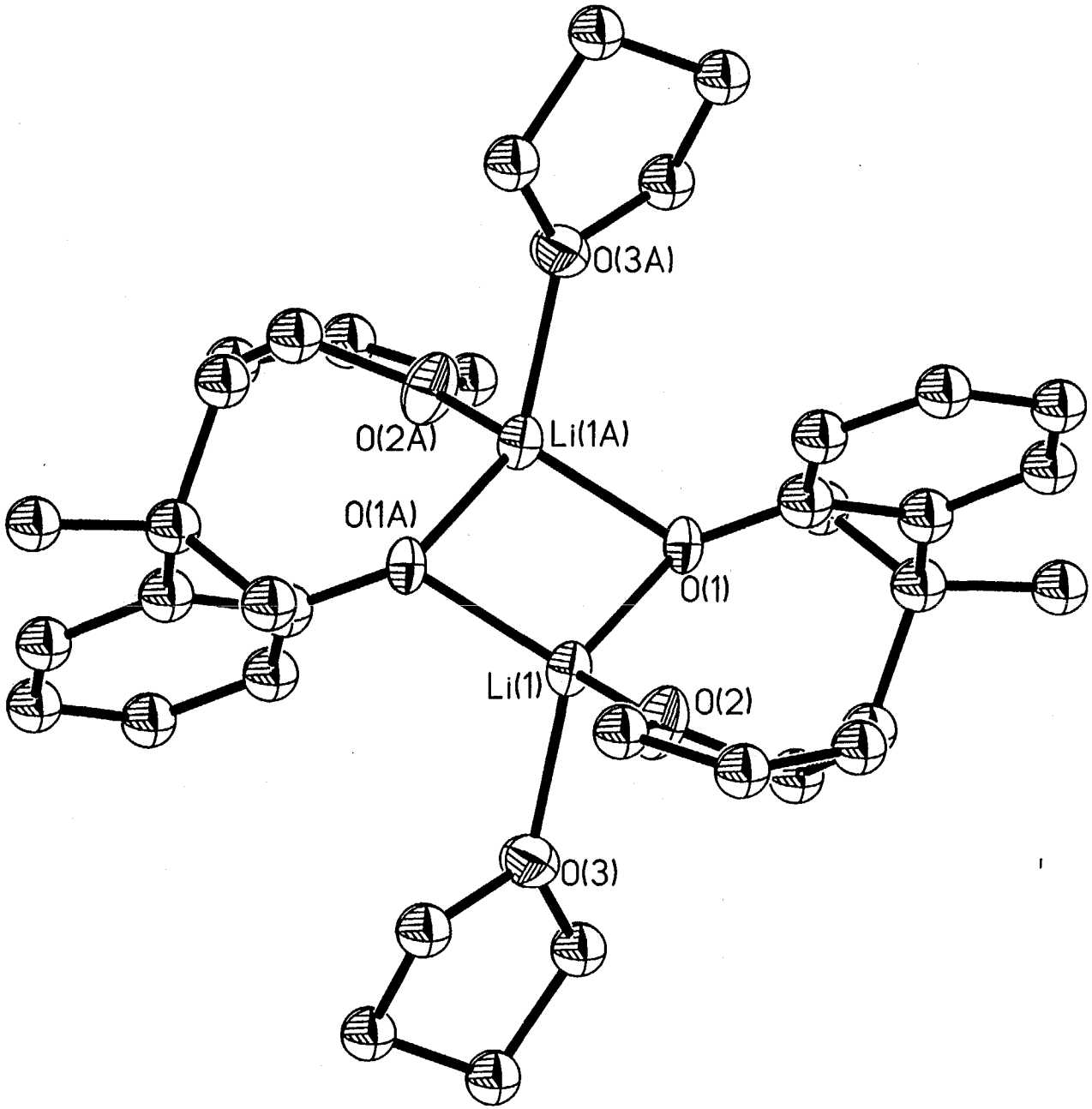
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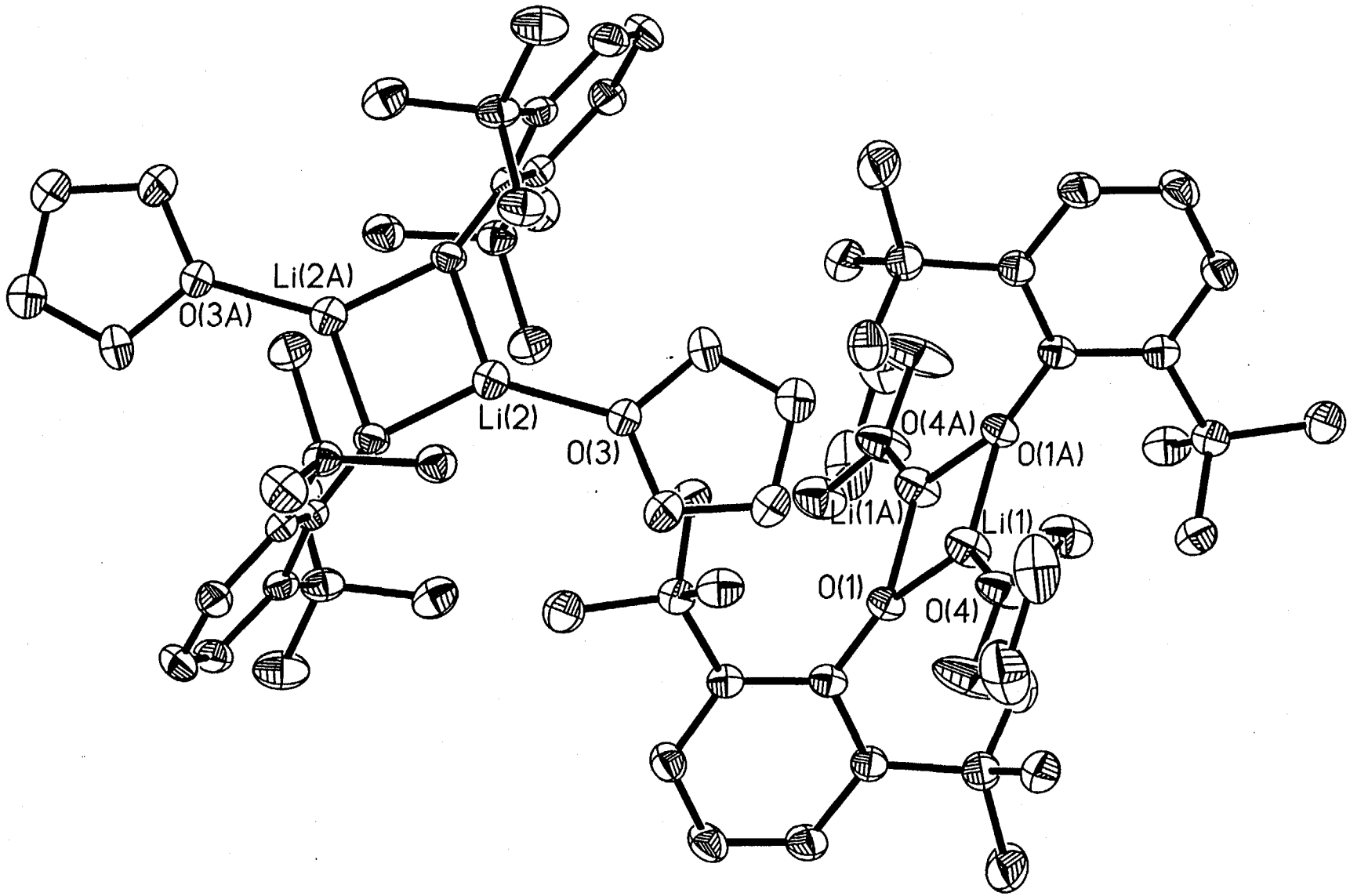
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Li(1A)
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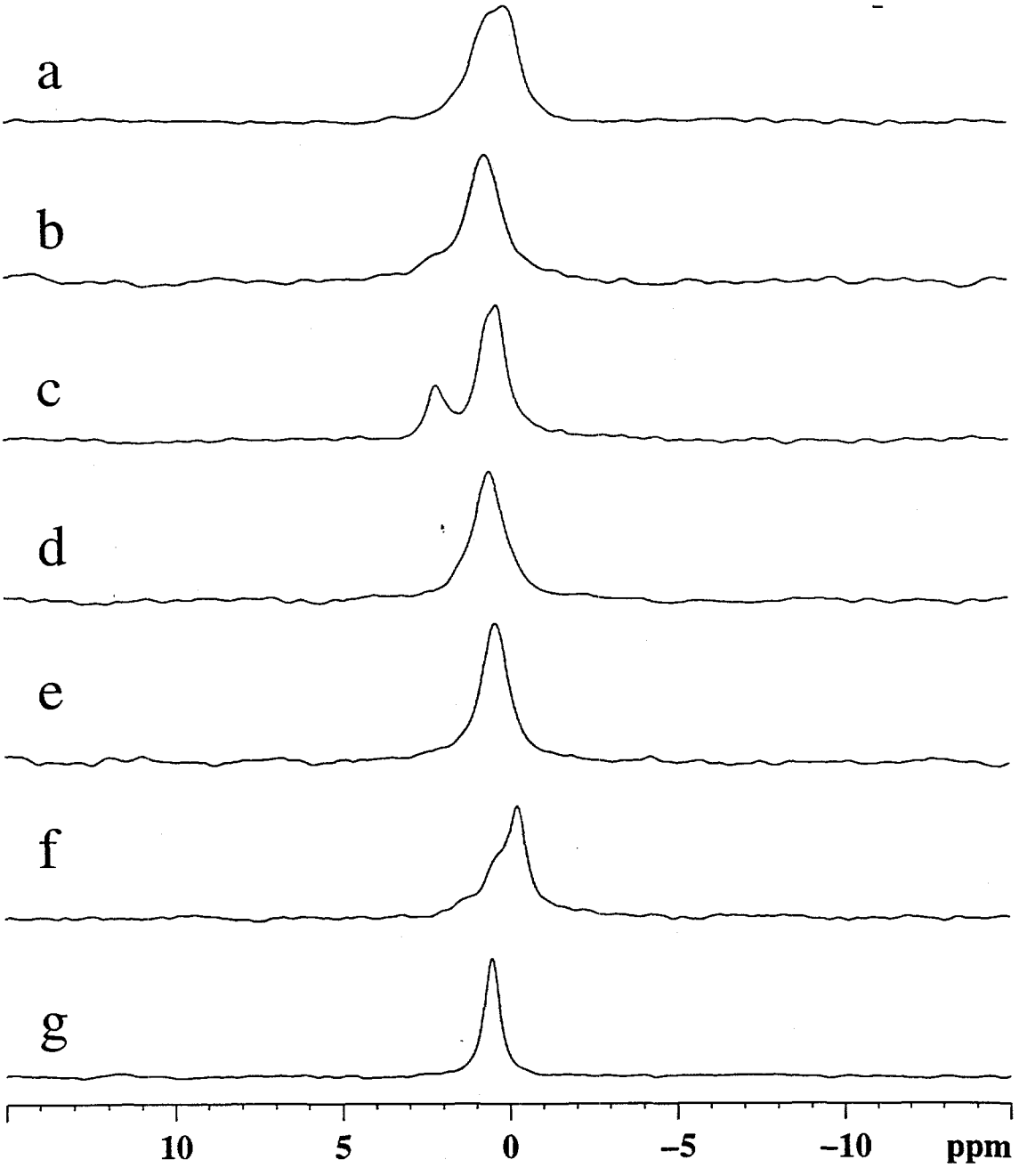


Figure 8. ^{6}Li MAS NMR spectra of **1** - **7** (a-g).

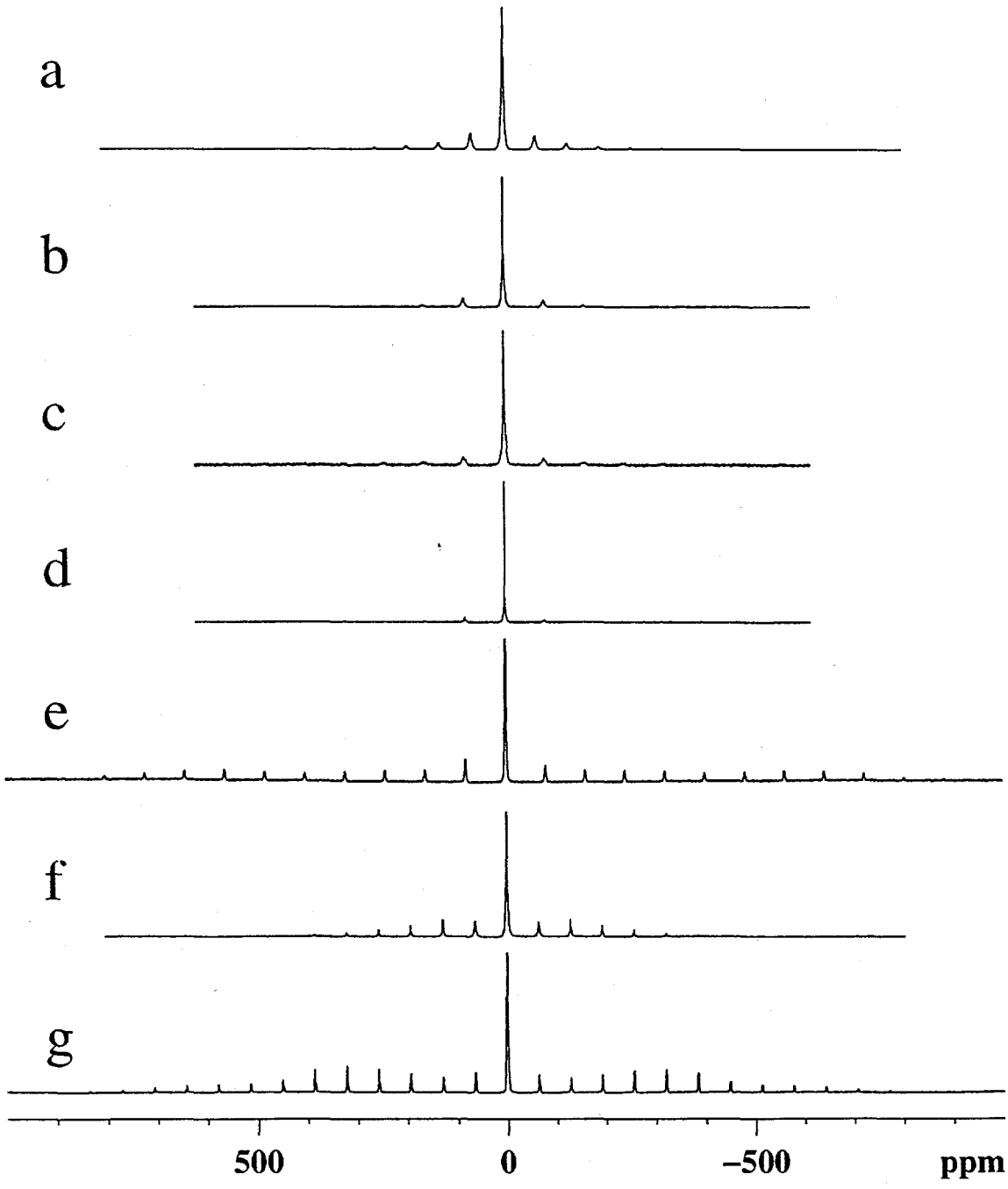


Figure 9. ^{7}Li MAS NMR spectra of **1** - **7** (a - g).

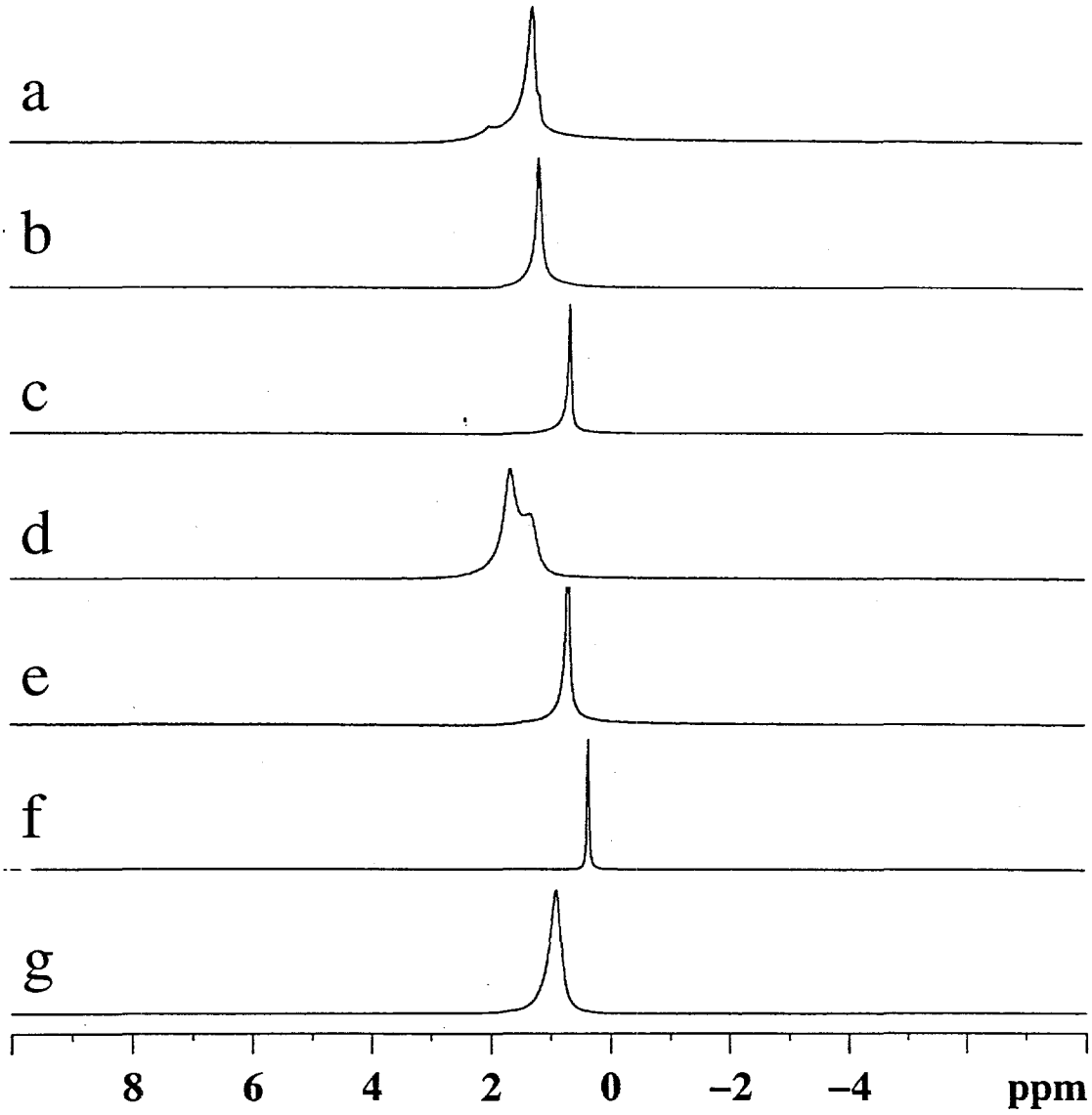
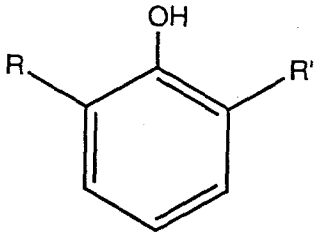


Figure 10. ^{7}Li solution (toluene-d_8) NMR spectra of **1** - **7** (a - g).

$$A(OR) + Ti(OR)_4 \xrightarrow{\text{toluene}} [ATi(OR)_5]_n \quad (1)$$

$$[ATi(OR)_5]_n + MCl_x \xrightarrow{\text{toluene}} \text{"}MTi(OR)_5(Cl)_{x-n}\text{"} + n\,ACl \quad (2)$$



$$+ \; LiN(SiMe_3)_2 \xrightarrow{THF} [Li(OAr)(THF)_x]_n + HN(SiMe_3)_2 \quad (3)$$

OAr	R	R'	Cmpd	n	x
OPh	H	H	**1**	6	1
oMP	Me	H	**2**	4	1
DMP	Me	Me	**3**	4	1
oPP	Pr^i	H	**4**	4	1
DIP	Pr^i	Pr^i	**5**	3	1
oBP	Bu^t	H	**6**	2	2
DBP	Bu^t	Bu^t	**7**	2	1

Supplemental Information for:

Structural Diversity in Lithium Aryloxides, Part 1. Structurally characterized $[Li(OAr)(THF)_x]_n$ where OAr = OC_6H_5, OC_6H_4(2-Me), OC_6H_3(2,6-Me)$_2$, OC_6H_4(2-Pr^i), OC_6H_3(2,6-Pr^i)$_2$, OC_6H_4(2-Bu^t), OC_6H_3(2,6-Bu^t)$_2$.

by:

Timothy J. Boyle*, Dawn M. Pedrotty, Todd M. Alam, Sara C. Vick, Mark A. Rodriguez

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$[Li(OPh)(THF)]_4$ (1)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group C2/c using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0541 and R2w=0.1252.

Table S1.1. Crystal data and structure refinement for **1**.

Empirical formula	C20 H26 Li2 O4
Formula weight	344.29
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 26.890(3) A alpha = 90 deg. b = 9.2373(9) A beta = 124.812(5) deg. c = 19.761(2) A gamma = 90 deg.
Volume	4030.0(7) A^3
Z, Calculated density	8, 1.135 Mg/m^3
Absorption coefficient	0.076 mm^-1
F(000)	1472
Crystal size	.4 x .2 x .4 mm
Theta range for data collection	1.84 to 28.32 deg.
Limiting indices	-35<=h<=31, -11<=k<=11, -15<=l<=26
Reflections collected / unique	12555 / 4727 [R(int) = 0.0683]
Completeness to theta = 28.32	94.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4727 / 0 / 235
Goodness-of-fit on F^2	0.829
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1252
R indices (all data)	R1 = 0.1570, wR2 = 0.1582
Largest diff. peak and hole	0.280 and -0.208 e.A^-3

Table S1.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	525(2)	7442(4)	2593(2)	50(1)
Li(2)	250(2)	5423(4)	3286(2)	48(1)
C(1)	588(1)	7936(2)	4147(1)	41(1)
C(2)	1219(1)	7921(2)	4666(1)	46(1)
C(3)	1521(1)	8240(3)	5497(2)	62(1)
C(4)	1204(2)	8601(3)	5825(2)	73(1)
C(5)	589(2)	8648(3)	5324(2)	73(1)
C(6)	282(1)	8322(3)	4493(2)	59(1)
C(7)	1106(1)	4873(2)	2807(1)	38(1)
C(8)	1182(1)	4525(3)	2182(1)	50(1)
C(9)	1744(1)	4166(3)	2363(2)	58(1)
C(10)	2246(1)	4131(3)	3165(2)	60(1)
C(11)	2177(1)	4440(3)	3790(2)	56(1)
C(12)	1620(1)	4797(2)	3615(1)	44(1)
C(13)	771(1)	4293(3)	5042(1)	68(1)
C(14)	1186(1)	3072(3)	5498(2)	79(1)
C(15)	1203(2)	2212(3)	4882(2)	92(1)
C(16)	654(1)	2670(3)	4077(2)	69(1)
C(17)	1703(1)	8485(3)	2831(2)	71(1)
C(18)	2111(1)	9677(4)	3371(2)	103(1)
C(19)	1743(2)	10544(4)	3550(2)	112(1)
C(20)	1120(2)	10162(3)	2925(3)	95(1)
O(1)	294(1)	7574(2)	3354(1)	48(1)
O(2)	575(1)	5297(2)	2637(1)	47(1)
O(3)	549(1)	4139(2)	4199(1)	56(1)
O(4)	1140(1)	8705(2)	2713(1)	61(1)

Table S1.3. Bond lengths [A] and angles [deg] for **1**.

Li(1)-O(1)#1	1.912(4)
Li(1)-O(4)	1.925(4)
Li(1)-O(1)	1.933(4)
Li(1)-O(2)	1.984(5)
Li(1)-Li(2)#1	2.589(5)
Li(1)-Li(1)#1	2.631(8)
Li(1)-Li(2)	2.656(6)
Li(1)-C(7)	2.738(5)
Li(2)-O(2)#1	1.907(4)
Li(2)-O(3)	1.912(4)
Li(2)-O(2)	1.922(4)
Li(2)-O(1)	1.990(4)
Li(2)-Li(2)#1	2.585(7)
Li(2)-Li(1)#1	2.589(5)
Li(2)-C(1)	2.710(4)
C(1)-O(1)	1.332(2)
C(1)-C(6)	1.384(3)
C(1)-C(2)	1.393(3)
C(2)-C(3)	1.385(3)
C(3)-C(4)	1.375(4)
C(4)-C(5)	1.359(4)
C(5)-C(6)	1.387(3)
C(7)-O(2)	1.326(2)
C(7)-C(12)	1.395(3)
C(7)-C(8)	1.399(3)
C(8)-C(9)	1.379(3)
C(9)-C(10)	1.376(3)
C(10)-C(11)	1.379(3)
C(11)-C(12)	1.372(3)
C(13)-O(3)	1.420(3)
C(13)-C(14)	1.478(4)
C(14)-C(15)	1.476(4)
C(15)-C(16)	1.485(4)
C(16)-O(3)	1.433(3)
C(17)-O(4)	1.409(3)
C(17)-C(18)	1.489(4)
C(18)-C(19)	1.466(5)
C(19)-C(20)	1.447(5)
C(20)-O(4)	1.419(3)
O(1)-Li(1)#1	1.912(4)
O(2)-Li(2)#1	1.907(4)
O(1)#1-Li(1)-O(4)	120.7(2)
O(1)#1-Li(1)-O(1)	93.21(18)
O(4)-Li(1)-O(1)	120.1(2)
O(1)#1-Li(1)-O(2)	96.76(18)
O(4)-Li(1)-O(2)	124.6(2)
O(1)-Li(1)-O(2)	94.12(18)
O(1)#1-Li(1)-Li(2)#1	49.74(13)
O(4)-Li(1)-Li(2)#1	145.6(2)
O(1)-Li(1)-Li(2)#1	94.23(18)

O(2)-Li(1)-Li(2)#1	47.05(13)
O(1)#1-Li(1)-Li(1)#1	47.16(12)
O(4)-Li(1)-Li(1)#1	142.68(14)
O(1)-Li(1)-Li(1)#1	46.51(13)
O(2)-Li(1)-Li(1)#1	92.64(12)
Li(2)#1-Li(1)-Li(1)#1	61.17(14)
O(1)#1-Li(1)-Li(2)	92.62(17)
O(4)-Li(1)-Li(2)	146.5(2)
O(1)-Li(1)-Li(2)	48.30(13)
O(2)-Li(1)-Li(2)	46.20(13)
Li(2)#1-Li(1)-Li(2)	59.04(17)
Li(1)#1-Li(1)-Li(2)	58.63(14)
O(1)#1-Li(1)-C(7)	116.27(18)
O(4)-Li(1)-C(7)	97.58(17)
O(1)-Li(1)-C(7)	110.07(17)
O(2)-Li(1)-C(7)	27.09(8)
Li(2)#1-Li(1)-C(7)	69.46(14)
Li(1)#1-Li(1)-C(7)	119.59(10)
Li(2)-Li(1)-C(7)	67.30(14)
O(2)#1-Li(2)-O(3)	119.9(2)
O(2)#1-Li(2)-O(2)	94.68(17)
O(3)-Li(2)-O(2)	119.0(2)
O(2)#1-Li(2)-O(1)	96.73(17)
O(3)-Li(2)-O(1)	125.34(19)
O(2)-Li(2)-O(1)	94.27(18)
O(2)#1-Li(2)-Li(2)#1	47.80(13)
O(3)-Li(2)-Li(2)#1	141.62(12)
O(2)-Li(2)-Li(2)#1	47.31(14)
O(1)-Li(2)-Li(2)#1	92.99(11)
O(2)#1-Li(2)-Li(1)#1	49.58(13)
O(3)-Li(2)-Li(1)#1	145.5(2)
O(2)-Li(2)-Li(1)#1	95.43(17)
O(1)-Li(2)-Li(1)#1	47.17(13)
Li(2)#1-Li(2)-Li(1)#1	61.78(13)
O(2)#1-Li(2)-Li(1)	93.66(16)
O(3)-Li(2)-Li(1)	146.2(2)
O(2)-Li(2)-Li(1)	48.15(13)
O(1)-Li(2)-Li(1)	46.49(13)
Li(2)#1-Li(2)-Li(1)	59.18(14)
Li(1)#1-Li(2)-Li(1)	60.20(19)
O(2)#1-Li(2)-C(1)	116.28(18)
O(3)-Li(2)-C(1)	97.43(15)
O(2)-Li(2)-C(1)	110.67(18)
O(1)-Li(2)-C(1)	27.93(8)
Li(2)#1-Li(2)-C(1)	120.81(9)
Li(1)#1-Li(2)-C(1)	69.95(14)
Li(1)-Li(2)-C(1)	68.28(14)
O(1)-C(1)-C(6)	121.5(2)
O(1)-C(1)-C(2)	121.4(2)
C(6)-C(1)-C(2)	117.1(2)
O(1)-C(1)-Li(2)	44.39(12)
C(6)-C(1)-Li(2)	116.71(19)
C(2)-C(1)-Li(2)	106.57(17)
C(3)-C(2)-C(1)	121.0(2)
C(4)-C(3)-C(2)	120.5(3)
C(5)-C(4)-C(3)	119.3(3)
C(4)-C(5)-C(6)	120.6(3)

C(1)-C(6)-C(5)	121.4(3)
O(2)-C(7)-C(12)	121.6(2)
O(2)-C(7)-C(8)	121.61(19)
C(12)-C(7)-C(8)	116.7(2)
O(2)-C(7)-Li(1)	42.93(13)
C(12)-C(7)-Li(1)	109.01(16)
C(8)-C(7)-Li(1)	114.90(17)
C(9)-C(8)-C(7)	121.1(2)
C(10)-C(9)-C(8)	120.9(2)
C(9)-C(10)-C(11)	118.8(2)
C(12)-C(11)-C(10)	120.6(2)
C(11)-C(12)-C(7)	121.8(2)
O(3)-C(13)-C(14)	107.7(2)
C(15)-C(14)-C(13)	106.0(2)
C(14)-C(15)-C(16)	104.5(2)
O(3)-C(16)-C(15)	105.1(2)
O(4)-C(17)-C(18)	107.1(2)
C(19)-C(18)-C(17)	104.7(3)
C(20)-C(19)-C(18)	105.8(3)
O(4)-C(20)-C(19)	105.2(3)
C(1)-O(1)-Li(1)#1	138.26(18)
C(1)-O(1)-Li(1)	133.71(18)
Li(1)#1-O(1)-Li(1)	86.33(18)
C(1)-O(1)-Li(2)	107.68(16)
Li(1)#1-O(1)-Li(2)	83.09(17)
Li(1)-O(1)-Li(2)	85.21(18)
C(7)-O(2)-Li(2)#1	139.11(18)
C(7)-O(2)-Li(2)	133.07(17)
Li(2)#1-O(2)-Li(2)	84.90(17)
C(7)-O(2)-Li(1)	109.98(17)
Li(2)#1-O(2)-Li(1)	83.37(16)
Li(2)-O(2)-Li(1)	85.66(17)
C(13)-O(3)-C(16)	107.49(17)
C(13)-O(3)-Li(2)	135.53(19)
C(16)-O(3)-Li(2)	116.53(18)
C(17)-O(4)-C(20)	107.8(2)
C(17)-O(4)-Li(1)	134.4(2)
C(20)-O(4)-Li(1)	115.9(2)

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

Table S1.4. Anisotropic displacement parameters (A^2 x 10^3) for **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	40(2)	64(3)	43(2)	0(2)	21(2)	-3(2)
Li(2)	42(2)	58(3)	37(2)	1(2)	18(2)	5(2)
C(1)	45(1)	39(1)	37(1)	0(1)	22(1)	0(1)
C(2)	42(1)	43(1)	44(1)	-3(1)	19(1)	-2(1)
C(3)	56(2)	45(2)	47(2)	1(1)	7(1)	-1(1)
C(4)	98(3)	59(2)	42(2)	-6(1)	29(2)	4(2)
C(5)	97(2)	82(2)	55(2)	-2(2)	52(2)	12(2)
C(6)	57(2)	73(2)	50(2)	-3(1)	33(1)	5(1)
C(7)	38(1)	37(1)	38(1)	-1(1)	22(1)	-2(1)
C(8)	48(2)	61(2)	40(1)	-7(1)	25(1)	-2(1)
C(9)	60(2)	66(2)	64(2)	-12(1)	45(2)	-4(1)
C(10)	48(2)	61(2)	77(2)	-2(1)	39(2)	6(1)
C(11)	39(2)	64(2)	50(2)	5(1)	18(1)	5(1)
C(12)	45(1)	48(2)	36(1)	0(1)	21(1)	2(1)
C(13)	94(2)	66(2)	43(2)	8(1)	38(2)	18(2)
C(14)	79(2)	81(2)	60(2)	13(2)	30(2)	18(2)
C(15)	127(3)	60(2)	82(2)	18(2)	56(2)	36(2)
C(16)	98(2)	49(2)	64(2)	-7(1)	48(2)	-5(2)
C(17)	64(2)	66(2)	101(2)	-16(2)	57(2)	-10(2)
C(18)	65(2)	78(2)	132(3)	-24(2)	36(2)	-16(2)
C(19)	165(4)	79(3)	137(3)	-50(2)	113(3)	-48(3)
C(20)	116(3)	48(2)	169(4)	2(2)	109(3)	4(2)
O(1)	42(1)	62(1)	34(1)	-7(1)	19(1)	-2(1)
O(2)	38(1)	61(1)	39(1)	-1(1)	20(1)	5(1)
O(3)	69(1)	55(1)	39(1)	5(1)	28(1)	13(1)
O(4)	48(1)	60(1)	78(1)	-9(1)	37(1)	-6(1)

Table S1.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	1444	7689	4447	56
H(3)	1951	8210	5842	74
H(4)	1412	8815	6395	87
H(5)	367	8907	5546	88
H(6)	-148	8364	4153	70
H(8)	841	4536	1624	60
H(9)	1784	3941	1928	69
H(10)	2633	3897	3287	72
H(11)	2519	4406	4347	67
H(12)	1583	4997	4056	53
H(13A)	430	4279	5103	82
H(13B)	988	5224	5259	82
H(14A)	1596	3433	5931	95
H(14B)	1035	2476	5762	95
H(15A)	1190	1163	4972	110
H(15B)	1574	2425	4907	110
H(16A)	723	2610	3637	83
H(16B)	303	2052	3925	83
H(17A)	1654	8505	2295	85
H(17B)	1874	7535	3095	85
H(18A)	2473	9285	3885	124
H(18B)	2245	10266	3084	124
H(19A)	1846	10315	4106	134
H(19B)	1810	11590	3525	134
H(20A)	869	10246	3143	114
H(20B)	949	10801	2438	114

$[Li(oMP)(THF)]_4$ (2)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P2(1)/c using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. Subsequent refinement confirmed the original atom identification. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0864 and R2w=0.2760

Table S2.1. Crystal data and structure refinement for **2**.

Empirical formula	C44 H60 Li4 O8
Formula weight	744.68
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 16.187(7) A alpha = 90 deg. b = 14.941(7) A beta = 108.425(12) deg. c = 18.920(10) A gamma = 90 deg.
Volume	4341(4) A^3
Z, Calculated density	4, 1.139 Mg/m^3
Absorption coefficient	0.075 mm^-1
F(000)	1600
Crystal size	.2 x .3 x .2 mm
Theta range for data collection	1.33 to 28.16 deg.
Limiting indices	-21<=h<=18, -19<=k<=18, -21<=l<=25
Reflections collected / unique	25189 / 9686 [R(int) = 0.0619]
Completeness to theta = 28.16	91.1 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9686 / 0 / 509
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0864, wR2 = 0.2760
R indices (all data)	R1 = 0.1900, wR2 = 0.3087
Largest diff. peak and hole	0.323 and -0.234 e.A^-3

Table S2.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	2532(5)	6854(5)	3012(4)	39(2)
Li(2)	1715(4)	7671(5)	1770(4)	37(2)
Li(3)	2448(5)	8596(5)	3000(4)	41(2)
Li(4)	3403(5)	7756(5)	2309(4)	38(2)
O(1)	2607(2)	6749(2)	1994(2)	37(1)
O(2)	1548(2)	7676(2)	2762(2)	35(1)
O(3)	2528(2)	8681(2)	1984(2)	38(1)
O(4)	3416(2)	7758(2)	3360(2)	38(1)
O(5)	2626(2)	5836(2)	3683(2)	43(1)
O(6)	810(2)	7544(2)	822(2)	44(1)
O(7)	2310(2)	9607(2)	3588(2)	46(1)
O(8)	4415(2)	7900(2)	1991(2)	49(1)
C(1)	2673(3)	5954(3)	1712(2)	38(1)
C(2)	3443(3)	5720(3)	1524(3)	52(1)
C(3)	3556(4)	4892(4)	1256(3)	66(2)
C(4)	2931(4)	4248(4)	1166(3)	62(2)
C(5)	2182(4)	4429(3)	1329(3)	56(1)
C(6)	2026(3)	5287(3)	1593(3)	48(1)
C(7)	1213(3)	5480(3)	1730(3)	52(1)
C(8)	2926(3)	5954(3)	4473(3)	50(1)
C(9)	3343(3)	5078(3)	4795(3)	56(1)
C(10)	2810(4)	4403(3)	4233(3)	62(2)
C(11)	2529(4)	4905(3)	3519(3)	77(2)
C(12)	751(3)	7585(3)	2812(2)	39(1)
C(13)	526(3)	6796(3)	3150(3)	48(1)
C(14)	-303(3)	6665(3)	3179(3)	54(1)
C(15)	-936(3)	7297(3)	2889(3)	49(1)
C(16)	-750(3)	8063(3)	2566(3)	46(1)
C(17)	87(3)	8232(3)	2532(2)	41(1)
C(18)	284(3)	9074(3)	2201(3)	50(1)
C(19)	-113(3)	7589(4)	661(3)	65(2)
C(20)	-513(3)	7184(3)	-99(3)	55(1)
C(21)	215(3)	6657(4)	-245(3)	58(1)
C(22)	1004(3)	7185(4)	191(3)	58(1)
C(23)	2476(3)	9482(3)	1661(2)	37(1)
C(24)	1759(3)	9680(3)	1014(3)	52(1)
C(25)	1656(4)	10491(4)	667(3)	63(2)
C(26)	2271(4)	11153(4)	966(4)	64(2)
C(27)	2965(3)	10999(3)	1571(3)	49(1)
C(28)	3100(3)	10158(3)	1937(3)	50(1)
C(29)	3867(3)	9996(4)	2587(3)	60(1)
C(30)	1984(4)	9411(4)	4203(3)	64(2)
C(31)	1378(4)	10168(4)	4217(3)	66(2)
C(32)	1782(4)	10945(4)	3940(4)	78(2)
C(33)	2258(4)	10546(3)	3454(3)	62(2)
C(34)	4184(3)	7814(3)	3904(2)	39(1)

C(35)	4362(3)	8547(3)	4395(3)	51(1)
C(36)	5145(3)	8646(4)	4958(3)	61(2)
C(37)	5787(3)	8002(4)	5023(3)	65(2)
C(38)	5640(3)	7276(3)	4558(3)	54(1)
C(39)	4828(3)	7159(3)	4001(3)	43(1)
C(40)	4668(3)	6350(3)	3523(3)	53(1)
C(41)	5329(3)	7962(5)	2393(4)	79(2)
C(42)	5760(4)	8302(6)	1879(4)	111(3)
C(43)	5064(4)	8659(5)	1234(4)	83(2)
C(44)	4269(3)	8150(4)	1230(3)	61(2)

Table S2.3. Bond lengths [A] and angles [deg] for **2**.

Li(1)-O(4)	1.926(8)
Li(1)-O(2)	1.947(7)
Li(1)-O(5)	1.958(7)
Li(1)-O(1)	1.974(8)
Li(1)-Li(4)	2.599(10)
Li(1)-Li(3)	2.606(10)
Li(1)-Li(2)	2.606(10)
Li(2)-O(6)	1.933(7)
Li(2)-O(1)	1.943(8)
Li(2)-O(3)	1.958(7)
Li(2)-O(2)	1.979(8)
Li(2)-Li(4)	2.599(10)
Li(2)-Li(3)	2.644(10)
Li(3)-O(7)	1.930(8)
Li(3)-O(2)	1.950(8)
Li(3)-O(4)	1.953(8)
Li(3)-O(3)	1.972(8)
Li(3)-Li(4)	2.637(11)
Li(4)-O(8)	1.928(8)
Li(4)-O(3)	1.935(7)
Li(4)-O(1)	1.947(8)
Li(4)-O(4)	1.982(8)
O(1)-C(1)	1.319(5)
O(2)-C(12)	1.330(5)
O(3)-C(23)	1.335(5)
O(4)-C(34)	1.342(5)
O(5)-C(11)	1.423(6)
O(5)-C(8)	1.429(5)
O(6)-C(19)	1.428(6)
O(6)-C(22)	1.432(6)
O(7)-C(33)	1.423(6)
O(7)-C(30)	1.451(6)
O(8)-C(44)	1.432(6)
O(8)-C(41)	1.436(6)
C(1)-C(6)	1.412(6)
C(1)-C(2)	1.442(7)
C(2)-C(3)	1.371(7)
C(3)-C(4)	1.368(8)
C(4)-C(5)	1.368(8)
C(5)-C(6)	1.428(7)
C(6)-C(7)	1.448(7)
C(8)-C(9)	1.510(7)
C(9)-C(10)	1.520(7)
C(10)-C(11)	1.485(7)
C(12)-C(17)	1.418(6)
C(12)-C(13)	1.442(6)
C(13)-C(14)	1.375(7)
C(14)-C(15)	1.374(7)
C(15)-C(16)	1.375(7)
C(16)-C(17)	1.400(6)
C(17)-C(18)	1.484(6)
C(19)-C(20)	1.504(7)
C(20)-C(21)	1.513(7)

C(21)-C(22)	1.506(7)
C(23)-C(28)	1.407(6)
C(23)-C(24)	1.425(6)
C(24)-C(25)	1.364(7)
C(25)-C(26)	1.390(8)
C(26)-C(27)	1.348(7)
C(27)-C(28)	1.418(7)
C(28)-C(29)	1.466(7)
C(30)-C(31)	1.504(8)
C(31)-C(32)	1.505(8)
C(32)-C(33)	1.499(8)
C(34)-C(39)	1.399(6)
C(34)-C(35)	1.406(7)
C(35)-C(36)	1.382(7)
C(36)-C(37)	1.393(8)
C(37)-C(38)	1.369(8)
C(38)-C(39)	1.412(6)
C(39)-C(40)	1.483(7)
C(41)-C(42)	1.457(8)
C(42)-C(43)	1.474(9)
C(43)-C(44)	1.491(8)

O(4)-Li(1)-O(2)	96.0(3)
O(4)-Li(1)-O(5)	115.2(4)
O(2)-Li(1)-O(5)	122.5(4)
O(4)-Li(1)-O(1)	97.0(4)
O(2)-Li(1)-O(1)	96.4(3)
O(5)-Li(1)-O(1)	123.7(4)
O(4)-Li(1)-Li(4)	49.2(2)
O(2)-Li(1)-Li(4)	94.8(3)
O(5)-Li(1)-Li(4)	142.4(4)
O(1)-Li(1)-Li(4)	48.0(2)
O(4)-Li(1)-Li(3)	48.2(2)
O(2)-Li(1)-Li(3)	48.1(2)
O(5)-Li(1)-Li(3)	140.8(4)
O(1)-Li(1)-Li(3)	95.2(3)
Li(4)-Li(1)-Li(3)	60.9(3)
O(4)-Li(1)-Li(2)	95.2(3)
O(2)-Li(1)-Li(2)	48.9(2)
O(5)-Li(1)-Li(2)	149.6(4)
O(1)-Li(1)-Li(2)	47.8(2)
Li(4)-Li(1)-Li(2)	59.9(3)
Li(3)-Li(1)-Li(2)	61.0(3)
O(6)-Li(2)-O(1)	115.2(4)
O(6)-Li(2)-O(3)	122.0(4)
O(1)-Li(2)-O(3)	95.6(3)
O(6)-Li(2)-O(2)	126.1(4)
O(1)-Li(2)-O(2)	96.4(3)
O(3)-Li(2)-O(2)	94.9(3)
O(6)-Li(2)-Li(4)	139.8(4)
O(1)-Li(2)-Li(4)	48.1(2)
O(3)-Li(2)-Li(4)	47.7(2)
O(2)-Li(2)-Li(4)	94.0(3)
O(6)-Li(2)-Li(1)	144.1(4)
O(1)-Li(2)-Li(1)	48.8(2)
O(3)-Li(2)-Li(1)	93.3(3)
O(2)-Li(2)-Li(1)	47.9(2)

Li(4)-Li(2)-Li(1)	59.9(3)
O(6)-Li(2)-Li(3)	149.9(4)
O(1)-Li(2)-Li(3)	94.8(3)
O(3)-Li(2)-Li(3)	47.9(2)
O(2)-Li(2)-Li(3)	47.2(2)
Li(4)-Li(2)-Li(3)	60.4(3)
Li(1)-Li(2)-Li(3)	59.5(3)
O(7)-Li(3)-O(2)	118.1(4)
O(7)-Li(3)-O(4)	121.9(4)
O(2)-Li(3)-O(4)	95.0(3)
O(7)-Li(3)-O(3)	124.5(4)
O(2)-Li(3)-O(3)	95.4(3)
O(4)-Li(3)-O(3)	95.1(4)
O(7)-Li(3)-Li(1)	142.4(4)
O(2)-Li(3)-Li(1)	48.0(2)
O(4)-Li(3)-Li(1)	47.3(2)
O(3)-Li(3)-Li(1)	93.0(3)
O(7)-Li(3)-Li(4)	148.3(4)
O(2)-Li(3)-Li(4)	93.5(3)
O(4)-Li(3)-Li(4)	48.4(2)
O(3)-Li(3)-Li(4)	47.0(2)
Li(1)-Li(3)-Li(4)	59.4(3)
O(7)-Li(3)-Li(2)	144.6(4)
O(2)-Li(3)-Li(2)	48.2(2)
O(4)-Li(3)-Li(2)	93.4(3)
O(3)-Li(3)-Li(2)	47.5(2)
Li(1)-Li(3)-Li(2)	59.5(3)
Li(4)-Li(3)-Li(2)	59.0(3)
O(8)-Li(4)-O(3)	115.5(4)
O(8)-Li(4)-O(1)	122.4(4)
O(3)-Li(4)-O(1)	96.2(3)
O(8)-Li(4)-O(4)	124.9(4)
O(3)-Li(4)-O(4)	95.3(3)
O(1)-Li(4)-O(4)	96.0(3)
O(8)-Li(4)-Li(1)	150.4(4)
O(3)-Li(4)-Li(1)	94.1(3)
O(1)-Li(4)-Li(1)	48.9(2)
O(4)-Li(4)-Li(1)	47.4(2)
O(8)-Li(4)-Li(2)	140.8(4)
O(3)-Li(4)-Li(2)	48.5(2)
O(1)-Li(4)-Li(2)	48.0(2)
O(4)-Li(4)-Li(2)	94.1(3)
Li(1)-Li(4)-Li(2)	60.2(3)
O(8)-Li(4)-Li(3)	142.3(4)
O(3)-Li(4)-Li(3)	48.1(2)
O(1)-Li(4)-Li(3)	94.9(3)
O(4)-Li(4)-Li(3)	47.5(2)
Li(1)-Li(4)-Li(3)	59.7(3)
Li(2)-Li(4)-Li(3)	60.7(3)
C(1)-O(1)-Li(2)	134.3(3)
C(1)-O(1)-Li(4)	133.6(3)
Li(2)-O(1)-Li(4)	83.8(3)
C(1)-O(1)-Li(1)	120.3(3)
Li(2)-O(1)-Li(1)	83.4(3)
Li(4)-O(1)-Li(1)	83.0(3)
C(12)-O(2)-Li(1)	131.0(3)
C(12)-O(2)-Li(3)	136.5(3)

Li(1)-O(2)-Li(3)	83.9(3)
C(12)-O(2)-Li(2)	119.6(3)
Li(1)-O(2)-Li(2)	83.2(3)
Li(3)-O(2)-Li(2)	84.6(3)
C(23)-O(3)-Li(4)	136.1(3)
C(23)-O(3)-Li(2)	130.9(3)
Li(4)-O(3)-Li(2)	83.8(3)
C(23)-O(3)-Li(3)	119.4(3)
Li(4)-O(3)-Li(3)	84.9(3)
Li(2)-O(3)-Li(3)	84.6(3)
C(34)-O(4)-Li(1)	135.6(3)
C(34)-O(4)-Li(3)	132.3(3)
Li(1)-O(4)-Li(3)	84.4(3)
C(34)-O(4)-Li(4)	118.9(3)
Li(1)-O(4)-Li(4)	83.4(3)
Li(3)-O(4)-Li(4)	84.2(3)
C(11)-O(5)-C(8)	109.1(3)
C(11)-O(5)-Li(1)	129.6(4)
C(8)-O(5)-Li(1)	120.9(3)
C(19)-O(6)-C(22)	109.2(3)
C(19)-O(6)-Li(2)	129.0(4)
C(22)-O(6)-Li(2)	120.6(3)
C(33)-O(7)-C(30)	109.0(4)
C(33)-O(7)-Li(3)	132.8(4)
C(30)-O(7)-Li(3)	116.2(4)
C(44)-O(8)-C(41)	109.3(4)
C(44)-O(8)-Li(4)	117.1(3)
C(41)-O(8)-Li(4)	132.5(4)
O(1)-C(1)-C(6)	123.3(4)
O(1)-C(1)-C(2)	120.3(4)
C(6)-C(1)-C(2)	116.4(4)
C(3)-C(2)-C(1)	122.5(5)
C(4)-C(3)-C(2)	120.1(6)
C(3)-C(4)-C(5)	120.4(5)
C(4)-C(5)-C(6)	121.6(5)
C(1)-C(6)-C(5)	119.0(5)
C(1)-C(6)-C(7)	120.1(4)
C(5)-C(6)-C(7)	120.9(4)
O(5)-C(8)-C(9)	106.0(4)
C(8)-C(9)-C(10)	102.2(4)
C(11)-C(10)-C(9)	104.1(4)
O(5)-C(11)-C(10)	108.3(4)
O(2)-C(12)-C(17)	122.8(4)
O(2)-C(12)-C(13)	120.1(4)
C(17)-C(12)-C(13)	117.1(4)
C(14)-C(13)-C(12)	121.4(5)
C(15)-C(14)-C(13)	120.0(5)
C(14)-C(15)-C(16)	120.6(5)
C(15)-C(16)-C(17)	121.5(5)
C(16)-C(17)-C(12)	119.3(4)
C(16)-C(17)-C(18)	120.8(4)
C(12)-C(17)-C(18)	119.8(4)
O(6)-C(19)-C(20)	107.0(4)
C(19)-C(20)-C(21)	104.9(4)
C(22)-C(21)-C(20)	101.6(4)
O(6)-C(22)-C(21)	106.3(4)
O(3)-C(23)-C(28)	122.6(4)

O(3)-C(23)-C(24)	119.7(4)
C(28)-C(23)-C(24)	117.7(4)
C(25)-C(24)-C(23)	122.7(5)
C(24)-C(25)-C(26)	118.2(5)
C(27)-C(26)-C(25)	121.5(5)
C(26)-C(27)-C(28)	121.6(5)
C(23)-C(28)-C(27)	118.2(5)
C(23)-C(28)-C(29)	120.8(4)
C(27)-C(28)-C(29)	120.9(5)
O(7)-C(30)-C(31)	105.5(4)
C(30)-C(31)-C(32)	102.4(5)
C(33)-C(32)-C(31)	105.8(5)
O(7)-C(33)-C(32)	107.2(5)
O(4)-C(34)-C(39)	121.9(4)
O(4)-C(34)-C(35)	120.1(4)
C(39)-C(34)-C(35)	118.0(4)
C(36)-C(35)-C(34)	122.6(5)
C(35)-C(36)-C(37)	118.1(5)
C(38)-C(37)-C(36)	121.2(5)
C(37)-C(38)-C(39)	120.5(5)
C(34)-C(39)-C(38)	119.5(4)
C(34)-C(39)-C(40)	120.7(4)
C(38)-C(39)-C(40)	119.9(4)
O(8)-C(41)-C(42)	107.4(5)
C(41)-C(42)-C(43)	106.0(5)
C(42)-C(43)-C(44)	104.6(5)
O(8)-C(44)-C(43)	105.0(4)

Table S2.4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	39(4)	32(4)	41(4)	5(3)	6(3)	3(3)
Li(2)	35(4)	38(4)	33(4)	0(3)	5(3)	-2(3)
Li(3)	47(4)	40(4)	35(4)	-4(3)	10(3)	-4(3)
Li(4)	39(4)	37(4)	38(4)	10(3)	14(3)	5(3)
O(1)	36(2)	36(2)	38(2)	-7(1)	10(1)	2(1)
O(2)	27(2)	37(2)	42(2)	4(1)	12(1)	1(1)
O(3)	34(2)	36(2)	42(2)	10(1)	11(1)	1(1)
O(4)	34(2)	38(2)	35(2)	1(1)	4(1)	1(1)
O(5)	50(2)	37(2)	38(2)	6(1)	10(2)	2(1)
O(6)	32(2)	58(2)	38(2)	-1(1)	5(1)	-1(1)
O(7)	55(2)	41(2)	43(2)	-5(1)	20(2)	2(2)
O(8)	42(2)	63(2)	44(2)	8(2)	18(2)	1(2)
C(1)	41(3)	43(3)	27(2)	-2(2)	8(2)	-1(2)
C(2)	58(3)	51(3)	47(3)	0(2)	18(3)	12(2)
C(3)	58(3)	76(4)	59(3)	-7(3)	11(3)	14(3)
C(4)	71(4)	64(4)	47(3)	-8(3)	11(3)	4(3)
C(5)	73(4)	46(3)	38(3)	-7(2)	2(3)	-7(3)
C(6)	48(3)	45(3)	40(3)	3(2)	0(2)	-7(2)
C(7)	44(3)	57(3)	48(3)	4(2)	4(2)	-7(2)
C(8)	66(3)	49(3)	41(3)	5(2)	22(2)	-1(2)
C(9)	60(3)	64(3)	42(3)	10(2)	11(2)	-2(3)
C(10)	90(4)	44(3)	54(3)	2(2)	27(3)	0(3)
C(11)	112(5)	40(3)	59(4)	4(3)	-2(3)	-4(3)
C(12)	37(3)	41(3)	34(2)	-4(2)	6(2)	2(2)
C(13)	47(3)	53(3)	46(3)	-3(2)	18(2)	2(2)
C(14)	63(3)	51(3)	55(3)	-3(2)	28(3)	-11(3)
C(15)	41(3)	57(3)	53(3)	-8(3)	20(2)	-5(2)
C(16)	32(2)	62(3)	44(3)	-10(2)	11(2)	1(2)
C(17)	42(3)	44(3)	37(2)	-3(2)	10(2)	7(2)
C(18)	48(3)	49(3)	54(3)	-1(2)	18(2)	5(2)
C(19)	40(3)	89(4)	58(3)	-21(3)	5(3)	0(3)
C(20)	47(3)	64(3)	50(3)	-6(3)	9(2)	-7(2)
C(21)	69(4)	61(3)	38(3)	-5(2)	10(3)	13(3)
C(22)	42(3)	91(4)	38(3)	0(3)	12(2)	8(3)
C(23)	40(2)	38(3)	42(3)	2(2)	23(2)	1(2)
C(24)	56(3)	48(3)	59(3)	16(2)	30(3)	10(2)
C(25)	58(3)	73(4)	61(3)	21(3)	25(3)	13(3)
C(26)	63(4)	52(3)	90(4)	9(3)	42(3)	6(3)
C(27)	51(3)	47(3)	58(3)	5(2)	31(3)	3(2)
C(28)	50(3)	48(3)	59(3)	-9(2)	28(3)	0(2)
C(29)	57(3)	59(3)	65(3)	0(3)	24(3)	-10(3)
C(30)	77(4)	69(4)	54(3)	1(3)	30(3)	2(3)
C(31)	59(3)	78(4)	68(4)	-16(3)	30(3)	-4(3)
C(32)	95(5)	55(4)	104(5)	-8(3)	61(4)	7(3)
C(33)	76(4)	45(3)	78(4)	-11(3)	41(3)	-4(3)
C(34)	36(2)	42(3)	38(2)	11(2)	8(2)	-2(2)
C(35)	49(3)	55(3)	42(3)	0(2)	5(2)	-8(2)
C(36)	60(3)	61(3)	54(3)	-6(3)	7(3)	-10(3)

C(37)	41(3)	70(4)	64(4)	11(3)	-10(3)	-9(3)
C(38)	38(3)	58(3)	58(3)	15(3)	6(2)	-3(2)
C(39)	45(3)	42(3)	41(3)	12(2)	14(2)	1(2)
C(40)	43(3)	54(3)	62(3)	7(3)	18(2)	9(2)
C(41)	36(3)	121(5)	81(4)	38(4)	19(3)	3(3)
C(42)	70(4)	198(9)	78(5)	30(5)	41(4)	-23(5)
C(43)	100(5)	86(5)	80(5)	19(4)	50(4)	1(4)
C(44)	58(3)	87(4)	44(3)	15(3)	24(3)	5(3)

Table S2.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(2)	3888	6156	1590	62
H(3)	4069	4767	1132	79
H(4)	3017	3671	990	75
H(5)	1756	3972	1265	67
H(7A)	1334	5759	2221	78
H(7B)	890	4922	1715	78
H(7C)	865	5889	1345	78
H(8A)	2434	6097	4658	60
H(8B)	3356	6447	4613	60
H(9A)	3293	4972	5296	68
H(9B)	3964	5060	4826	68
H(10A)	3169	3878	4198	74
H(10B)	2301	4196	4372	74
H(11A)	2891	4731	3206	92
H(11B)	1914	4766	3242	92
H(13)	960	6357	3358	57
H(14)	-439	6137	3400	65
H(15)	-1508	7203	2911	59
H(16)	-1199	8487	2362	56
H(18A)	-256	9412	1982	75
H(18B)	545	8932	1812	75
H(18C)	693	9435	2589	75
H(19A)	-302	8218	664	78
H(19B)	-293	7251	1037	78
H(20A)	-728	7657	-480	66
H(20B)	-1005	6787	-106	66
H(21A)	238	6036	-56	69
H(21B)	153	6643	-782	69
H(22A)	1523	6793	354	69
H(22B)	1119	7674	-119	69
H(24)	1337	9227	817	62
H(25)	1176	10601	232	75
H(26)	2199	11727	738	77
H(27)	3375	11466	1758	58
H(29A)	3682	9772	3000	89
H(29B)	4190	10557	2736	89
H(29C)	4243	9552	2461	89
H(30A)	2469	9381	4678	77
H(30B)	1670	8833	4122	77
H(31A)	1360	10277	4729	79
H(31B)	780	10047	3884	79
H(32A)	1327	11365	3652	93
H(32B)	2189	11272	4363	93
H(33A)	1941	10670	2923	75
H(33B)	2849	10806	3577	75
H(35)	3926	8992	4337	61
H(36)	5242	9139	5291	73
H(37)	6336	8068	5396	78

H(38)	6089	6847	4611	64
H(40A)	4207	5990	3616	79
H(40B)	5203	5995	3638	79
H(40C)	4488	6530	2998	79
H(41A)	5563	7365	2582	95
H(41B)	5427	8372	2822	95
H(42A)	6078	7816	1721	133
H(42B)	6179	8780	2117	133
H(43A)	5201	8559	766	100
H(43B)	4982	9308	1293	100
H(44A)	3743	8529	1046	73
H(44B)	4195	7613	909	73

[Li(DMP)(THF)]$_4$ (3)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P(2)1/n using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. Subsequent refinement confirmed the original atom identification. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0901 and R2w=0.2480.

Table S3.1. Crystal data and structure refinement for **3**.

Identification code	d:\frames\xtal\dmtp007m
Empirical formula	C48 H68 Li4 O8
Formula weight	800.78
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.5624(14) A alpha = 90 deg. b = 20.819(3) A beta = 91.769(2) deg. c = 17.135(2) A gamma = 90 deg.
Volume	4479.2(9) A^3
Z, Calculated density	4, 1.187 Mg/m^3
Absorption coefficient	0.077 mm^-1
F(000)	1728
Crystal size	.2 x .2 x .4mm mm
Theta range for data collection	1.54 to 23.34 deg.
Limiting indices	-13<=h<=11, -21<=k<=23, -18<=l<=19
Reflections collected / unique	20813 / 6431 [R(int) = 0.0929]
Completeness to theta = 23.34	99.1 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6431 / 0 / 549
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0901, wR2 = 0.2480
R indices (all data)	R1 = 0.1112, wR2 = 0.2768
Largest diff. peak and hole	3.619 and -1.179 e.A^-3

Table S3.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	7029(6)	1981(3)	2767(4)	33(2)
Li(2)	8960(5)	1422(3)	2835(4)	32(2)
Li(3)	7691(6)	1291(3)	1530(4)	34(2)
Li(4)	7159(5)	711(3)	2883(4)	33(2)
C(1)	6762(5)	3393(2)	3380(3)	51(1)
C(2)	6842(6)	3630(3)	4215(4)	69(2)
C(3)	6337(4)	3119(3)	4706(3)	50(1)
C(4)	5885(4)	2638(2)	4111(3)	40(1)
C(5)	7945(3)	1582(2)	4305(2)	30(1)
C(6)	8603(3)	2112(2)	4523(2)	33(1)
C(7)	8786(4)	2250(2)	5312(3)	42(1)
C(8)	8361(4)	1884(3)	5890(3)	46(1)
C(9)	7706(4)	1378(2)	5684(3)	43(1)
C(10)	7470(3)	1221(2)	4901(2)	34(1)
C(11)	9113(4)	2521(2)	3913(3)	40(1)
C(12)	6706(4)	696(2)	4700(3)	42(1)
C(13)	10594(4)	1060(2)	4208(3)	41(1)
C(14)	11404(4)	525(2)	4235(3)	43(1)
C(15)	12109(4)	698(3)	3567(3)	59(1)
C(16)	11394(3)	1076(3)	3006(3)	44(1)
C(17)	9220(3)	200(2)	2201(2)	28(1)
C(18)	9457(3)	-221(2)	2830(2)	33(1)
C(19)	10301(4)	-649(2)	2781(3)	42(1)
C(20)	10916(4)	-681(2)	2131(3)	52(1)
C(21)	10670(4)	-282(2)	1503(3)	46(1)
C(22)	9825(3)	153(2)	1523(2)	34(1)
C(23)	8823(4)	-198(2)	3563(3)	40(1)
C(24)	9581(4)	586(2)	846(3)	42(1)
C(25)	8519(3)	2528(2)	1576(2)	29(1)
C(26)	9593(3)	2658(2)	1413(2)	32(1)
C(27)	9837(4)	3111(2)	841(2)	37(1)
C(28)	9045(4)	3438(2)	427(3)	42(1)
C(29)	7998(4)	3325(2)	608(2)	37(1)
C(30)	7713(3)	2888(2)	1174(2)	31(1)
C(31)	10470(4)	2306(2)	1842(3)	41(1)
C(32)	6563(3)	2794(2)	1356(3)	35(1)
C(33)	8311(3)	1752(2)	-199(2)	37(1)
C(34)	7762(18)	2047(12)	-928(4)	550(3)
C(35)	6751(4)	1625(3)	-985(3)	46(1)
C(36)	6471(4)	1595(3)	-139(3)	47(1)
C(37)	5453(3)	1078(2)	1782(2)	31(1)
C(38)	5417(3)	561(2)	1248(2)	34(1)
C(39)	4446(4)	382(2)	897(3)	41(1)
C(40)	3517(4)	701(3)	1052(3)	44(1)
C(41)	3547(4)	1204(2)	1578(3)	42(1)
C(42)	4490(3)	1389(2)	1953(2)	35(1)
C(43)	6415(4)	202(2)	1050(3)	38(1)

C(44)	4485(4)	1915(2)	2561(3)	44(1)
C(45)	6275(4)	-681(2)	2723(3)	45(1)
C(46)	5220(4)	-883(2)	2355(3)	54(1)
C(47)	4405(4)	-461(3)	2766(3)	59(2)
C(48)	5062(4)	-2(2)	3267(3)	47(1)
O(1)	6525(2)	2714(1)	3432(2)	36(1)
O(2)	7764(2)	1428(1)	3553(2)	29(1)
O(3)	10405(2)	1187(2)	3390(2)	37(1)
O(4)	8458(2)	645(1)	2250(2)	30(1)
O(5)	8271(2)	2066(1)	2083(2)	30(1)
O(6)	7474(2)	1522(2)	293(2)	37(1)
O(7)	6377(2)	1263(1)	2128(2)	30(1)
O(8)	6123(2)	-29(1)	2985(2)	37(1)

Table S3.3. Bond lengths [A] and angles [deg] for **3**.

Li(1)-O(2)	1.977(7)
Li(1)-O(5)	1.989(7)
Li(1)-O(7)	2.013(7)
Li(1)-O(1)	2.018(7)
Li(1)-Li(4)	2.656(10)
Li(1)-Li(2)	2.690(10)
Li(1)-Li(3)	2.711(10)
Li(2)-O(2)	1.971(7)
Li(2)-O(4)	1.994(7)
Li(2)-O(5)	2.033(7)
Li(2)-O(3)	2.082(8)
Li(2)-Li(4)	2.708(10)
Li(2)-Li(3)	2.718(10)
Li(2)-C(17)	2.789(8)
Li(3)-O(7)	1.970(7)
Li(3)-O(5)	1.996(8)
Li(3)-O(4)	2.046(8)
Li(3)-O(6)	2.183(8)
Li(3)-Li(4)	2.716(9)
Li(3)-C(25)	2.777(8)
Li(4)-O(7)	1.971(7)
Li(4)-O(4)	1.992(7)
Li(4)-O(2)	2.018(7)
Li(4)-O(8)	2.027(7)
C(1)-O(1)	1.449(6)
C(1)-C(2)	1.513(8)
C(2)-C(3)	1.508(8)
C(3)-C(4)	1.527(7)
C(4)-O(1)	1.444(5)
C(5)-O(2)	1.341(5)
C(5)-C(10)	1.415(6)
C(5)-C(6)	1.422(6)
C(6)-C(7)	1.393(6)
C(6)-C(11)	1.506(6)
C(7)-C(8)	1.371(7)
C(8)-C(9)	1.376(7)
C(9)-C(10)	1.403(6)
C(10)-C(12)	1.487(6)
C(13)-O(3)	1.439(5)
C(13)-C(14)	1.507(6)
C(14)-C(15)	1.512(7)
C(15)-C(16)	1.515(7)
C(16)-O(3)	1.442(5)
C(17)-O(4)	1.336(5)
C(17)-C(22)	1.412(6)
C(17)-C(18)	1.413(6)
C(18)-C(19)	1.391(6)
C(18)-C(23)	1.509(6)
C(19)-C(20)	1.376(7)
C(20)-C(21)	1.388(7)
C(21)-C(22)	1.396(6)
C(22)-C(24)	1.493(6)
C(25)-O(5)	1.339(5)
C(25)-C(26)	1.412(6)

C(25)-C(30)	1.420(6)
C(26)-C(27)	1.400(6)
C(26)-C(31)	1.498(6)
C(27)-C(28)	1.384(7)
C(28)-C(29)	1.381(6)
C(29)-C(30)	1.385(6)
C(30)-C(32)	1.501(6)
C(33)-O(6)	1.449(5)
C(33)-C(34)	1.54(2)
C(34)-C(35)	1.545(9)
C(35)-C(36)	1.503(7)
C(36)-O(6)	1.449(6)
C(37)-O(7)	1.342(5)
C(37)-C(42)	1.411(6)
C(37)-C(38)	1.414(6)
C(38)-C(39)	1.393(6)
C(38)-C(43)	1.507(6)
C(39)-C(40)	1.377(7)
C(40)-C(41)	1.381(7)
C(41)-C(42)	1.385(6)
C(42)-C(44)	1.510(6)
C(45)-O(8)	1.444(5)
C(45)-C(46)	1.510(7)
C(46)-C(47)	1.538(8)
C(47)-C(48)	1.512(7)
C(48)-O(8)	1.433(5)

O(2)-Li(1)-O(5)	95.4(3)
O(2)-Li(1)-O(7)	96.5(3)
O(5)-Li(1)-O(7)	93.4(3)
O(2)-Li(1)-O(1)	101.8(3)
O(5)-Li(1)-O(1)	122.1(4)
O(7)-Li(1)-O(1)	137.7(4)
O(2)-Li(1)-Li(4)	49.0(2)
O(5)-Li(1)-Li(4)	94.9(3)
O(7)-Li(1)-Li(4)	47.5(2)
O(1)-Li(1)-Li(4)	137.0(4)
O(2)-Li(1)-Li(2)	47.0(2)
O(5)-Li(1)-Li(2)	48.7(2)
O(7)-Li(1)-Li(2)	93.1(3)
O(1)-Li(1)-Li(2)	127.0(4)
Li(4)-Li(1)-Li(2)	60.9(3)
O(2)-Li(1)-Li(3)	94.4(3)
O(5)-Li(1)-Li(3)	47.2(2)
O(7)-Li(1)-Li(3)	46.4(2)
O(1)-Li(1)-Li(3)	161.9(4)
Li(4)-Li(1)-Li(3)	60.8(2)
Li(2)-Li(1)-Li(3)	60.4(3)
O(2)-Li(2)-O(4)	94.8(3)
O(2)-Li(2)-O(5)	94.2(3)
O(4)-Li(2)-O(5)	95.4(3)
O(2)-Li(2)-O(3)	112.8(3)
O(4)-Li(2)-O(3)	107.3(3)
O(5)-Li(2)-O(3)	142.4(4)
O(2)-Li(2)-Li(1)	47.1(2)
O(4)-Li(2)-Li(1)	93.3(3)
O(5)-Li(2)-Li(1)	47.3(2)

O(3)-Li(2)-Li(1)	153.4(4)
O(2)-Li(2)-Li(4)	48.0(2)
O(4)-Li(2)-Li(4)	47.2(2)
O(5)-Li(2)-Li(4)	92.3(3)
O(3)-Li(2)-Li(4)	125.1(3)
Li(1)-Li(2)-Li(4)	58.9(2)
O(2)-Li(2)-Li(3)	94.3(3)
O(4)-Li(2)-Li(3)	48.5(2)
O(5)-Li(2)-Li(3)	47.0(2)
O(3)-Li(2)-Li(3)	146.4(3)
Li(1)-Li(2)-Li(3)	60.2(3)
Li(4)-Li(2)-Li(3)	60.1(2)
O(2)-Li(2)-C(17)	110.5(3)
O(4)-Li(2)-C(17)	26.34(14)
O(5)-Li(2)-C(17)	114.0(3)
O(3)-Li(2)-C(17)	81.5(2)
Li(1)-Li(2)-C(17)	119.6(3)
Li(4)-Li(2)-C(17)	67.7(2)
Li(3)-Li(2)-C(17)	70.2(2)
O(7)-Li(3)-O(5)	94.5(3)
O(7)-Li(3)-O(4)	93.1(3)
O(5)-Li(3)-O(4)	95.0(3)
O(7)-Li(3)-O(6)	115.4(3)
O(5)-Li(3)-O(6)	108.4(3)
O(4)-Li(3)-O(6)	140.6(4)
O(7)-Li(3)-Li(1)	47.8(2)
O(5)-Li(3)-Li(1)	47.0(2)
O(4)-Li(3)-Li(1)	91.5(3)
O(6)-Li(3)-Li(1)	127.7(3)
O(7)-Li(3)-Li(4)	46.4(2)
O(5)-Li(3)-Li(4)	92.9(3)
O(4)-Li(3)-Li(4)	46.9(2)
O(6)-Li(3)-Li(4)	154.2(4)
Li(1)-Li(3)-Li(4)	58.6(2)
O(7)-Li(3)-Li(2)	93.2(3)
O(5)-Li(3)-Li(2)	48.2(2)
O(4)-Li(3)-Li(2)	46.9(2)
O(6)-Li(3)-Li(2)	146.0(4)
Li(1)-Li(3)-Li(2)	59.4(3)
Li(4)-Li(3)-Li(2)	59.8(3)
O(7)-Li(3)-C(25)	109.4(3)
O(5)-Li(3)-C(25)	26.71(15)
O(4)-Li(3)-C(25)	115.1(3)
O(6)-Li(3)-C(25)	81.9(2)
Li(1)-Li(3)-C(25)	67.1(2)
Li(4)-Li(3)-C(25)	119.4(3)
Li(2)-Li(3)-C(25)	71.0(2)
O(7)-Li(4)-O(4)	94.8(3)
O(7)-Li(4)-O(2)	96.5(3)
O(4)-Li(4)-O(2)	93.4(3)
O(7)-Li(4)-O(8)	101.0(3)
O(4)-Li(4)-O(8)	122.3(4)
O(2)-Li(4)-O(8)	138.2(4)
O(7)-Li(4)-Li(1)	48.9(2)
O(4)-Li(4)-Li(1)	94.4(3)
O(2)-Li(4)-Li(1)	47.7(2)
O(8)-Li(4)-Li(1)	136.4(4)

O(7)-Li(4)-Li(2)	93.5(3)
O(4)-Li(4)-Li(2)	47.2(2)
O(2)-Li(4)-Li(2)	46.5(2)
O(8)-Li(4)-Li(2)	163.2(4)
Li(1)-Li(4)-Li(2)	60.2(3)
O(7)-Li(4)-Li(3)	46.4(2)
O(4)-Li(4)-Li(3)	48.6(2)
O(2)-Li(4)-Li(3)	93.3(3)
O(8)-Li(4)-Li(3)	126.0(3)
Li(1)-Li(4)-Li(3)	60.6(3)
Li(2)-Li(4)-Li(3)	60.2(2)
O(1)-C(1)-C(2)	105.5(4)
C(3)-C(2)-C(1)	106.4(4)
C(2)-C(3)-C(4)	104.1(4)
O(1)-C(4)-C(3)	105.2(4)
O(2)-C(5)-C(10)	120.4(4)
O(2)-C(5)-C(6)	121.2(4)
C(10)-C(5)-C(6)	118.5(4)
C(7)-C(6)-C(5)	119.5(4)
C(7)-C(6)-C(11)	119.7(4)
C(5)-C(6)-C(11)	120.8(4)
C(8)-C(7)-C(6)	122.0(5)
C(7)-C(8)-C(9)	118.9(4)
C(8)-C(9)-C(10)	122.0(4)
C(9)-C(10)-C(5)	119.0(4)
C(9)-C(10)-C(12)	120.5(4)
C(5)-C(10)-C(12)	120.4(4)
O(3)-C(13)-C(14)	104.8(4)
C(13)-C(14)-C(15)	102.3(4)
C(14)-C(15)-C(16)	104.7(4)
O(3)-C(16)-C(15)	107.2(4)
O(4)-C(17)-C(22)	120.3(4)
O(4)-C(17)-C(18)	121.1(4)
C(22)-C(17)-C(18)	118.6(4)
O(4)-C(17)-Li(2)	41.5(2)
C(22)-C(17)-Li(2)	117.1(3)
C(18)-C(17)-Li(2)	107.1(3)
C(19)-C(18)-C(17)	119.7(4)
C(19)-C(18)-C(23)	119.5(4)
C(17)-C(18)-C(23)	120.7(4)
C(20)-C(19)-C(18)	121.8(4)
C(19)-C(20)-C(21)	118.8(4)
C(20)-C(21)-C(22)	121.4(4)
C(21)-C(22)-C(17)	119.6(4)
C(21)-C(22)-C(24)	120.7(4)
C(17)-C(22)-C(24)	119.7(4)
O(5)-C(25)-C(26)	120.6(4)
O(5)-C(25)-C(30)	121.1(4)
C(26)-C(25)-C(30)	118.3(4)
O(5)-C(25)-Li(3)	42.0(2)
C(26)-C(25)-Li(3)	122.1(3)
C(30)-C(25)-Li(3)	102.3(3)
C(27)-C(26)-C(25)	120.0(4)
C(27)-C(26)-C(31)	120.0(4)
C(25)-C(26)-C(31)	120.0(4)
C(28)-C(27)-C(26)	121.4(4)
C(29)-C(28)-C(27)	118.4(4)

C(28)-C(29)-C(30)	122.5(4)
C(29)-C(30)-C(25)	119.4(4)
C(29)-C(30)-C(32)	120.1(4)
C(25)-C(30)-C(32)	120.5(4)
O(6)-C(33)-C(34)	106.8(6)
C(33)-C(34)-C(35)	99.8(8)
C(36)-C(35)-C(34)	100.3(4)
O(6)-C(36)-C(35)	105.7(4)
O(7)-C(37)-C(42)	120.8(4)
O(7)-C(37)-C(38)	120.9(4)
C(42)-C(37)-C(38)	118.3(4)
C(39)-C(38)-C(37)	119.6(4)
C(39)-C(38)-C(43)	119.6(4)
C(37)-C(38)-C(43)	120.9(4)
C(40)-C(39)-C(38)	121.6(4)
C(39)-C(40)-C(41)	119.0(4)
C(40)-C(41)-C(42)	121.4(4)
C(41)-C(42)-C(37)	120.1(4)
C(41)-C(42)-C(44)	120.0(4)
C(37)-C(42)-C(44)	119.8(4)
O(8)-C(45)-C(46)	105.6(4)
C(45)-C(46)-C(47)	103.7(4)
C(48)-C(47)-C(46)	105.2(4)
O(8)-C(48)-C(47)	106.3(4)
C(4)-O(1)-C(1)	106.1(3)
C(4)-O(1)-Li(1)	124.3(3)
C(1)-O(1)-Li(1)	129.5(3)
C(5)-O(2)-Li(2)	119.4(3)
C(5)-O(2)-Li(1)	125.3(3)
Li(2)-O(2)-Li(1)	85.9(3)
C(5)-O(2)-Li(4)	140.6(3)
Li(2)-O(2)-Li(4)	85.5(3)
Li(1)-O(2)-Li(4)	83.3(3)
C(13)-O(3)-C(16)	107.2(3)
C(13)-O(3)-Li(2)	127.1(3)
C(16)-O(3)-Li(2)	125.5(3)
C(17)-O(4)-Li(4)	133.0(3)
C(17)-O(4)-Li(2)	112.2(3)
Li(4)-O(4)-Li(2)	85.6(3)
C(17)-O(4)-Li(3)	137.9(3)
Li(4)-O(4)-Li(3)	84.5(3)
Li(2)-O(4)-Li(3)	84.5(3)
C(25)-O(5)-Li(1)	130.4(3)
C(25)-O(5)-Li(3)	111.3(3)
Li(1)-O(5)-Li(3)	85.8(3)
C(25)-O(5)-Li(2)	141.4(3)
Li(1)-O(5)-Li(2)	83.9(3)
Li(3)-O(5)-Li(2)	84.9(3)
C(33)-O(6)-C(36)	107.7(3)
C(33)-O(6)-Li(3)	124.5(3)
C(36)-O(6)-Li(3)	126.9(3)
C(37)-O(7)-Li(3)	120.4(3)
C(37)-O(7)-Li(4)	121.9(3)
Li(3)-O(7)-Li(4)	87.1(3)
C(37)-O(7)-Li(1)	141.7(3)
Li(3)-O(7)-Li(1)	85.8(3)
Li(4)-O(7)-Li(1)	83.6(3)

C(48)-O(8)-C(45)	106.0(3)
C(48)-O(8)-Li(4)	127.3(3)
C(45)-O(8)-Li(4)	126.6(3)

Table S3.4. Anisotropic displacement parameters (A^2 x 10^3) for **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	37(4)	27(4)	36(4)	4(3)	4(3)	0(3)
Li(2)	33(4)	31(4)	33(4)	-6(3)	2(3)	0(3)
Li(3)	33(4)	34(4)	36(4)	0(3)	3(3)	-1(3)
Li(4)	36(4)	33(4)	29(4)	0(3)	5(3)	0(3)
C(1)	74(4)	27(2)	53(3)	7(2)	5(3)	-1(2)
C(2)	96(5)	40(3)	70(4)	-16(3)	5(3)	-4(3)
C(3)	49(3)	60(3)	42(3)	-11(2)	1(2)	12(2)
C(4)	41(3)	43(3)	36(2)	-3(2)	12(2)	4(2)
C(5)	30(2)	32(2)	26(2)	0(2)	2(2)	7(2)
C(6)	30(2)	35(2)	33(2)	-8(2)	1(2)	6(2)
C(7)	36(2)	49(3)	39(3)	-10(2)	-7(2)	9(2)
C(8)	47(3)	59(3)	31(2)	-9(2)	-6(2)	13(2)
C(9)	45(3)	55(3)	28(2)	7(2)	4(2)	15(2)
C(10)	36(2)	37(2)	30(2)	3(2)	6(2)	9(2)
C(11)	40(3)	32(2)	46(3)	-9(2)	2(2)	-4(2)
C(12)	45(3)	46(3)	37(2)	6(2)	11(2)	-1(2)
C(13)	44(3)	45(3)	33(2)	-4(2)	-3(2)	5(2)
C(14)	45(3)	40(3)	42(3)	-4(2)	-9(2)	6(2)
C(15)	43(3)	73(4)	60(3)	1(3)	1(2)	20(3)
C(16)	34(2)	53(3)	46(3)	-3(2)	4(2)	6(2)
C(17)	29(2)	23(2)	33(2)	-3(2)	-2(2)	1(2)
C(18)	35(2)	29(2)	35(2)	-4(2)	-4(2)	-4(2)
C(19)	50(3)	33(2)	43(3)	-2(2)	-8(2)	10(2)
C(20)	56(3)	45(3)	53(3)	-12(2)	-3(2)	20(2)
C(21)	46(3)	49(3)	43(3)	-16(2)	8(2)	7(2)
C(22)	36(2)	34(2)	30(2)	-6(2)	1(2)	1(2)
C(23)	41(3)	41(3)	38(2)	9(2)	2(2)	1(2)
C(24)	46(3)	45(3)	34(2)	-4(2)	8(2)	2(2)
C(25)	40(2)	26(2)	22(2)	-4(2)	5(2)	-3(2)
C(26)	35(2)	33(2)	28(2)	-5(2)	0(2)	-5(2)
C(27)	38(2)	37(3)	36(2)	-1(2)	6(2)	-11(2)
C(28)	55(3)	36(3)	34(2)	7(2)	4(2)	-11(2)
C(29)	44(3)	35(2)	32(2)	3(2)	-4(2)	2(2)
C(30)	40(2)	26(2)	27(2)	-2(2)	-2(2)	-2(2)
C(31)	38(3)	45(3)	39(3)	0(2)	2(2)	-1(2)
C(32)	37(2)	34(2)	35(2)	2(2)	-1(2)	4(2)
C(33)	37(2)	37(2)	35(2)	-3(2)	4(2)	-3(2)
C(34)	713(12)	927(16)	13(3)	-35(10)	38(8)	-793
C(35)	44(3)	55(3)	38(3)	0(2)	-2(2)	3(2)
C(36)	39(3)	58(3)	44(3)	7(2)	1(2)	-1(2)
C(37)	32(2)	33(2)	26(2)	6(2)	3(2)	-3(2)
C(38)	38(2)	34(2)	28(2)	2(2)	3(2)	-4(2)
C(39)	42(3)	47(3)	34(2)	-3(2)	1(2)	-11(2)
C(40)	34(3)	60(3)	39(3)	2(2)	-2(2)	-8(2)
C(41)	31(2)	52(3)	42(3)	5(2)	3(2)	0(2)
C(42)	31(2)	39(2)	34(2)	3(2)	3(2)	-1(2)
C(43)	43(3)	38(2)	33(2)	-6(2)	0(2)	-3(2)
C(44)	42(3)	40(3)	52(3)	-6(2)	6(2)	2(2)

C(45)	58(3)	28(2)	48(3)	2(2)	-3(2)	5(2)
C(46)	70(4)	38(3)	54(3)	7(2)	-4(3)	-15(3)
C(47)	46(3)	75(4)	55(3)	3(3)	-1(2)	-22(3)
C(48)	46(3)	48(3)	48(3)	6(2)	13(2)	-5(2)
O(1)	46(2)	28(2)	35(2)	-1(1)	9(1)	0(1)
O(2)	36(2)	28(2)	25(2)	-1(1)	2(1)	1(1)
O(3)	34(2)	45(2)	33(2)	-3(1)	0(1)	5(1)
O(4)	32(2)	27(2)	30(2)	-2(1)	2(1)	5(1)
O(5)	35(2)	29(2)	26(1)	3(1)	3(1)	-4(1)
O(6)	37(2)	43(2)	32(2)	3(1)	1(1)	-5(1)
O(7)	28(2)	30(2)	32(2)	0(1)	-1(1)	-4(1)
O(8)	39(2)	32(2)	42(2)	1(1)	6(1)	-2(1)

Table S3.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(1A)	6188	3622	3085	62
H(1B)	7442	3463	3116	62
H(2A)	7596	3693	4381	82
H(2B)	6461	4043	4267	82
H(3A)	5764	3304	5021	60
H(3B)	6872	2914	5061	60
H(4A)	5943	2194	4317	48
H(4B)	5128	2731	3983	48
H(7)	9218	2608	5453	50
H(8)	8516	1978	6424	55
H(9)	7404	1127	6084	51
H(11A)	9254	2950	4126	59
H(11B)	8633	2554	3454	59
H(11C)	9785	2323	3764	59
H(12A)	6421	518	5181	64
H(12B)	7073	357	4417	64
H(12C)	6121	868	4372	64
H(13A)	9929	925	4456	49
H(13B)	10876	1446	4480	49
H(14A)	11061	102	4151	51
H(14B)	11811	521	4739	51
H(15A)	12382	306	3314	70
H(15B)	12721	962	3754	70
H(16A)	11733	1490	2875	53
H(16B)	11264	830	2518	53
H(19)	10458	-928	3208	51
H(20)	11498	-972	2113	62
H(21)	11085	-304	1050	55
H(23A)	8137	-414	3469	60
H(23B)	8700	250	3709	60
H(23C)	9219	-417	3987	60
H(24A)	10115	523	447	62
H(24B)	9596	1033	1022	62
H(24C)	8873	484	624	62
H(27)	10562	3194	735	44
H(28)	9217	3734	29	50
H(29)	7452	3556	333	45
H(31A)	11159	2482	1697	61
H(31B)	10437	1849	1705	61
H(31C)	10386	2355	2406	61
H(32A)	6428	2973	1873	53
H(32B)	6395	2334	1354	53
H(32C)	6113	3014	962	53
H(33A)	8780	1392	-348	44
H(33B)	8750	2078	82	44
H(34A)	8201	2001	-1395	660
H(34B)	7587	2506	-849	660
H(35A)	6180	1830	-1308	55
H(35B)	6905	1194	-1196	55

H(36A)	6107	1995	18	56
H(36B)	5996	1226	-43	56
H(39)	4425	30	543	49
H(40)	2864	578	800	53
H(41)	2908	1427	1685	50
H(43A)	6228	-234	877	57
H(43B)	6891	178	1513	57
H(43C)	6775	427	631	57
H(44A)	3754	2066	2623	67
H(44B)	4931	2272	2393	67
H(44C)	4766	1746	3060	67
H(45A)	6473	-964	3169	54
H(45B)	6845	-701	2337	54
H(46A)	5083	-1345	2449	65
H(46B)	5201	-803	1785	65
H(47A)	3956	-223	2379	71
H(47B)	3939	-726	3093	71
H(48A)	4775	440	3221	57
H(48B)	5055	-133	3822	57

[Li(oPP)(THF)]$_4$ (4)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P2(1)/c using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. Subsequent refinement confirmed the original atom identification. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0859 and R2w=0.2324.

Table S4.1. Crystal data and structure refinement for **4**.

Empirical formula	C52 H76 Li4 O8
Formula weight	856.89
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.9466(18) A alpha = 90 deg. b = 15.119(2) A beta = 101.012(3) deg. c = 27.015(4) A gamma = 90 deg.
Volume	5190.3(12) A^3
Z, Calculated density	4, 1.097 Mg/m^3
Absorption coefficient	0.070 mm^-1
F(000)	1856
Crystal size	.2 x .2 x .2 mm
Theta range for data collection	1.55 to 28.28 deg.
Limiting indices	-15<=h<=16, -16<=k<=20, -35<=l<=22
Reflections collected / unique	33430 / 12261 [R(int) = 0.1278]
Completeness to theta = 28.28	95.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12261 / 0 / 585
Goodness-of-fit on F^2	0.927
Final R indices [I>2sigma(I)]	R1 = 0.0859, wR2 = 0.2324
R indices (all data)	R1 = 0.1793, wR2 = 0.2924
Largest diff. peak and hole	0.985 and -0.403 e.A^-3

Table S4.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	2012(4)	3465(3)	1320(2)	46(1)
Li(2)	3441(4)	2180(3)	1560(2)	48(1)
Li(3)	1877(4)	2071(3)	772(2)	45(1)
Li(4)	1496(4)	1961(3)	1703(2)	48(1)
C(1)	2657(2)	466(2)	1204(1)	43(1)
C(2)	3134(3)	411(2)	784(1)	54(1)
C(3)	3419(3)	-381(3)	600(1)	65(1)
C(4)	3233(3)	-1156(2)	834(2)	67(1)
C(5)	2781(3)	-1115(2)	1256(2)	61(1)
C(6)	2483(2)	-319(2)	1455(1)	47(1)
C(7)	2033(3)	-295(2)	1931(1)	56(1)
C(8)	1502(4)	-1174(3)	2021(2)	105(2)
C(9)	2800(4)	-59(4)	2364(2)	108(2)
C(10)	990(4)	1475(3)	2706(2)	95(2)
C(11)	161(5)	1751(4)	2983(2)	116(2)
C(12)	-849(5)	1622(4)	2587(2)	119(2)
C(13)	-492(4)	1851(3)	2116(2)	101(2)
C(14)	2481(3)	3227(2)	2401(1)	47(1)
C(15)	1619(3)	3764(2)	2432(1)	56(1)
C(16)	1481(4)	4129(2)	2887(2)	73(1)
C(17)	2191(4)	3968(3)	3320(2)	87(1)
C(19)	3051(4)	3436(3)	3299(1)	81(1)
C(20)	3218(3)	3059(2)	2847(1)	58(1)
C(21)	4170(3)	2482(3)	2830(1)	64(1)
C(22)	5092(3)	3061(3)	2734(2)	89(1)
C(23)	4494(4)	1894(3)	3287(2)	99(2)
C(24)	-165(2)	2465(2)	944(1)	44(1)
C(25)	-458(3)	1589(2)	821(1)	61(1)
C(26)	-1481(3)	1356(2)	635(2)	73(1)
C(27)	-2259(3)	1984(3)	572(2)	71(1)
C(28)	-1997(3)	2849(2)	701(1)	59(1)
C(29)	-967(2)	3102(2)	888(1)	44(1)
C(30)	-721(3)	4065(2)	1035(1)	52(1)
C(31)	-1331(4)	4375(3)	1431(2)	89(1)
C(32)	-953(4)	4672(3)	579(2)	83(1)
C(33)	1045(3)	1008(2)	-195(2)	72(1)
C(34)	112(4)	1115(3)	-603(2)	93(1)
C(35)	4(5)	2055(3)	-683(2)	131(2)
C(36)	511(3)	2492(2)	-212(1)	67(1)
C(37)	2031(3)	5097(2)	733(1)	73(1)
C(38)	2591(5)	5982(3)	832(2)	115(2)
C(39)	2434(4)	6245(3)	1336(2)	90(1)
C(40)	2470(3)	5391(2)	1601(2)	74(1)
C(41)	3818(2)	3370(2)	845(1)	43(1)
C(42)	4146(2)	3323(2)	377(1)	50(1)

C(43)	3597(3)	2720(2)	-40(1)	57(1)
C(45)	4323(3)	1992(3)	-169(2)	79(1)
C(46)	3129(3)	3243(3)	-516(2)	80(1)
C(47)	4999(3)	3844(2)	310(2)	67(1)
C(48)	5534(3)	4380(2)	681(2)	72(1)
C(49)	5236(3)	4417(2)	1144(2)	64(1)
C(50)	4377(2)	3908(2)	1218(1)	53(1)
C(51)	5710(3)	1889(3)	1438(2)	98(2)
C(52)	6536(6)	1299(7)	1617(4)	285(8)
C(53)	6259(4)	809(5)	2048(3)	159(3)
C(54)	5152(3)	883(3)	1960(2)	80(1)
O(1)	2579(2)	2868(1)	1961(1)	46(1)
O(2)	2999(2)	2895(1)	942(1)	43(1)
O(3)	2372(2)	1257(1)	1362(1)	47(1)
O(4)	850(2)	2672(1)	1114(1)	46(1)
O(6)	1180(2)	1835(1)	79(1)	54(1)
O(7)	2047(2)	4742(1)	1230(1)	54(1)
O(8)	4865(2)	1683(2)	1683(1)	61(1)
O(9)	603(2)	1665(2)	2187(1)	69(1)

Table S4.3. Bond lengths [A] and angles [deg] for **4**.

Li(1)-O(4)	1.921(5)
Li(1)-O(7)	1.948(5)
Li(1)-O(1)	1.967(5)
Li(1)-O(2)	1.979(5)
Li(1)-Li(3)	2.563(7)
Li(1)-Li(4)	2.636(7)
Li(1)-Li(2)	2.676(7)
Li(2)-O(8)	1.960(5)
Li(2)-O(3)	1.965(5)
Li(2)-O(2)	1.980(6)
Li(2)-O(1)	1.990(5)
Li(2)-Li(4)	2.640(7)
Li(2)-Li(3)	2.648(7)
Li(2)-C(41)	2.751(6)
Li(3)-O(2)	1.902(5)
Li(3)-O(6)	1.948(6)
Li(3)-O(4)	1.979(5)
Li(3)-O(3)	2.019(6)
Li(3)-Li(4)	2.659(7)
Li(4)-O(3)	1.915(5)
Li(4)-O(9)	1.955(5)
Li(4)-O(4)	1.969(6)
Li(4)-O(1)	1.990(5)
Li(4)-C(24)	2.778(6)
C(1)-O(3)	1.346(3)
C(1)-C(2)	1.395(4)
C(1)-C(6)	1.406(4)
C(2)-C(3)	1.373(5)
C(3)-C(4)	1.375(5)
C(4)-C(5)	1.380(5)
C(5)-C(6)	1.401(5)
C(6)-C(7)	1.508(4)
C(7)-C(9)	1.428(6)
C(7)-C(8)	1.537(5)
C(10)-O(9)	1.424(5)
C(10)-C(11)	1.482(6)
C(11)-C(12)	1.536(8)
C(12)-C(13)	1.476(6)
C(13)-O(9)	1.422(5)
C(14)-O(1)	1.334(3)
C(14)-C(15)	1.396(4)
C(14)-C(20)	1.411(5)
C(15)-C(16)	1.388(5)
C(16)-C(17)	1.364(6)
C(17)-C(19)	1.384(6)
C(19)-C(20)	1.399(5)
C(20)-C(21)	1.518(5)
C(21)-C(23)	1.515(5)
C(21)-C(22)	1.541(6)
C(24)-O(4)	1.343(3)
C(24)-C(25)	1.400(4)
C(24)-C(29)	1.403(4)

C(25)-C(26)	1.370(5)
C(26)-C(27)	1.370(5)
C(27)-C(28)	1.380(5)
C(28)-C(29)	1.387(4)
C(29)-C(30)	1.526(4)
C(30)-C(32)	1.519(5)
C(30)-C(31)	1.520(5)
C(33)-O(6)	1.447(4)
C(33)-C(34)	1.480(5)
C(34)-C(35)	1.440(6)
C(35)-C(36)	1.472(6)
C(36)-O(6)	1.448(4)
C(37)-O(7)	1.444(4)
C(37)-C(38)	1.520(6)
C(38)-C(39)	1.470(7)
C(39)-C(40)	1.472(5)
C(40)-O(7)	1.435(4)
C(41)-O(2)	1.346(3)
C(41)-C(50)	1.387(4)
C(41)-C(42)	1.413(4)
C(42)-C(47)	1.396(5)
C(42)-C(43)	1.515(5)
C(43)-C(45)	1.531(5)
C(43)-C(46)	1.532(5)
C(47)-C(48)	1.369(5)
C(48)-C(49)	1.380(5)
C(49)-C(50)	1.397(5)
C(51)-C(52)	1.406(7)
C(51)-O(8)	1.418(4)
C(52)-C(53)	1.481(8)
C(53)-C(54)	1.412(6)
C(54)-O(8)	1.434(4)

O(4)-Li(1)-O(7)	128.1(3)
O(4)-Li(1)-O(1)	96.2(2)
O(7)-Li(1)-O(1)	123.5(3)
O(4)-Li(1)-O(2)	97.2(2)
O(7)-Li(1)-O(2)	109.6(2)
O(1)-Li(1)-O(2)	94.9(2)
O(4)-Li(1)-Li(3)	49.91(17)
O(7)-Li(1)-Li(3)	138.0(3)
O(1)-Li(1)-Li(3)	96.0(2)
O(2)-Li(1)-Li(3)	47.38(16)
O(4)-Li(1)-Li(4)	48.11(17)
O(7)-Li(1)-Li(4)	156.6(3)
O(1)-Li(1)-Li(4)	48.60(17)
O(2)-Li(1)-Li(4)	93.7(2)
Li(3)-Li(1)-Li(4)	61.5(2)
O(4)-Li(1)-Li(2)	94.8(2)
O(7)-Li(1)-Li(2)	136.0(3)
O(1)-Li(1)-Li(2)	47.82(16)
O(2)-Li(1)-Li(2)	47.50(16)
Li(3)-Li(1)-Li(2)	60.69(19)
Li(4)-Li(1)-Li(2)	59.59(18)
O(8)-Li(2)-O(3)	111.4(3)
O(8)-Li(2)-O(2)	117.5(3)
O(3)-Li(2)-O(2)	94.8(2)

O(8)-Li(2)-O(1)	135.7(3)
O(3)-Li(2)-O(1)	94.6(2)
O(2)-Li(2)-O(1)	94.1(2)
O(8)-Li(2)-Li(4)	145.1(3)
O(3)-Li(2)-Li(4)	46.33(16)
O(2)-Li(2)-Li(4)	93.5(2)
O(1)-Li(2)-Li(4)	48.45(16)
O(8)-Li(2)-Li(3)	131.4(3)
O(3)-Li(2)-Li(3)	49.21(17)
O(2)-Li(2)-Li(3)	45.76(16)
O(1)-Li(2)-Li(3)	92.8(2)
Li(4)-Li(2)-Li(3)	60.38(19)
O(8)-Li(2)-Li(1)	154.6(3)
O(3)-Li(2)-Li(1)	91.8(2)
O(2)-Li(2)-Li(1)	47.46(16)
O(1)-Li(2)-Li(1)	47.09(16)
Li(4)-Li(2)-Li(1)	59.46(18)
Li(3)-Li(2)-Li(1)	57.55(18)
O(8)-Li(2)-C(41)	94.7(2)
O(3)-Li(2)-C(41)	118.9(2)
O(2)-Li(2)-C(41)	27.36(11)
O(1)-Li(2)-C(41)	103.5(2)
Li(4)-Li(2)-C(41)	119.1(2)
Li(3)-Li(2)-C(41)	71.73(18)
Li(1)-Li(2)-C(41)	64.01(16)
O(2)-Li(3)-O(6)	123.0(3)
O(2)-Li(3)-O(4)	97.8(2)
O(6)-Li(3)-O(4)	107.6(2)
O(2)-Li(3)-O(3)	95.5(2)
O(6)-Li(3)-O(3)	131.7(3)
O(4)-Li(3)-O(3)	92.9(2)
O(2)-Li(3)-Li(1)	49.97(17)
O(6)-Li(3)-Li(1)	132.3(3)
O(4)-Li(3)-Li(1)	47.94(16)
O(3)-Li(3)-Li(1)	93.9(2)
O(2)-Li(3)-Li(2)	48.23(17)
O(6)-Li(3)-Li(2)	157.9(3)
O(4)-Li(3)-Li(2)	94.3(2)
O(3)-Li(3)-Li(2)	47.47(16)
Li(1)-Li(3)-Li(2)	61.76(19)
O(2)-Li(3)-Li(4)	94.8(2)
O(6)-Li(3)-Li(4)	139.5(3)
O(4)-Li(3)-Li(4)	47.49(17)
O(3)-Li(3)-Li(4)	45.83(16)
Li(1)-Li(3)-Li(4)	60.60(19)
Li(2)-Li(3)-Li(4)	59.64(19)
O(3)-Li(4)-O(9)	132.4(3)
O(3)-Li(4)-O(4)	96.6(2)
O(9)-Li(4)-O(4)	116.9(3)
O(3)-Li(4)-O(1)	96.2(2)
O(9)-Li(4)-O(1)	112.9(3)
O(4)-Li(4)-O(1)	94.0(2)
O(3)-Li(4)-Li(1)	94.2(2)
O(9)-Li(4)-Li(1)	133.3(3)
O(4)-Li(4)-Li(1)	46.58(16)
O(1)-Li(4)-Li(1)	47.86(16)
O(3)-Li(4)-Li(2)	47.94(16)

O(9)-Li(4)-Li(2)	145.9(3)
O(4)-Li(4)-Li(2)	94.8(2)
O(1)-Li(4)-Li(2)	48.46(16)
Li(1)-Li(4)-Li(2)	60.95(19)
O(3)-Li(4)-Li(3)	49.15(17)
O(9)-Li(4)-Li(3)	152.5(3)
O(4)-Li(4)-Li(3)	47.83(16)
O(1)-Li(4)-Li(3)	92.5(2)
Li(1)-Li(4)-Li(3)	57.90(18)
Li(2)-Li(4)-Li(3)	59.98(18)
O(3)-Li(4)-C(24)	104.1(2)
O(9)-Li(4)-C(24)	94.8(2)
O(4)-Li(4)-C(24)	26.50(11)
O(1)-Li(4)-C(24)	117.7(2)
Li(1)-Li(4)-C(24)	72.10(18)
Li(2)-Li(4)-C(24)	118.9(2)
Li(3)-Li(4)-C(24)	62.77(16)
O(3)-C(1)-C(2)	120.1(3)
O(3)-C(1)-C(6)	121.2(3)
C(2)-C(1)-C(6)	118.7(3)
C(3)-C(2)-C(1)	122.4(3)
C(2)-C(3)-C(4)	119.7(3)
C(3)-C(4)-C(5)	118.7(3)
C(4)-C(5)-C(6)	123.2(3)
C(5)-C(6)-C(1)	117.3(3)
C(5)-C(6)-C(7)	121.8(3)
C(1)-C(6)-C(7)	120.9(3)
C(9)-C(7)-C(6)	112.5(3)
C(9)-C(7)-C(8)	110.4(4)
C(6)-C(7)-C(8)	111.7(3)
O(9)-C(10)-C(11)	106.7(4)
C(10)-C(11)-C(12)	102.4(4)
C(13)-C(12)-C(11)	101.9(4)
O(9)-C(13)-C(12)	107.8(4)
O(1)-C(14)-C(15)	120.3(3)
O(1)-C(14)-C(20)	121.6(3)
C(15)-C(14)-C(20)	118.1(3)
C(16)-C(15)-C(14)	121.6(4)
C(17)-C(16)-C(15)	120.5(4)
C(16)-C(17)-C(19)	119.0(4)
C(17)-C(19)-C(20)	122.1(4)
C(19)-C(20)-C(14)	118.7(3)
C(19)-C(20)-C(21)	121.5(3)
C(14)-C(20)-C(21)	119.8(3)
C(23)-C(21)-C(20)	114.3(3)
C(23)-C(21)-C(22)	111.6(3)
C(20)-C(21)-C(22)	109.8(3)
O(4)-C(24)-C(25)	120.3(3)
O(4)-C(24)-C(29)	122.2(3)
C(25)-C(24)-C(29)	117.5(3)
O(4)-C(24)-Li(4)	40.84(16)
C(25)-C(24)-Li(4)	93.0(2)
C(29)-C(24)-Li(4)	136.0(2)
C(26)-C(25)-C(24)	122.0(3)
C(27)-C(26)-C(25)	120.2(3)
C(26)-C(27)-C(28)	119.0(3)
C(27)-C(28)-C(29)	121.8(3)

C(28)-C(29)-C(24)	119.4(3)
C(28)-C(29)-C(30)	119.7(3)
C(24)-C(29)-C(30)	120.9(3)
C(32)-C(30)-C(31)	109.6(3)
C(32)-C(30)-C(29)	111.5(3)
C(31)-C(30)-C(29)	111.5(3)
O(6)-C(33)-C(34)	106.8(3)
C(35)-C(34)-C(33)	105.1(4)
C(34)-C(35)-C(36)	107.4(4)
O(6)-C(36)-C(35)	106.5(3)
O(7)-C(37)-C(38)	104.0(4)
C(39)-C(38)-C(37)	104.8(4)
C(38)-C(39)-C(40)	102.5(3)
O(7)-C(40)-C(39)	106.7(3)
O(2)-C(41)-C(50)	119.5(3)
O(2)-C(41)-C(42)	122.0(3)
C(50)-C(41)-C(42)	118.4(3)
O(2)-C(41)-Li(2)	42.53(16)
C(50)-C(41)-Li(2)	90.7(2)
C(42)-C(41)-Li(2)	136.1(2)
C(47)-C(42)-C(41)	117.9(3)
C(47)-C(42)-C(43)	120.9(3)
C(41)-C(42)-C(43)	121.1(3)
C(42)-C(43)-C(45)	112.4(3)
C(42)-C(43)-C(46)	111.5(3)
C(45)-C(43)-C(46)	110.0(3)
C(48)-C(47)-C(42)	122.8(4)
C(47)-C(48)-C(49)	119.8(3)
C(48)-C(49)-C(50)	118.4(4)
C(41)-C(50)-C(49)	122.6(3)
C(52)-C(51)-O(8)	107.6(4)
C(51)-C(52)-C(53)	107.8(5)
C(54)-C(53)-C(52)	102.6(5)
C(53)-C(54)-O(8)	108.0(4)
C(14)-O(1)-Li(1)	120.9(2)
C(14)-O(1)-Li(4)	114.4(2)
Li(1)-O(1)-Li(4)	83.5(2)
C(14)-O(1)-Li(2)	148.9(2)
Li(1)-O(1)-Li(2)	85.1(2)
Li(4)-O(1)-Li(2)	83.1(2)
C(41)-O(2)-Li(3)	153.5(2)
C(41)-O(2)-Li(1)	118.6(2)
Li(3)-O(2)-Li(1)	82.6(2)
C(41)-O(2)-Li(2)	110.1(2)
Li(3)-O(2)-Li(2)	86.0(2)
Li(1)-O(2)-Li(2)	85.0(2)
C(1)-O(3)-Li(4)	150.5(2)
C(1)-O(3)-Li(2)	119.8(2)
Li(4)-O(3)-Li(2)	85.7(2)
C(1)-O(3)-Li(3)	110.9(2)
Li(4)-O(3)-Li(3)	85.0(2)
Li(2)-O(3)-Li(3)	83.3(2)
C(24)-O(4)-Li(1)	154.8(2)
C(24)-O(4)-Li(4)	112.7(2)
Li(1)-O(4)-Li(4)	85.3(2)
C(24)-O(4)-Li(3)	115.7(2)
Li(1)-O(4)-Li(3)	82.2(2)

Li(4)-O(4)-Li(3)	84.7(2)
C(33)-O(6)-C(36)	108.2(2)
C(33)-O(6)-Li(3)	129.7(2)
C(36)-O(6)-Li(3)	121.1(2)
C(40)-O(7)-C(37)	109.3(3)
C(40)-O(7)-Li(1)	127.3(3)
C(37)-O(7)-Li(1)	119.2(3)
C(51)-O(8)-C(54)	106.5(3)
C(51)-O(8)-Li(2)	128.5(3)
C(54)-O(8)-Li(2)	123.6(3)
C(13)-O(9)-C(10)	109.1(3)
C(13)-O(9)-Li(4)	124.5(3)
C(10)-O(9)-Li(4)	124.2(3)

Table S2.4. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	48(3)	48(3)	42(3)	-2(2)	12(2)	0(2)
Li(2)	44(3)	54(3)	45(3)	-1(2)	10(2)	3(2)
Li(3)	41(3)	49(3)	46(3)	-4(2)	7(2)	4(2)
Li(4)	51(3)	47(3)	49(3)	3(2)	19(2)	0(2)
C(1)	42(2)	40(2)	47(2)	-2(1)	9(1)	4(1)
C(2)	61(2)	53(2)	50(2)	7(2)	16(2)	14(2)
C(3)	72(2)	76(3)	47(2)	-6(2)	14(2)	18(2)
C(4)	78(3)	57(2)	65(2)	-18(2)	13(2)	14(2)
C(5)	64(2)	42(2)	75(3)	3(2)	8(2)	0(2)
C(6)	47(2)	41(2)	53(2)	5(2)	9(2)	3(1)
C(7)	64(2)	44(2)	65(2)	14(2)	26(2)	7(2)
C(8)	128(4)	112(4)	78(3)	6(3)	31(3)	-48(3)
C(9)	87(3)	177(5)	65(3)	-35(3)	27(2)	-20(3)
C(10)	118(4)	94(3)	86(3)	34(3)	55(3)	15(3)
C(11)	150(5)	117(4)	101(4)	29(3)	75(4)	48(4)
C(12)	140(5)	96(4)	154(6)	5(4)	111(5)	2(3)
C(13)	77(3)	122(4)	119(4)	22(3)	58(3)	6(3)
C(14)	60(2)	47(2)	35(2)	0(1)	14(2)	-3(2)
C(15)	64(2)	56(2)	50(2)	4(2)	20(2)	5(2)
C(16)	97(3)	61(2)	71(3)	-2(2)	43(2)	9(2)
C(17)	138(4)	78(3)	52(3)	-14(2)	39(3)	4(3)
C(19)	121(4)	82(3)	37(2)	-4(2)	7(2)	10(3)
C(20)	82(2)	54(2)	38(2)	1(2)	10(2)	3(2)
C(21)	71(2)	74(2)	41(2)	-2(2)	-4(2)	11(2)
C(22)	78(3)	110(4)	75(3)	-11(3)	3(2)	3(2)
C(23)	122(4)	106(4)	63(3)	25(3)	5(3)	31(3)
C(24)	43(2)	44(2)	44(2)	-7(1)	10(1)	-1(1)
C(25)	54(2)	51(2)	80(3)	-16(2)	21(2)	0(2)
C(26)	59(2)	64(2)	101(3)	-32(2)	26(2)	-16(2)
C(27)	47(2)	82(3)	84(3)	-32(2)	13(2)	-11(2)
C(28)	48(2)	71(2)	57(2)	-13(2)	7(2)	10(2)
C(29)	47(2)	49(2)	35(2)	-6(1)	7(1)	5(1)
C(30)	55(2)	43(2)	56(2)	-2(2)	7(2)	9(1)
C(31)	122(4)	73(3)	81(3)	-33(2)	41(3)	2(2)
C(32)	99(3)	69(3)	80(3)	17(2)	18(2)	15(2)
C(33)	87(3)	58(2)	64(2)	-17(2)	-5(2)	1(2)
C(34)	95(3)	86(3)	85(3)	-25(3)	-17(3)	2(2)
C(35)	168(5)	84(3)	103(4)	4(3)	-70(4)	0(3)
C(36)	79(2)	62(2)	57(2)	7(2)	6(2)	12(2)
C(37)	91(3)	66(2)	62(2)	24(2)	12(2)	17(2)
C(38)	146(5)	76(3)	133(5)	39(3)	49(4)	-11(3)
C(39)	103(3)	48(2)	118(4)	5(2)	16(3)	-4(2)
C(40)	99(3)	48(2)	80(3)	-15(2)	28(2)	-3(2)
C(41)	44(2)	39(2)	47(2)	6(1)	13(1)	5(1)
C(42)	52(2)	51(2)	52(2)	14(2)	20(2)	8(2)
C(43)	63(2)	67(2)	46(2)	3(2)	22(2)	6(2)

C(45)	101(3)	72(3)	70(3)	0(2)	33(2)	17(2)
C(46)	93(3)	86(3)	60(2)	5(2)	16(2)	12(2)
C(47)	60(2)	73(2)	74(3)	19(2)	31(2)	5(2)
C(48)	50(2)	60(2)	107(3)	24(2)	18(2)	-5(2)
C(49)	48(2)	49(2)	92(3)	7(2)	2(2)	1(2)
C(50)	48(2)	49(2)	61(2)	1(2)	9(2)	0(2)
C(51)	67(3)	116(4)	119(4)	57(3)	36(3)	32(2)
C(52)	151(6)	408(14)	346(13)	303(12)	170(8)	179(8)
C(53)	106(4)	212(7)	175(6)	122(6)	67(4)	- 81(4)
C(54)	61(2)	78(3)	100(3)	25(2)	17(2)	12(2)
O(1)	50(1)	53(1)	34(1)	1(1)	10(1)	2(1)
O(2)	51(1)	42(1)	40(1)	0(1)	17(1)	-3(1)
O(3)	53(1)	37(1)	54(1)	3(1)	18(1)	5(1)
O(4)	43(1)	42(1)	52(1)	-6(1)	8(1)	1(1)
O(6)	63(1)	48(1)	49(1)	-6(1)	1(1)	5(1)
O(7)	67(1)	40(1)	54(1)	1(1)	10(1)	-2(1)
O(8)	45(1)	69(2)	71(2)	17(1)	17(1)	15(1)
O(9)	81(2)	62(2)	78(2)	13(1)	45(2)	4(1)

Table S4.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(2)	3264	931	621	65
H(3)	3736	-392	319	78
H(4)	3408	-1698	710	80
H(5)	2668	-1640	1417	73
H(7)	1487	163	1885	67
H(8A)	2032	-1606	2146	157
H(8B)	1086	-1379	1709	157
H(8C)	1058	-1087	2263	157
H(9A)	3228	-564	2478	162
H(9B)	2451	140	2627	162
H(9C)	3237	408	2277	162
H(10A)	1636	1799	2827	113
H(10B)	1133	847	2752	113
H(11A)	249	2363	3089	139
H(11B)	161	1380	3276	139
H(12A)	-1097	1016	2581	143
H(12B)	-1404	2016	2647	143
H(13A)	-873	1505	1838	121
H(13B)	-619	2473	2039	121
H(15)	1125	3881	2142	67
H(16)	900	4485	2896	88
H(17)	2099	4212	3624	104
H(19)	3534	3325	3594	98
H(21)	3980	2091	2537	77
H(22A)	5316	3443	3019	134
H(22B)	4867	3412	2437	134
H(22C)	5666	2689	2688	134
H(23A)	4811	2248	3571	148
H(23B)	4991	1462	3219	148
H(23C)	3885	1600	3362	148
H(25)	57	1153	866	73
H(26)	-1649	770	552	88
H(27)	-2954	1828	443	85
H(28)	-2525	3274	662	71
H(30)	31	4108	1179	62
H(31A)	-1154	4980	1517	134
H(31B)	-1151	4013	1727	134
H(31C)	-2072	4330	1299	134
H(32A)	-1686	4634	428	124
H(32B)	-537	4496	337	124
H(32C)	-783	5270	683	124
H(33A)	937	528	27	86
H(33B)	1664	878	-336	86
H(34A)	218	819	-908	112
H(34B)	-510	872	-502	112
H(35A)	-734	2216	-767	157
H(35B)	340	2234	-958	157

H(36A)	925	2994	-285	80
H(36B)	-15	2701	-28	80
H(37A)	1315	5177	552	88
H(37B)	2401	4711	539	88
H(38A)	3334	5921	826	139
H(38B)	2287	6415	581	139
H(39A)	1760	6535	1320	108
H(39B)	2990	6636	1499	108
H(40A)	3189	5244	1754	89
H(40B)	2055	5418	1864	89
H(43)	3014	2432	81	69
H(45A)	4876	2252	-312	118
H(45B)	3925	1592	-408	118
H(45C)	4623	1674	132	118
H(46A)	2705	3718	-429	120
H(46B)	2701	2858	-753	120
H(46C)	3688	3480	-664	120
H(47)	5214	3826	1	80
H(48)	6096	4719	620	86
H(49)	5598	4771	1401	77
H(50)	4173	3932	1530	64
H(51A)	5490	1828	1075	118
H(51B)	5940	2494	1511	118
H(52A)	7188	1621	1724	343
H(52B)	6629	890	1352	343
H(53A)	6477	195	2048	191
H(53B)	6577	1079	2367	191
H(54A)	4908	901	2278	95
H(54B)	4832	378	1768	95

[Li(DIP)(THF)]$_3$ (5)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P2(1)/n using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. Subsequent refinement confirmed the original atom identification. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0626 and R2w=0.1566.

Table S5.1. Crystal data and structure refinement for **5**.

Empirical formula	C48 H75 Li3 O6
Formula weight	768.90
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 13.316(2) A alpha = 90 deg. b = 16.148(3) A beta = 90.000(4) deg. c = 22.427(3) A gamma = 90 deg.
Volume	4822.4(13) A^3
Z, Calculated density	4, 1.059 Mg/m^3
Absorption coefficient	0.066 mm^-1
F(000)	1680
Crystal size	0.2 mm x .2mm x 0.4mm
Theta range for data collection	1.55 to 28.29 deg.
Limiting indices	-17<=h<=12, -21<=k<=19, -28<=l<=24
Reflections collected / unique	30409 / 11234 [R(int) = 0.1066]
Completeness to theta = 28.29	93.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11234 / 0 / 526
Goodness-of-fit on F^2	0.811
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1566
R indices (all data)	R1 = 0.2620, wR2 = 0.2179
Largest diff. peak and hole	0.246 and -0.233 e.A^-3

Table S5.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	3167(4)	1869(4)	1456(2)	63(2)
Li(2)	1452(4)	2213(4)	513(2)	59(2)
Li(3)	3673(4)	2344(4)	176(2)	62(2)
C(1)	-786(3)	1711(2)	514(2)	71(1)
C(2)	-1732(3)	2070(3)	244(2)	86(1)
C(3)	-1409(4)	2744(4)	-100(4)	244(5)
C(4)	-388(3)	2858(3)	-75(2)	124(2)
C(5)	1079(2)	1615(2)	1598(1)	44(1)
C(6)	427(2)	2173(2)	1887(1)	45(1)
C(7)	-347(2)	1853(2)	2242(1)	54(1)
C(8)	-494(3)	1019(3)	2310(2)	62(1)
C(9)	138(3)	469(2)	2016(1)	57(1)
C(10)	929(2)	749(2)	1662(1)	49(1)
C(11)	1634(3)	165(2)	1343(2)	63(1)
C(12)	585(3)	3094(2)	1814(1)	57(1)
C(13)	1350(3)	76(2)	682(2)	85(1)
C(14)	1714(3)	-698(2)	1630(2)	85(1)
C(15)	1319(3)	3434(2)	2273(2)	102(2)
C(16)	-385(3)	3608(2)	1812(2)	88(1)
C(17)	2777(3)	1331(4)	2701(2)	128(2)
C(18)	3247(4)	1230(4)	3241(2)	149(2)
C(19)	4230(4)	1519(5)	3192(2)	195(4)
C(20)	4422(3)	1737(4)	2604(2)	142(2)
C(21)	2174(2)	3040(2)	-506(2)	51(1)
C(22)	2073(3)	3893(3)	-420(2)	65(1)
C(23)	1903(3)	4416(3)	-909(2)	84(1)
C(24)	1829(3)	4090(3)	-1476(2)	84(1)
C(25)	1924(3)	3250(3)	-1562(2)	69(1)
C(26)	2088(2)	2707(2)	-1091(2)	54(1)
C(27)	2168(4)	4263(3)	203(2)	94(1)
C(30)	2183(3)	1786(2)	-1178(2)	63(1)
C(31)	5679(3)	2363(3)	-352(2)	96(2)
C(32)	6143(4)	2495(3)	-935(2)	108(2)
C(33)	5605(3)	3238(3)	-1171(2)	96(1)
C(34)	4622(3)	3182(4)	-901(2)	146(2)
C(35)	2576(4)	1531(3)	-1789(2)	116(2)
C(36)	1204(3)	1334(3)	-1040(2)	101(2)
C(37)	5099(3)	2041(2)	1134(1)	54(1)
C(38)	6579(3)	1321(4)	1477(2)	95(2)
C(39)	5527(3)	2792(3)	1328(2)	68(1)
C(40)	5641(5)	4338(3)	1130(3)	196(3)
C(42)	5645(3)	1299(3)	1195(2)	67(1)
C(43)	4967(3)	3593(3)	1241(2)	92(1)
C(44)	6973(4)	2043(5)	1684(2)	108(2)
C(45)	6471(4)	2764(4)	1604(2)	94(2)

C(46)	5215(3)	497(3)	966(2)	86(1)
C(47)	5979(4)	12(3)	584(2)	110(2)
C(49)	1253(5)	4685(4)	435(3)	173(3)
C(50)	3061(4)	4817(4)	275(2)	158(2)
C(51)	4811(4)	-50(3)	1478(2)	134(2)
C(52)	4259(5)	3789(3)	1760(3)	173(3)
O(1)	1834(2)	1897(1)	1259(1)	51(1)
O(2)	2356(2)	2535(1)	-41(1)	57(1)
O(3)	4170(2)	2032(1)	902(1)	51(1)
O(4)	3488(2)	1650(2)	2284(1)	87(1)
O(5)	20(2)	2237(2)	317(1)	73(1)
O(6)	4675(2)	2658(2)	-397(1)	77(1)

Table S5.3. Bond lengths [A] and angles [deg] for **5**.

Li(1)-O(1)	1.830(6)
Li(1)-O(3)	1.844(6)
Li(1)-O(4)	1.937(6)
Li(1)-C(37)	2.687(7)
Li(1)-Li(3)	3.048(8)
Li(1)-Li(2)	3.162(8)
Li(2)-O(2)	1.807(6)
Li(2)-O(1)	1.822(6)
Li(2)-O(5)	1.958(6)
Li(2)-C(5)	2.665(6)
Li(2)-Li(3)	3.060(8)
Li(3)-O(3)	1.829(6)
Li(3)-O(2)	1.846(6)
Li(3)-O(6)	1.920(6)
Li(3)-C(21)	2.754(7)
C(1)-O(5)	1.439(4)
C(1)-C(2)	1.513(5)
C(2)-C(3)	1.402(6)
C(3)-C(4)	1.373(6)
C(4)-O(5)	1.439(4)
C(5)-O(1)	1.340(3)
C(5)-C(6)	1.410(4)
C(5)-C(10)	1.420(4)
C(6)-C(7)	1.400(4)
C(6)-C(12)	1.510(4)
C(7)-C(8)	1.370(4)
C(8)-C(9)	1.390(4)
C(9)-C(10)	1.394(4)
C(10)-C(11)	1.511(4)
C(11)-C(13)	1.537(5)
C(11)-C(14)	1.538(4)
C(12)-C(15)	1.522(5)
C(12)-C(16)	1.535(5)
C(17)-C(18)	1.373(5)
C(17)-O(4)	1.428(4)
C(18)-C(19)	1.395(6)
C(19)-C(20)	1.388(5)
C(20)-O(4)	1.444(4)
C(21)-O(2)	1.345(3)
C(21)-C(22)	1.397(4)
C(21)-C(26)	1.423(4)
C(22)-C(23)	1.403(5)
C(22)-C(27)	1.524(5)
C(23)-C(24)	1.380(5)
C(24)-C(25)	1.375(5)
C(25)-C(26)	1.392(4)
C(26)-C(30)	1.504(4)
C(27)-C(49)	1.489(6)
C(27)-C(50)	1.497(6)
C(30)-C(35)	1.522(5)
C(30)-C(36)	1.527(5)
C(31)-O(6)	1.423(4)
C(31)-C(32)	1.462(5)
C(32)-C(33)	1.494(5)

C(33)-C(34)	1.445(5)
C(34)-O(6)	1.414(4)
C(37)-O(3)	1.341(4)
C(37)-C(42)	1.408(5)
C(37)-C(39)	1.410(5)
C(38)-C(44)	1.361(6)
C(38)-C(42)	1.396(5)
C(39)-C(45)	1.402(6)
C(39)-C(43)	1.506(5)
C(40)-C(43)	1.523(6)
C(42)-C(46)	1.506(5)
C(43)-C(52)	1.531(6)
C(44)-C(45)	1.354(6)
C(46)-C(47)	1.544(5)
C(46)-C(51)	1.545(5)

O(1)-Li(1)-O(3)	122.5(3)
O(1)-Li(1)-O(4)	116.7(3)
O(3)-Li(1)-O(4)	120.8(3)
O(1)-Li(1)-C(37)	149.5(3)
O(3)-Li(1)-C(37)	27.10(12)
O(4)-Li(1)-C(37)	93.7(2)
O(1)-Li(1)-Li(3)	88.9(2)
O(3)-Li(1)-Li(3)	33.77(16)
O(4)-Li(1)-Li(3)	154.1(3)
C(37)-Li(1)-Li(3)	60.57(17)
O(1)-Li(1)-Li(2)	29.96(15)
O(3)-Li(1)-Li(2)	92.7(2)
O(4)-Li(1)-Li(2)	146.4(3)
C(37)-Li(1)-Li(2)	119.6(2)
Li(3)-Li(1)-Li(2)	59.01(18)
O(2)-Li(2)-O(1)	121.8(3)
O(2)-Li(2)-O(5)	119.3(3)
O(1)-Li(2)-O(5)	118.9(3)
O(2)-Li(2)-C(5)	148.9(3)
O(1)-Li(2)-C(5)	27.33(12)
O(5)-Li(2)-C(5)	91.8(2)
O(2)-Li(2)-Li(3)	33.51(16)
O(1)-Li(2)-Li(3)	88.7(2)
O(5)-Li(2)-Li(3)	152.2(3)
C(5)-Li(2)-Li(3)	115.5(2)
O(2)-Li(2)-Li(1)	91.7(2)
O(1)-Li(2)-Li(1)	30.10(16)
O(5)-Li(2)-Li(1)	149.0(3)
C(5)-Li(2)-Li(1)	57.32(16)
Li(3)-Li(2)-Li(1)	58.63(18)
O(3)-Li(3)-O(2)	128.7(3)
O(3)-Li(3)-O(6)	114.7(3)
O(2)-Li(3)-O(6)	116.1(3)
O(3)-Li(3)-C(21)	150.4(3)
O(2)-Li(3)-C(21)	25.41(12)
O(6)-Li(3)-C(21)	91.4(2)
O(3)-Li(3)-Li(1)	34.08(16)
O(2)-Li(3)-Li(1)	94.6(2)
O(6)-Li(3)-Li(1)	148.3(3)
C(21)-Li(3)-Li(1)	117.7(2)
O(3)-Li(3)-Li(2)	96.4(2)

O(2)-Li(3)-Li(2)	32.70(16)
O(6)-Li(3)-Li(2)	148.8(3)
C(21)-Li(3)-Li(2)	57.63(17)
Li(1)-Li(3)-Li(2)	62.36(18)
O(5)-C(1)-C(2)	105.7(3)
C(3)-C(2)-C(1)	105.2(4)
C(4)-C(3)-C(2)	112.7(5)
C(3)-C(4)-O(5)	107.7(4)
O(1)-C(5)-C(6)	120.4(3)
O(1)-C(5)-C(10)	119.8(3)
C(6)-C(5)-C(10)	119.8(3)
O(1)-C(5)-Li(2)	38.65(17)
C(6)-C(5)-Li(2)	107.7(2)
C(10)-C(5)-Li(2)	118.4(2)
C(7)-C(6)-C(5)	118.6(3)
C(7)-C(6)-C(12)	121.8(3)
C(5)-C(6)-C(12)	119.6(3)
C(8)-C(7)-C(6)	122.1(3)
C(7)-C(8)-C(9)	119.3(3)
C(8)-C(9)-C(10)	121.4(3)
C(9)-C(10)-C(5)	118.9(3)
C(9)-C(10)-C(11)	122.5(3)
C(5)-C(10)-C(11)	118.6(3)
C(10)-C(11)-C(13)	111.2(3)
C(10)-C(11)-C(14)	114.2(3)
C(13)-C(11)-C(14)	109.6(3)
C(6)-C(12)-C(15)	111.8(3)
C(6)-C(12)-C(16)	114.5(3)
C(15)-C(12)-C(16)	110.3(3)
C(18)-C(17)-O(4)	108.7(4)
C(17)-C(18)-C(19)	108.5(4)
C(20)-C(19)-C(18)	109.5(4)
C(19)-C(20)-O(4)	106.8(4)
O(2)-C(21)-C(22)	120.6(3)
O(2)-C(21)-C(26)	119.9(3)
C(22)-C(21)-C(26)	119.5(3)
O(2)-C(21)-Li(3)	36.09(17)
C(22)-C(21)-Li(3)	113.3(3)
C(26)-C(21)-Li(3)	114.5(3)
C(21)-C(22)-C(23)	120.1(4)
C(21)-C(22)-C(27)	120.3(4)
C(23)-C(22)-C(27)	119.6(4)
C(24)-C(23)-C(22)	120.2(4)
C(25)-C(24)-C(23)	119.9(4)
C(24)-C(25)-C(26)	122.0(4)
C(25)-C(26)-C(21)	118.3(3)
C(25)-C(26)-C(30)	122.5(3)
C(21)-C(26)-C(30)	119.2(3)
C(49)-C(27)-C(50)	109.8(4)
C(49)-C(27)-C(22)	115.6(4)
C(50)-C(27)-C(22)	113.5(4)
C(26)-C(30)-C(35)	114.4(3)
C(26)-C(30)-C(36)	112.0(3)
C(35)-C(30)-C(36)	110.2(3)
O(6)-C(31)-C(32)	106.5(3)
C(31)-C(32)-C(33)	103.4(4)
C(34)-C(33)-C(32)	103.6(4)

O(6)-C(34)-C(33)	109.1(3)
O(3)-C(37)-C(42)	120.3(3)
O(3)-C(37)-C(39)	120.1(4)
C(42)-C(37)-C(39)	119.5(4)
O(3)-C(37)-Li(1)	38.77(17)
C(42)-C(37)-Li(1)	112.4(3)
C(39)-C(37)-Li(1)	113.1(3)
C(44)-C(38)-C(42)	121.3(5)
C(45)-C(39)-C(37)	118.1(4)
C(45)-C(39)-C(43)	122.0(4)
C(37)-C(39)-C(43)	119.9(4)
C(38)-C(42)-C(37)	118.9(4)
C(38)-C(42)-C(46)	121.0(4)
C(37)-C(42)-C(46)	120.1(3)
C(39)-C(43)-C(40)	114.0(4)
C(39)-C(43)-C(52)	112.6(4)
C(40)-C(43)-C(52)	108.9(4)
C(45)-C(44)-C(38)	120.1(5)
C(44)-C(45)-C(39)	121.9(5)
C(42)-C(46)-C(47)	112.0(4)
C(42)-C(46)-C(51)	111.7(4)
C(47)-C(46)-C(51)	110.5(3)
C(5)-O(1)-Li(2)	114.0(3)
C(5)-O(1)-Li(1)	125.6(2)
Li(2)-O(1)-Li(1)	119.9(3)
C(21)-O(2)-Li(2)	125.9(3)
C(21)-O(2)-Li(3)	118.5(2)
Li(2)-O(2)-Li(3)	113.8(3)
C(37)-O(3)-Li(3)	132.5(3)
C(37)-O(3)-Li(1)	114.1(2)
Li(3)-O(3)-Li(1)	112.1(3)
C(17)-O(4)-C(20)	106.2(3)
C(17)-O(4)-Li(1)	123.2(3)
C(20)-O(4)-Li(1)	130.5(3)
C(4)-O(5)-C(1)	108.6(3)
C(4)-O(5)-Li(2)	121.2(3)
C(1)-O(5)-Li(2)	130.2(3)
C(34)-O(6)-C(31)	107.7(3)
C(34)-O(6)-Li(3)	131.2(3)
C(31)-O(6)-Li(3)	121.1(3)

Table S5.4. Anisotropic displacement parameters (A^2 x 10^3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	48(4)	88(4)	52(3)	8(3)	-1(3)	-6(3)
Li(2)	53(4)	72(4)	53(3)	4(3)	-4(3)	1(3)
Li(3)	47(4)	87(4)	51(3)	13(3)	0(3)	-2(3)
C(1)	57(3)	95(3)	62(2)	5(2)	-12(2)	-14(2)
C(2)	54(3)	123(4)	81(3)	11(3)	-11(2)	-3(3)
C(3)	63(4)	297(9)	371(11)	248(9)	-63(5)	-48(5)
C(4)	63(3)	147(5)	161(5)	92(4)	-16(3)	2(3)
C(5)	35(2)	60(3)	36(2)	5(2)	-2(2)	1(2)
C(6)	39(2)	59(2)	37(2)	2(2)	-7(2)	-2(2)
C(7)	42(2)	72(3)	46(2)	-2(2)	3(2)	3(2)
C(8)	48(3)	80(3)	59(2)	14(2)	5(2)	-7(2)
C(9)	54(3)	57(2)	60(2)	12(2)	1(2)	-5(2)
C(10)	38(2)	61(3)	49(2)	8(2)	-5(2)	0(2)
C(11)	54(3)	60(3)	74(3)	2(2)	2(2)	2(2)
C(12)	61(3)	60(3)	51(2)	-7(2)	-1(2)	-1(2)
C(13)	100(4)	78(3)	77(3)	-9(2)	14(2)	14(2)
C(14)	77(3)	70(3)	108(3)	11(2)	6(2)	23(2)
C(15)	103(4)	79(3)	123(4)	-21(3)	-41(3)	-12(3)
C(16)	79(3)	75(3)	111(3)	7(2)	4(3)	18(2)
C(17)	65(3)	253(6)	66(3)	56(4)	-1(3)	-37(4)
C(18)	77(4)	300(8)	69(3)	49(4)	3(3)	0(4)
C(19)	77(4)	442(11)	67(4)	75(5)	-10(3)	-59(5)
C(20)	68(4)	303(8)	57(3)	29(4)	-17(3)	-58(4)
C(21)	30(2)	62(3)	62(3)	12(2)	1(2)	2(2)
C(22)	54(3)	68(3)	72(3)	6(2)	4(2)	-4(2)
C(23)	81(3)	65(3)	108(4)	14(3)	-8(3)	3(2)
C(24)	75(3)	82(4)	94(4)	38(3)	-17(3)	4(3)
C(25)	64(3)	85(3)	57(2)	20(2)	-7(2)	5(2)
C(26)	38(2)	72(3)	52(2)	9(2)	-3(2)	5(2)
C(27)	112(4)	78(3)	91(3)	-6(3)	3(3)	-1(3)
C(30)	61(3)	78(3)	51(2)	6(2)	-5(2)	3(2)
C(31)	64(3)	144(4)	82(3)	40(3)	22(2)	34(3)
C(32)	87(4)	138(4)	98(4)	15(3)	28(3)	24(3)
C(33)	70(3)	138(4)	79(3)	28(3)	15(2)	10(3)
C(34)	57(3)	245(6)	137(4)	130(5)	30(3)	27(4)
C(35)	168(5)	105(4)	76(3)	4(3)	39(3)	40(3)
C(36)	89(4)	95(3)	117(4)	-19(3)	4(3)	-20(3)
C(37)	43(2)	84(3)	35(2)	4(2)	4(2)	-9(2)
C(38)	53(3)	158(5)	75(3)	34(3)	-5(2)	14(3)
C(39)	53(3)	108(4)	43(2)	-10(2)	7(2)	-19(3)
C(40)	155(6)	124(5)	309(9)	26(5)	39(6)	-59(4)
C(42)	48(3)	99(3)	53(2)	20(2)	-4(2)	2(2)
C(43)	88(4)	93(3)	94(3)	-33(3)	15(3)	-21(3)
C(44)	52(3)	205(7)	67(3)	5(4)	-8(2)	-22(4)
C(45)	70(4)	155(5)	56(3)	-27(3)	7(3)	-44(3)
C(46)	67(3)	80(3)	111(3)	15(3)	-9(3)	22(3)
C(47)	103(4)	99(4)	127(4)	17(3)	-5(3)	30(3)
C(49)	135(6)	207(7)	177(6)	-93(5)	21(5)	3(5)

C(50)	122(5)	220(7)	131(5)	-66(4)	-3(4)	-51(5)
C(51)	137(5)	94(4)	170(5)	47(3)	45(4)	3(3)
C(52)	184(7)	150(5)	185(6)	-66(4)	100(5)	-19(4)
O(1)	39(1)	68(2)	46(1)	4(1)	5(1)	-2(1)
O(2)	43(2)	80(2)	48(1)	17(1)	-1(1)	-3(1)
O(3)	38(1)	73(2)	43(1)	5(1)	-3(1)	-1(1)
O(4)	50(2)	168(3)	44(1)	21(2)	-2(1)	-15(2)
O(5)	42(2)	107(2)	71(2)	21(2)	-1(1)	-3(1)
O(6)	43(2)	125(2)	63(2)	34(2)	8(1)	8(2)

Table S5.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(1A)	-830	1711	955	86
H(1B)	-681	1136	376	86
H(2A)	-2075	1654	-9	103
H(2B)	-2201	2254	560	103
H(3A)	-1611	2654	-520	292
H(3B)	-1747	3253	43	292
H(4A)	-231	3418	78	148
H(4B)	-92	2802	-478	148
H(7)	-783	2227	2442	64
H(8)	-1023	819	2555	75
H(9)	29	-110	2057	69
H(11)	2318	419	1358	75
H(12)	904	3174	1415	69
H(13A)	692	-193	649	127
H(13B)	1856	-262	477	127
H(13C)	1320	625	497	127
H(14A)	1885	-639	2053	128
H(14B)	2238	-1018	1428	128
H(14C)	1070	-986	1593	128
H(15A)	1010	3418	2669	153
H(15B)	1490	4007	2171	153
H(15C)	1931	3096	2273	153
H(16A)	-864	3364	1531	132
H(16B)	-232	4177	1691	132
H(16C)	-677	3610	2213	132
H(17A)	2207	1720	2743	154
H(17B)	2513	793	2559	154
H(18A)	3249	637	3354	178
H(18B)	2885	1543	3554	178
H(19A)	4324	2007	3453	235
H(19B)	4705	1083	3320	235
H(20A)	4940	1369	2431	171
H(20B)	4665	2315	2581	171
H(23)	1839	4996	-850	101
H(24)	1711	4445	-1807	100
H(25)	1876	3035	-1955	83
H(27)	2287	3783	475	112
H(30)	2687	1588	-880	76
H(31A)	5684	1767	-248	116
H(31B)	6049	2671	-40	116
H(32A)	6041	2009	-1198	129
H(32B)	6871	2603	-896	129
H(33A)	5950	3755	-1051	115
H(33B)	5558	3219	-1612	115
H(34A)	4391	3740	-780	176
H(34B)	4135	2956	-1193	176
H(35A)	2083	1682	-2095	174
H(35B)	2685	931	-1796	174
H(35C)	3211	1817	-1868	174

H(36A)	967	1493	-643	151
H(36B)	1319	734	-1052	151
H(36C)	696	1483	-1338	151
H(38)	6948	821	1525	114
H(40A)	6092	4415	1471	295
H(40B)	5227	4835	1078	295
H(40C)	6040	4245	769	295
H(43)	4539	3524	878	110
H(44)	7600	2042	1886	130
H(45)	6768	3265	1739	113
H(46)	4633	639	703	103
H(47A)	6222	366	260	164
H(47B)	5653	-480	416	164
H(47C)	6546	-159	834	164
H(49A)	1367	4856	848	259
H(49B)	683	4302	418	259
H(49C)	1108	5173	190	259
H(50A)	2958	5327	46	236
H(50B)	3663	4532	129	236
H(50C)	3148	4954	697	236
H(51A)	5364	-201	1744	200
H(51B)	4511	-554	1311	200
H(51C)	4301	257	1702	200
H(52A)	3746	3355	1791	259
H(52B)	3933	4324	1690	259
H(52C)	4644	3813	2132	259

$[Li(oBP)(THF)_2]_2$ (6)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P2(1)/n using direct methods. This solution yielded the positions of the Li, O, N, and C atoms as Q peaks. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0527 and R2w=0.1471.

Table S6.1. Crystal data and structure refinement for **6**.

Empirical formula	C18 H29 Li O3
Formula weight	300.35
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 9.1510(7) A alpha = 90 deg. b = 14.4287(12) A beta = 105.3260(10) deg. c = 14.1346(12) A gamma = 90 deg.
Volume	1799.9(3) A^3
Z, Calculated density	4, 1.108 Mg/m^3
Absorption coefficient	0.072 mm^-1
F(000)	656
Crystal size	.2 x ? x .35 mm
Theta range for data collection	2.06 to 28.27 deg.
Limiting indices	-11<=h<=11, -12<=k<=18, -17<=l<=17
Reflections collected / unique	11255 / 4149 [R(int) = 0.0261]
Completeness to theta = 28.27	93.0 %
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4149 / 0 / 202
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.1471
R indices (all data)	R1 = 0.0916, wR2 = 0.1724
Largest diff. peak and hole	0.282 and -0.221 e.A^-3

Table S6.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	5925(3)	23(2)	5840(2)	43(1)
O(1)	4970(1)	991(1)	4978(1)	40(1)
O(2)	5648(2)	241(1)	7181(1)	64(1)
O(3)	8176(2)	-172(1)	6352(1)	59(1)
C(1)	4243(2)	1711(1)	5215(1)	36(1)
C(2)	4644(2)	2647(1)	5081(1)	37(1)
C(3)	3802(2)	3346(1)	5379(1)	50(1)
C(4)	2609(2)	3166(2)	5785(1)	60(1)
C(5)	2218(2)	2267(2)	5909(1)	56(1)
C(6)	3016(2)	1559(1)	5625(1)	50(1)
C(7)	5954(2)	2873(1)	4640(1)	46(1)
C(8)	7440(2)	2483(1)	5291(2)	64(1)
C(9)	5656(2)	2457(1)	3608(1)	60(1)
C(10)	6168(3)	3924(1)	4548(2)	71(1)
C(11)	6125(3)	1124(2)	7630(2)	79(1)
C(12)	5194(3)	1261(2)	8331(2)	75(1)
C(13)	5124(3)	306(2)	8722(2)	69(1)
C(14)	5181(3)	-300(2)	7879(1)	60(1)
C(15)	9480(2)	331(2)	6306(2)	74(1)
C(16)	10830(3)	-272(2)	6784(2)	85(1)
C(17)	10181(2)	-1217(2)	6729(2)	65(1)
C(18)	8653(2)	-1031(2)	6865(2)	65(1)

Table S6.3. Bond lengths [A] and angles [deg] for **6**.

Li(1)-O(1)	1.907(3)
Li(1)-O(1)#1	1.911(3)
Li(1)-O(2)	2.002(3)
Li(1)-O(3)	2.014(3)
Li(1)-Li(1)#1	2.527(6)
O(1)-C(1)	1.3230(19)
O(1)-Li(1)#1	1.911(3)
O(2)-C(14)	1.410(2)
O(2)-C(11)	1.438(2)
O(3)-C(15)	1.413(3)
O(3)-C(18)	1.444(2)
C(1)-C(6)	1.409(2)
C(1)-C(2)	1.426(2)
C(2)-C(3)	1.399(2)
C(2)-C(7)	1.525(2)
C(3)-C(4)	1.386(3)
C(4)-C(5)	1.369(3)
C(5)-C(6)	1.375(3)
C(7)-C(8)	1.534(3)
C(7)-C(9)	1.534(3)
C(7)-C(10)	1.539(3)
C(11)-C(12)	1.481(3)
C(12)-C(13)	1.492(3)
C(13)-C(14)	1.490(3)
C(15)-C(16)	1.516(3)
C(16)-C(17)	1.481(3)
C(17)-C(18)	1.485(3)
O(1)-Li(1)-O(1)#1	97.10(13)
O(1)-Li(1)-O(2)	109.81(14)
O(1)#1-Li(1)-O(2)	123.47(15)
O(1)-Li(1)-O(3)	125.77(15)
O(1)#1-Li(1)-O(3)	110.16(14)
O(2)-Li(1)-O(3)	93.14(13)
O(1)-Li(1)-Li(1)#1	48.61(10)
O(1)#1-Li(1)-Li(1)#1	48.48(10)
O(2)-Li(1)-Li(1)#1	132.3(2)
O(3)-Li(1)-Li(1)#1	134.56(19)
C(1)-O(1)-Li(1)	126.08(13)
C(1)-O(1)-Li(1)#1	126.19(13)
Li(1)-O(1)-Li(1)#1	82.90(13)
C(14)-O(2)-C(11)	107.11(15)
C(14)-O(2)-Li(1)	135.50(15)
C(11)-O(2)-Li(1)	117.17(14)
C(15)-O(3)-C(18)	108.48(15)
C(15)-O(3)-Li(1)	135.02(15)
C(18)-O(3)-Li(1)	116.45(14)
O(1)-C(1)-C(6)	119.40(15)
O(1)-C(1)-C(2)	123.05(14)
C(6)-C(1)-C(2)	117.55(15)
C(3)-C(2)-C(1)	117.47(16)
C(3)-C(2)-C(7)	121.56(15)
C(1)-C(2)-C(7)	120.97(14)

C(4)-C(3)-C(2)	123.14(18)
C(5)-C(4)-C(3)	119.37(18)
C(4)-C(5)-C(6)	119.32(18)
C(5)-C(6)-C(1)	123.14(18)
C(2)-C(7)-C(8)	110.17(15)
C(2)-C(7)-C(9)	110.11(14)
C(8)-C(7)-C(9)	109.48(16)
C(2)-C(7)-C(10)	112.14(15)
C(8)-C(7)-C(10)	107.44(16)
C(9)-C(7)-C(10)	107.41(16)
O(2)-C(11)-C(12)	104.64(18)
C(11)-C(12)-C(13)	102.32(18)
C(14)-C(13)-C(12)	103.37(17)
O(2)-C(14)-C(13)	108.42(18)
O(3)-C(15)-C(16)	106.47(18)
C(17)-C(16)-C(15)	103.70(19)
C(16)-C(17)-C(18)	101.83(18)
O(3)-C(18)-C(17)	105.14(17)

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

Table S6.4. Anisotropic displacement parameters (A^2 x 10^3) for **6**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	53(2)	34(1)	42(2)	-3(1)	15(1)	-3(1)
O(1)	52(1)	24(1)	48(1)	-2(1)	18(1)	-2(1)
O(2)	97(1)	57(1)	45(1)	-10(1)	30(1)	-13(1)
O(3)	51(1)	54(1)	66(1)	8(1)	5(1)	4(1)
C(1)	39(1)	32(1)	37(1)	-4(1)	8(1)	-3(1)
C(2)	40(1)	30(1)	39(1)	-3(1)	4(1)	2(1)
C(3)	59(1)	35(1)	51(1)	-7(1)	6(1)	9(1)
C(4)	58(1)	73(2)	49(1)	-11(1)	12(1)	25(1)
C(5)	46(1)	81(2)	45(1)	-4(1)	16(1)	6(1)
C(6)	48(1)	54(1)	50(1)	-4(1)	19(1)	-10(1)
C(7)	47(1)	27(1)	65(1)	2(1)	16(1)	-4(1)
C(8)	41(1)	53(1)	94(2)	7(1)	14(1)	-4(1)
C(9)	74(1)	51(1)	63(1)	5(1)	37(1)	-8(1)
C(10)	76(1)	34(1)	105(2)	6(1)	28(1)	-12(1)
C(11)	114(2)	72(2)	50(1)	-7(1)	22(1)	-38(1)
C(12)	104(2)	66(2)	46(1)	-12(1)	2(1)	26(1)
C(13)	79(1)	75(2)	60(1)	-6(1)	29(1)	-1(1)
C(14)	71(1)	60(1)	51(1)	3(1)	19(1)	1(1)
C(15)	61(1)	59(1)	99(2)	14(1)	15(1)	1(1)
C(16)	57(1)	80(2)	111(2)	27(2)	13(1)	5(1)
C(17)	73(1)	63(1)	56(1)	7(1)	9(1)	19(1)
C(18)	62(1)	64(1)	63(1)	21(1)	5(1)	2(1)

Table S6.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6**.

	x	y	z	U(eq)
H(3)	4055	3960	5300	60
H(4)	2078	3652	5972	72
H(5)	1422	2135	6182	67
H(6)	2732	952	5706	60
H(8A)	7634	2750	5934	95
H(8B)	8257	2632	5009	95
H(8C)	7360	1822	5337	95
H(9A)	5553	1797	3644	89
H(9B)	6488	2600	3338	89
H(9C)	4739	2714	3196	89
H(10A)	5250	4191	4148	107
H(10B)	6980	4036	4249	107
H(10C)	6408	4201	5188	107
H(11A)	5940	1613	7142	94
H(11B)	7195	1115	7969	94
H(12A)	4192	1489	8002	90
H(12B)	5676	1689	8849	90
H(13A)	5979	188	9283	83
H(13B)	4192	212	8913	83
H(14A)	5890	-804	8102	72
H(14B)	4189	-563	7588	72
H(15A)	9529	915	6653	89
H(15B)	9461	459	5629	89
H(16A)	11603	-237	6429	101
H(16B)	11269	-88	7459	101
H(17A)	10772	-1611	7247	78
H(17B)	10117	-1503	6099	78
H(18A)	7958	-1528	6588	79
H(18B)	8700	-970	7555	79

$[Li_2(DBP)_2(THF)]_2$ (7)

Experimental. A colorless crystal was mounted on a thin glass fiber from a pool of Fluorolube™ HO-125 and then immediately placed under a liquid N_2 stream on a Bruker AXS diffractometer. The radiation used was graphite monochromatized Mo Kα radiation (λ=0.71073 A). The lattice parameters were optimized from a least-squares calculation on 68 carefully centered reflections. Lattice determination and data collection were carried out using SMART Version 5.054 software. Data reduction was performed using SAINT+ 6.01 software. Structure solution was performed using SHELXTL 5.1 software. The structure refinement was performed using XSHELL 3.0 software. No absorption correction was performed due to the low absorption of the crystal. Data collection parameters are given in Table 1.

Structure Solution and Refinement. The structure was solved in the space group P2(1)/n using direct methods. This solution yielded the positions of the Li, O, and C atoms as Q peaks. The hydrogen atoms were fixed in positions of ideal geometry and refined within the XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms they were bonded to. The final refinement included anisotropic thermal parameters on all non-hydrogen atoms and converged to R1=0.0576 and R2w=0.1289

Table S7.1. Crystal data and structure refinement for **7**.

Empirical formula	C36 H58 Li2 N0 O4
Formula weight	568.70
Temperature	168(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.483(3) A alpha = 90 deg. b = 14.693(4) A beta = 107.993(4) deg. c = 20.207(5) A gamma = 90 deg.
Volume	3524.9(15) A^3
Z, Calculated density	4, 1.072 Mg/m^3
Absorption coefficient	0.066 mm^-1
F(000)	1248
Crystal size	.4 x .2 x .4mm
Theta range for data collection	1.72 to 28.51 deg.
Limiting indices	-14<=h<=16, -19<=k<=15, -26<=l<=24
Reflections collected / unique	22139 / 8264 [R(int) = 0.0767]
Completeness to theta = 28.51	92.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8264 / 0 / 391
Goodness-of-fit on F^2	0.833
Final R indices [I>2sigma(I)]	R1 = 0.0576, wR2 = 0.1289
R indices (all data)	R1 = 0.1714, wR2 = 0.1673
Largest diff. peak and hole	0.284 and -0.270 e.A^-3

Table S7.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	4532(4)	10214(3)	408(2)	53(1)
Li(2)	115(4)	5746(3)	253(2)	50(1)
C(1)	6531(2)	8964(2)	970(1)	37(1)
C(2)	7570(2)	9354(2)	1397(1)	42(1)
C(3)	8349(2)	8787(2)	1845(1)	50(1)
C(4)	8170(2)	7870(2)	1893(1)	52(1)
C(5)	7173(2)	7492(2)	1487(1)	47(1)
C(6)	6346(2)	8010(2)	1023(1)	37(1)
C(7)	7802(2)	10385(2)	1399(1)	50(1)
C(8)	8985(2)	10638(2)	1885(2)	80(1)
C(9)	6952(2)	10908(2)	1672(1)	60(1)
C(10)	7760(2)	10727(2)	674(2)	64(1)
C(11)	5238(2)	7547(2)	604(1)	41(1)
C(12)	4262(2)	7924(2)	834(1)	54(1)
C(13)	4997(2)	7684(2)	-184(1)	50(1)
C(14)	5267(2)	6511(2)	724(1)	57(1)
C(15)	732(2)	4101(1)	1234(1)	34(1)
C(16)	1878(2)	3820(2)	1499(1)	36(1)
C(17)	2154(2)	3183(2)	2037(1)	47(1)
C(18)	1376(2)	2842(2)	2332(1)	52(1)
C(19)	290(2)	3158(2)	2104(1)	44(1)
C(20)	-62(2)	3790(2)	1568(1)	37(1)
C(21)	2795(2)	4228(2)	1221(1)	46(1)
C(22)	3972(2)	3861(2)	1610(1)	67(1)
C(23)	2844(2)	5263(2)	1331(1)	55(1)
C(24)	2587(2)	4013(2)	445(1)	54(1)
C(25)	-1282(2)	4150(2)	1354(1)	43(1)
C(26)	-1956(2)	3772(2)	1825(2)	64(1)
C(27)	-1928(2)	3846(2)	605(1)	55(1)
C(28)	-1300(2)	5193(2)	1414(1)	49(1)
C(29)	744(3)	7333(2)	1228(1)	74(1)
C(30)	900(3)	8325(2)	1139(2)	81(1)
C(31)	91(3)	8545(2)	460(2)	83(1)
C(32)	-127(4)	7712(2)	74(2)	116(2)
C(33)	3965(3)	10208(3)	1738(2)	107(1)
C(34)	3031(4)	10496(2)	1978(2)	105(1)
C(35)	2125(3)	10783(2)	1343(2)	90(1)
C(36)	2747(2)	11068(2)	871(2)	69(1)
O(1)	5761(1)	9488(1)	526(1)	40(1)
O(2)	402(1)	4642(1)	674(1)	37(1)
O(3)	276(1)	6970(1)	544(1)	54(1)
O(4)	3729(1)	10507(1)	1035(1)	62(1)

Table S7.3. Bond lengths [A] and angles [deg] for **7**.

Li(1)-O(1)	1.822(4)
Li(1)-O(1)#1	1.862(4)
Li(1)-O(4)	1.891(5)
Li(1)-Li(1)#1	2.382(9)
Li(2)-O(2)	1.816(4)
Li(2)-O(2)#2	1.872(4)
Li(2)-O(3)	1.883(4)
Li(2)-Li(2)#2	2.399(8)
C(1)-O(1)	1.337(2)
C(1)-C(6)	1.430(3)
C(1)-C(2)	1.437(3)
C(2)-C(3)	1.383(3)
C(2)-C(7)	1.541(3)
C(3)-C(4)	1.375(3)
C(4)-C(5)	1.379(3)
C(5)-C(6)	1.387(3)
C(6)-C(11)	1.540(3)
C(7)-C(10)	1.535(4)
C(7)-C(8)	1.545(3)
C(7)-C(9)	1.544(4)
C(11)-C(12)	1.535(3)
C(11)-C(13)	1.538(3)
C(11)-C(14)	1.540(3)
C(15)-O(2)	1.339(2)
C(15)-C(16)	1.425(3)
C(15)-C(20)	1.435(3)
C(16)-C(17)	1.394(3)
C(16)-C(21)	1.543(3)
C(17)-C(18)	1.382(3)
C(18)-C(19)	1.371(3)
C(19)-C(20)	1.391(3)
C(20)-C(25)	1.542(3)
C(21)-C(23)	1.536(3)
C(21)-C(22)	1.535(3)
C(21)-C(24)	1.541(3)
C(25)-C(28)	1.539(3)
C(25)-C(27)	1.544(3)
C(25)-C(26)	1.554(3)
C(29)-O(3)	1.426(3)
C(29)-C(30)	1.488(4)
C(30)-C(31)	1.466(4)
C(31)-C(32)	1.432(4)
C(32)-O(3)	1.431(3)
C(33)-O(4)	1.429(3)
C(33)-C(34)	1.457(5)
C(34)-C(35)	1.485(5)
C(35)-C(36)	1.466(4)
C(36)-O(4)	1.428(3)
O(1)-Li(1)#1	1.862(4)
O(2)-Li(2)#2	1.872(4)
O(1)-Li(1)-O(1)#1	99.5(2)
O(1)-Li(1)-O(4)	130.2(2)
O(1)#1-Li(1)-O(4)	130.2(2)

O(1)-Li(1)-Li(1)#1	50.45(16)
O(1)#1-Li(1)-Li(1)#1	49.00(16)
O(4)-Li(1)-Li(1)#1	176.9(4)
O(2)-Li(2)-O(2)#2	98.86(19)
O(2)-Li(2)-O(3)	136.1(2)
O(2)#2-Li(2)-O(3)	125.0(2)
O(2)-Li(2)-Li(2)#2	50.43(15)
O(2)#2-Li(2)-Li(2)#2	48.43(15)
O(3)-Li(2)-Li(2)#2	173.3(3)
O(1)-C(1)-C(6)	121.09(19)
O(1)-C(1)-C(2)	120.1(2)
C(6)-C(1)-C(2)	118.85(19)
C(3)-C(2)-C(1)	118.3(2)
C(3)-C(2)-C(7)	119.7(2)
C(1)-C(2)-C(7)	121.86(19)
C(4)-C(3)-C(2)	122.7(2)
C(5)-C(4)-C(3)	119.2(2)
C(4)-C(5)-C(6)	121.9(2)
C(5)-C(6)-C(1)	119.0(2)
C(5)-C(6)-C(11)	119.0(2)
C(1)-C(6)-C(11)	121.99(19)
C(10)-C(7)-C(2)	111.6(2)
C(10)-C(7)-C(8)	105.8(2)
C(2)-C(7)-C(8)	112.3(2)
C(10)-C(7)-C(9)	110.7(2)
C(2)-C(7)-C(9)	109.9(2)
C(8)-C(7)-C(9)	106.3(2)
C(12)-C(11)-C(13)	110.25(19)
C(12)-C(11)-C(14)	106.9(2)
C(13)-C(11)-C(14)	106.30(19)
C(12)-C(11)-C(6)	109.61(19)
C(13)-C(11)-C(6)	111.52(19)
C(14)-C(11)-C(6)	112.08(19)
O(2)-C(15)-C(16)	120.1(2)
O(2)-C(15)-C(20)	120.6(2)
C(16)-C(15)-C(20)	119.4(2)
C(17)-C(16)-C(15)	117.7(2)
C(17)-C(16)-C(21)	120.8(2)
C(15)-C(16)-C(21)	121.4(2)
C(18)-C(17)-C(16)	122.9(2)
C(19)-C(18)-C(17)	119.0(2)
C(18)-C(19)-C(20)	122.0(2)
C(19)-C(20)-C(15)	118.7(2)
C(19)-C(20)-C(25)	119.6(2)
C(15)-C(20)-C(25)	121.7(2)
C(23)-C(21)-C(22)	106.5(2)
C(23)-C(21)-C(16)	109.5(2)
C(22)-C(21)-C(16)	112.2(2)
C(23)-C(21)-C(24)	109.7(2)
C(22)-C(21)-C(24)	106.5(2)
C(16)-C(21)-C(24)	112.36(19)
C(28)-C(25)-C(27)	110.44(19)
C(28)-C(25)-C(20)	110.84(18)
C(27)-C(25)-C(20)	110.34(19)
C(28)-C(25)-C(26)	106.5(2)
C(27)-C(25)-C(26)	106.2(2)
C(20)-C(25)-C(26)	112.4(2)

O(3)-C(29)-C(30)	106.2(2)
C(31)-C(30)-C(29)	104.5(2)
C(32)-C(31)-C(30)	106.3(2)
C(31)-C(32)-O(3)	108.7(3)
O(4)-C(33)-C(34)	107.6(3)
C(33)-C(34)-C(35)	105.6(3)
C(36)-C(35)-C(34)	103.2(3)
O(4)-C(36)-C(35)	105.9(2)
C(1)-O(1)-Li(1)	145.74(19)
C(1)-O(1)-Li(1)#1	133.69(19)
Li(1)-O(1)-Li(1)#1	80.5(2)
C(15)-O(2)-Li(2)	153.00(18)
C(15)-O(2)-Li(2)#2	125.85(17)
Li(2)-O(2)-Li(2)#2	81.14(19)
C(29)-O(3)-C(32)	108.2(2)
C(29)-O(3)-Li(2)	129.2(2)
C(32)-O(3)-Li(2)	122.5(2)
C(33)-O(4)-C(36)	107.9(2)
C(33)-O(4)-Li(1)	127.3(2)
C(36)-O(4)-Li(1)	124.82(19)

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

Table S7.4. Anisotropic displacement parameters (A^2 x 10^3) for 7.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Li(1)	51(3)	66(3)	47(3)	9(2)	20(2)	15(2)
Li(2)	57(3)	43(2)	47(3)	-3(2)	12(2)	2(2)
C(1)	30(1)	46(2)	36(1)	1(1)	11(1)	5(1)
C(2)	34(1)	43(2)	46(2)	0(1)	8(1)	2(1)
C(3)	32(1)	57(2)	53(2)	3(1)	1(1)	1(1)
C(4)	38(2)	51(2)	60(2)	12(1)	6(1)	9(1)
C(5)	44(2)	41(2)	54(2)	5(1)	13(1)	4(1)
C(6)	32(1)	43(2)	37(1)	-1(1)	12(1)	1(1)
C(7)	42(2)	45(2)	57(2)	1(1)	7(1)	-1(1)
C(8)	57(2)	55(2)	107(3)	0(2)	-4(2)	-11(2)
C(9)	66(2)	50(2)	59(2)	-8(1)	12(2)	3(1)
C(10)	71(2)	50(2)	76(2)	7(2)	31(2)	-9(1)
C(11)	37(2)	45(2)	41(1)	3(1)	14(1)	-2(1)
C(12)	40(2)	73(2)	51(2)	0(1)	16(1)	-6(1)
C(13)	52(2)	53(2)	45(2)	-5(1)	15(1)	-6(1)
C(14)	53(2)	54(2)	62(2)	5(1)	13(1)	-13(1)
C(15)	39(1)	32(1)	29(1)	-3(1)	6(1)	-4(1)
C(16)	37(1)	41(1)	28(1)	-5(1)	6(1)	0(1)
C(17)	45(2)	53(2)	38(1)	0(1)	5(1)	10(1)
C(18)	64(2)	46(2)	42(2)	14(1)	9(1)	9(1)
C(19)	50(2)	43(2)	39(1)	6(1)	13(1)	-3(1)
C(20)	40(1)	33(1)	32(1)	-5(1)	6(1)	-4(1)
C(21)	32(1)	62(2)	41(1)	-3(1)	7(1)	3(1)
C(22)	39(2)	105(2)	55(2)	2(2)	9(1)	5(2)
C(23)	47(2)	65(2)	56(2)	-7(1)	19(1)	-15(1)
C(24)	47(2)	72(2)	43(2)	0(1)	16(1)	7(1)
C(25)	37(1)	50(2)	41(1)	1(1)	11(1)	-4(1)
C(26)	47(2)	74(2)	74(2)	11(2)	23(2)	-3(2)
C(27)	44(2)	59(2)	56(2)	-4(1)	6(1)	-7(1)
C(28)	43(2)	54(2)	47(2)	-1(1)	12(1)	8(1)
C(29)	111(3)	48(2)	51(2)	-10(1)	7(2)	2(2)
C(30)	98(3)	50(2)	72(2)	-12(2)	-8(2)	-2(2)
C(31)	113(3)	50(2)	67(2)	-2(2)	0(2)	2(2)
C(32)	172(4)	37(2)	88(3)	-1(2)	-33(2)	17(2)
C(33)	101(3)	188(4)	38(2)	35(2)	29(2)	61(3)
C(34)	190(4)	79(2)	78(3)	19(2)	88(3)	23(3)
C(35)	84(3)	65(2)	146(4)	8(2)	74(3)	3(2)
C(36)	53(2)	91(2)	60(2)	1(2)	17(2)	26(2)
O(1)	35(1)	44(1)	38(1)	5(1)	9(1)	6(1)
O(2)	38(1)	40(1)	31(1)	3(1)	7(1)	0(1)
O(3)	68(1)	37(1)	46(1)	-4(1)	2(1)	1(1)
O(4)	56(1)	96(1)	38(1)	14(1)	18(1)	30(1)

Table S7.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(3)	9035	9043	2130	60
H(4)	8728	7500	2203	62
H(5)	7049	6859	1525	56
H(8A)	9104	11294	1858	120
H(8B)	9557	10307	1741	120
H(8C)	9043	10472	2365	120
H(9A)	6183	10766	1381	90
H(9B)	7085	11564	1655	90
H(9C)	7047	10726	2153	90
H(10A)	7003	10632	349	96
H(10B)	8309	10390	511	96
H(10C)	7943	11377	698	96
H(12A)	4389	7778	1325	81
H(12B)	3553	7649	551	81
H(12C)	4222	8586	771	81
H(13A)	4830	8327	-300	75
H(13B)	4350	7311	-437	75
H(13C)	5659	7502	-315	75
H(14A)	5918	6250	618	86
H(14B)	4574	6237	421	86
H(14C)	5330	6387	1211	86
H(17)	2910	2974	2207	57
H(18)	1590	2394	2688	63
H(19)	-238	2939	2318	53
H(22A)	4144	3982	2109	101
H(22B)	4532	4163	1436	101
H(22C)	3993	3203	1534	101
H(23A)	2092	5523	1121	83
H(23B)	3370	5530	1112	83
H(23C)	3102	5397	1831	83
H(24A)	2518	3354	373	81
H(24B)	3220	4240	302	81
H(24C)	1890	4310	167	81
H(26A)	-1578	3946	2309	96
H(26B)	-1995	3107	1789	96
H(26C)	-2720	4025	1675	96
H(27A)	-2708	4063	481	83
H(27B)	-1924	3180	578	83
H(27C)	-1564	4102	282	83
H(28A)	-847	5462	1146	73
H(28B)	-986	5370	1904	73
H(28C)	-2077	5412	1232	73
H(29A)	1476	7040	1466	89
H(29B)	229	7230	1507	89
H(30A)	737	8678	1514	97
H(30B)	1680	8457	1144	97
H(31A)	-613	8790	518	100
H(31B)	411	9005	216	100
H(32A)	261	7716	-286	139

H(32B)	-945	7644	-161	139
H(33A)	4678	10481	2033	129
H(33B)	4041	9537	1764	129
H(34A)	3261	11009	2310	126
H(34B)	2772	9988	2212	126
H(35A)	1610	10272	1145	108
H(35B)	1683	11294	1445	108
H(36A)	2283	10979	380	82
H(36B)	2959	11718	942	82