Dimerization upon Deprotonation: Formation of a *m*-Terphenyl substituted (R,S)-dilithium disiloxanolate disilanol†

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†This paper is dedicated to Prof. Dr. Manfred Scheer on the occasion of his 60th birthday

a) Crystallographic details for **6**, **7**, **4**, **4•THF** and **4•DMF** (CCDC 1059825-1059828 and 1062439).

b) MS data

Table S1. Summary of Crystal data for **6,4, 4•THF** and **4•DMF**.

	6	**4**	**4•THF**	**4•DMF**	**7**
Empirical formula	$C_{96}H_{104}Li_4O_{10}Si_4$	$(1-\delta)(C_{48}H_{54}O_5Si_2) \cdot 2\delta(C_{24}H_{25}I)$, $\delta = 0.0512(7)$	$C_{48}H_{54}O_5Si_2 \cdot C_4H_8O$	$C_{48}H_{54}O_5Si_2 \cdot C_3H_7NO$	$C_{96}H_{106}Na_2O_{10}Si_4 \cdot 0.5(C_6H_6)$
Formula weight	1557.91	772.91	839.19	840.18	1617.20
Crystal description	block, colorless	block, colorless	plate, colorless	block, colorless	block, colorless
Crystal size [mm]	0.48 x 0.35 x 0.30	0.36 x 0.34 x 0.30	0.38 x 0.36 x 0.36	0.22 x 0.16 x 0.16	0.06 x 0.10 x 0.12
Crystal system, space group	monoclinic, *I* 2/*a*	monoclinic, P 2_1/c	triclinic, P -1	triclinic, P 1	monoclinic, C2/c
Radiation and λ [Å]	MoK_α, 0.71073	MoK_α, 0.71073	MoK_α, 0.71073	MoK_α, 0.71073	CuK_α, 1.54186
Monochromator	graphite	graphite	graphite	graphite	Graded multilayer mirror
Temperature [K]	95	100	100	100	100
Unit cell dimensions:					
a [Å]	24.160(5)	9.0956(3)	10.6900(4)	11.0238(6)	22.4147(11)
b [Å]	15.240(3)	36.8415(11)	10.9103(4)	11.3839(6)	16.9077(11)
c [Å]	24.342(6)	12.6169(4)	21.4916(7)	11.6765(6)	46.234(2)
α [°]			91.6194(15)	61.913(2)	
β [°]	107.484(17)	101.9490(10)	101.2382(15)	66.372(2)	99.496(4)
γ [°]			113.3622(13)	65.614(2)	
Volume [Å³]	8549(3)	4136.3(2)	2241.41(14)	1137.92(11)	17281.7(16)
Z	4	4	2	1	8
Calculated density	1.210 Mg/m³	1.241 Mg/m³	1.243 Mg/m³	1.226 Mg/m³	1.243 Mg/m³
F(000)	3312	1647	900	450	6888
Linear absorption coefficient μ [mm^{-1}]	0.128	0.205	0.130	0.128	1.212
Absorption correction	empirical	semi-empirical	semi-empirical	semi-empirical	integration
Unit cell determination	$15.49 < \Theta < 16.46°$ 50 reflections used at 95 K	$3.14 < \Theta < 30.05°$ 9972 reflections used at 100 K	$2.27 < \Theta < 30.86°$ 9874 reflections used at 100 K	$2.28 < \Theta < 28.39°$ 7168 reflections used at 100 K	$1.94 < \Theta < 66.26$ 9839 reflections used at 100 K

Diffractometer	mod. Stoe Stadi-4	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Stoe Stadi Vari
Radiation source	sealed tube	sealed tube	sealed tube	sealed tube	sealed tube
Scan type	ω scans	ϕ and ω scans	ϕ and ω scans	ϕ and ω scans	ϕ and ω scans
Θ range for data collection	2.57 to 25.00°	2.36 to 28.00°	1.95 to 30.00°	2.05 to 27.00°	3.9 to 69.0°
Index ranges	-28 ≤ h ≤ 27, -1 ≤ k ≤ 18, -1 ≤ l ≤ 28	-12 ≤ h ≤ 11, -48 ≤ k ≤ 48, -16 ≤ l ≤ 15	-14 ≤ h ≤ 15, -15 ≤ k ≤ 15, -30 ≤ l ≤ 30	-12 ≤ h ≤ 14, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14	-26 ≤ h ≤ 26, -18 ≤ k ≤ 20, -55 ≤ l ≤ 28
Refl. collected / unique	8732 / 7517	37642 / 9822	34198 / 13054	14622 / 8431	35065 / 14942
Significant unique refl.	4841 with I > 2σ(I)	8179 with I > 2σ(I)	10988 with I > 2σ(I)	7511 with I > 2σ(I)	4841 with I > 2σ(I)
R(int), R(sigma)	0.0360, 0.1033	0.0415, 0.0414	0.0218, 0.0244	0.0278, 0.0416	0.157, 0.2261
Completeness to Θ = 26.0°	99.9%	98.4%	99.8%	99.2%	93.5%
Refinement method	full-matrix least-squares on F²	full-matrix least-squares on F²	full-matrix least-squares on F²	full-matrix least-squares on F²	full-matrix least-squares on F²
Data / parameters / restraints	7517 / 553 / 2	9822 / 564 / 5	13054 / 591 / 4	8431 / 589 / 7	14942 / 1079 / 7
Goodness-of-fit on F²	1.013	1.114	1.031	1.023	0.781
Final R indices [I > 2σ(I)]	R1 = 0.0545, wR2 = 0.1054	R1 = 0.0513, wR2 = 0.1122	R1 = 0.0377, wR2 = 0.1010	R1 = 0.0456, wR2 = 0.1168	R1 = 0.0606, wR2 = 0.1474
R indices (all data)	R1 = 0.1027, wR2 = 0.1251	R1 = 0.0624, wR2 = 0.1171	R1 = 0.0467, wR2 = 0.1073	R1 = 0.0540, wR2 = 0.1237	R1 = 0.1108, wR2 = 0.1912
Largest difference peak/hole	0.230 / -0.310 e/Å³	0.347 / -0.320 e/Å³	0.597 / -0.380 e/Å³	0.645 / -0.295 e/Å³	-0.39 / 0.23 e/Å³

X-ray diffraction data of 6. All the measurements were performed using graphite-monochromatized Mo K_α radiation at 95K: $C_{96}H_{104}Li_4O_{10}Si_4$, M_r 1557.91, monoclinic, space group I 2/a, a = 24.160(5)Å, b = 15.240(3)Å, c = 24.342(6)Å, β = 107.484(17)°, V = 8549(3)Å^3, Z = 4, d_{calc} = 1.210g cm^{-3}, μ = 0.128mm^{-1}. A total of 8732 reflections were collected (Θ_{max} = 25.0°), from which 7517 were unique (R_{int} = 0.0360), with 4841 having I > 2σ(I). The structure was solved by direct methods (SHELXS-97) and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/6). The non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints. The H atoms H2 and H5 bonded to the O atoms could be localized as the two strongest peaks in the difference Fourier map and were refined with individual isotropic displacement parameters. The O–H distances were fixed to a bond length of 0.84 Å but no further constraints were applied to these H atoms. The H atoms of the phenyl rings were put at the external bisector of the C–C–C angle at a C–H distance of 0.95Å and common isotropic displacement parameters were refined for the H atoms of the same phenyl group. The H atoms of the methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometry with tetrahedral angles, enabling rotation around the X–C bond, and C–H distances of 0.98Å. For 553 parameters final *R* indices of R1 = 0.0545 and wR^2 = 0.1251 (GOF = 1.013) were obtained. The largest peak in a difference Fourier map was 0.230eÅ^{-3}.

Table S2. Selected bond lengths [Å] and angles [°] for **6**.

Si(1)-O(3)	1.584(2)	O(6)-Si(2)-O(5)	103.41(11)
Si(1)-O(1)	1.6586(16)	O(4)-Si(2)-O(5)	105.10(8)
Si(1)-O(2)	1.678(2)	O(6)-Si(2)-C(41)	112.85(12)
Si(1)-C(11)	1.882(3)	O(4)-Si(2)-C(41)	109.60(12)
Si(2)-O(6)	1.577(2)	O(5)-Si(2)-C(41)	112.94(12)
Si(2)-O(4)	1.6590(16)	Si(1)-O(1)-Si(1)$^{i)}$	119.29(17)
Si(2)-O(5)	1.670(2)	Si(1)-O(2)-Li(2)$^{i)}$	92.67(17)
Si(2)-C(41)	1.893(3)	Si(1)-O(2)-H(2)	116.8(9)
O(2)-Li(2)$^{i)}$	2.092(6)	Si(1)-O(3)-Li(1)	137.4(2)
O(3)-Li(1)	1.856(6)	Si(1)-O(3)-Li(2)	119.9(2)
O(3)-Li(2)	1.901(6)	Li(1)-O(3)-Li(2)	92.0(2)
O(5)-Li(1)$^{i)}$	2.064(6)	Si(2)-O(4)-Si(2)$^{i)}$	119.20(17)
O(6)-Li(2)$^{i)}$	1.858(6)	Si(2)-O(5)-Li(1)$^{i)}$	94.97(18)
O(6)-Li(1)	1.917(6)	Si(2)-O(5)-H(5)	112.6(5)
Li(1)-Li(2)$^{i)}$	2.660(8)	Si(2)-O(6)-Li(2)$^{i)}$	138.4(2)
Li(1)-Li(2)	2.703(8)	Si(2)-O(6)-Li(1)	120.9(2)
		Li(2)$^{i)}$-O(6)-Li(1)	89.6(2)
O(3)-Si(1)-O(1)	112.85(11)	O(3)-Li(1)-O(6)	110.2(3)
O(3)-Si(1)-O(2)	103.58(10)	O(3)-Li(1)-O(5)$^{i)}$	121.7(3)
O(1)-Si(1)-O(2)	104.97(8)	O(6)-Li(1)-O(5)$^{i)}$	111.8(3)
O(3)-Si(1)-C(11)	110.57(12)	O(6)$^{i)}$-Li(2)-O(3)	110.2(3)
O(1)-Si(1)-C(11)	111.40(12)	O(3)-Li(2)-O(2)$^{i)}$	113.1(3)
O(2)-Si(1)-C(11)	113.15(12)	O(6)$^{i)}$-Li(2)-O(2)$^{i)}$	123.4(3)
O(6)-Si(2)-O(4)	112.60(11)		

$^{i)}$ 0.5-x, y, 1-z

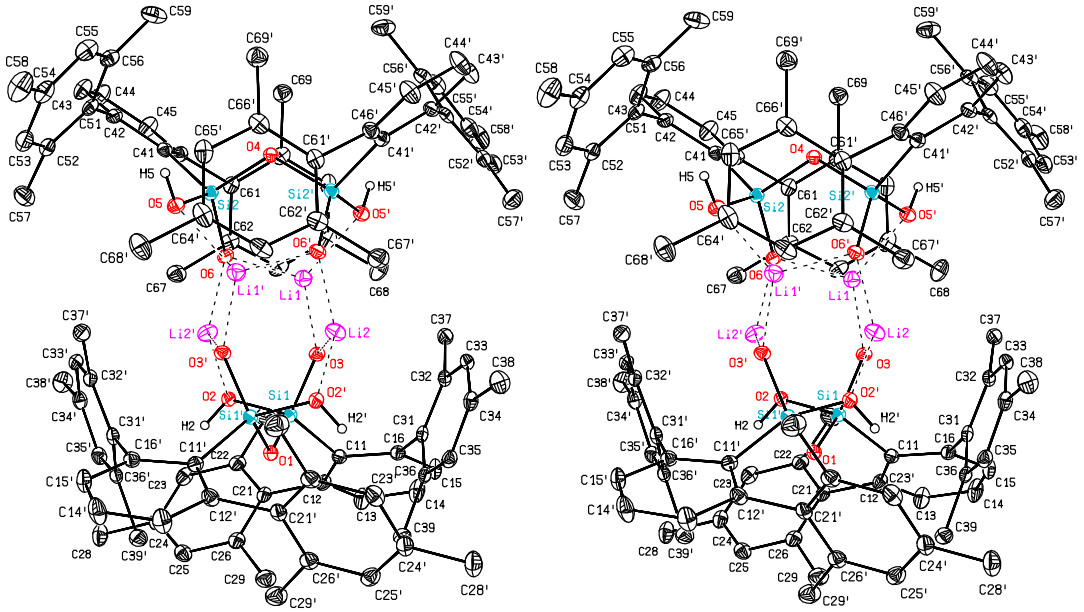


Figure S1. Stereoscopic ORTEP plot of **6** showing the atomic numbering scheme. The probability ellipsoids are drawn at the 30% probability level and the H atoms of the phenyl rings and of the methyl groups were omitted for clarity reasons. The shortest contacts between the Li atoms and the O atoms were plotted with dashed lines.

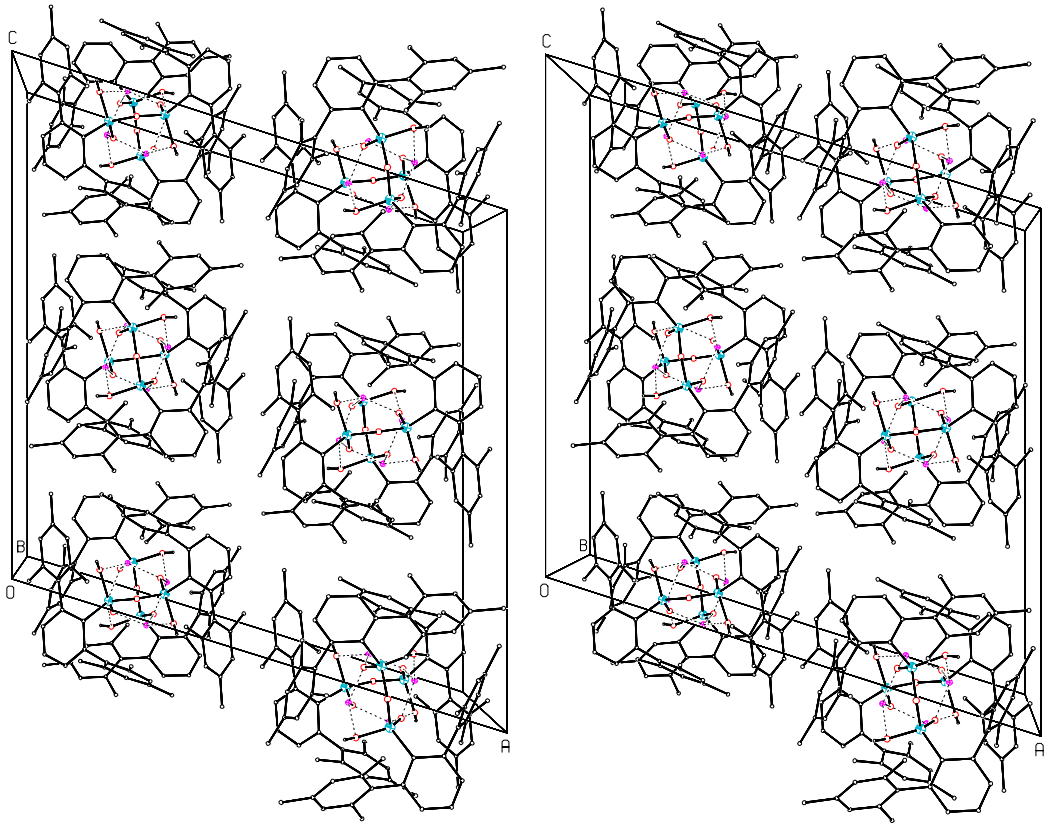


Figure S2. Stereoscopic ORTEP plot of the packing of **6** viewed along the monoclinic axis. The atoms are drawn with arbitrary radii. The H atoms of the phenyl rings and of the methyl groups were omitted for clarity reasons. The shortest contacts between the Li atoms and the O atoms were plotted with dashed lines.

X-ray diffraction data of 4. All the measurements were performed using graphite-monochromatized Mo K_α radiation at 100K: $(1\text{-}\delta)(C_{48}H_{54}O_5Si_2) \cdot 2\delta(C_{24}H_{25}I)$, δ = 0.0512(7), M_r 772.91, monoclinic, space group P $2_1/c$, a = 9.0956(3)Å, b = 36.8415(11)Å, c = 12.6169(4)Å, β = 101.9490(10)°, V = 4136.3(2)Å^3, Z = 4, d_{calc} = 1.241g cm^{-3}, μ = 0.205mm^{-1}. A total of 37642 reflections were collected (Θ_{max} = 28.0°), from which 9822 were unique (R_{int} = 0.0415), with 8179 having I > 2σ(I). The structure was solved by direct methods (SHELXS-97)[2] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/6)[2]. Since in the crystal under investigation about 5% of the 1,1,3,3-disiloxanetetrol bridges between two terphenyl ligands are substituted by two iodine atoms, site occupation factors SOF1 and 1-SOF1 were refined for the 1,1,3,3-disiloxanetetrol fragment and for the I atoms, respectively. The parameter SOF1 refined to 0.9488(7), the site occupation factors of the atoms of the terphenyl ligands were fixed at unity. The non-hydrogen atoms were refined with anisotropic displacement parameters without any further constraints. All the H atoms of OH groups could be localized in a difference Fourier map. The H atoms of the OH group O22 are disordered over two sites and were refined with site occupation factors of 0.5 with a common isotropic displacement parameter. The other H atoms of the OH groups were refined with individual isotropic displacement parameters. The O–H distances were fixed to a bond length of 0.84Å but no further constraints were applied to these H atoms. The H atoms of the phenyl rings were put at the external bisector of the C–C–C angle at a C–H distance of 0.95Å and common isotropic displacement parameters were refined for the H atoms of the same phenyl group. The H atoms of the methyl group C67 are disordered over two orientations and were refined with site occupation factors of 0.5 at two positions rotated from each other by 60° with common isotropic displacement parameters for the H atoms and idealized geometry with tetrahedral angles, enabling rotation around the C–C bond, and C–H distances of 0.98Å. The H atoms of the other methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometry with tetrahedral angles, enabling rotation around the C–C bond, and C–H distances of 0.98Å. For 564 parameters final *R* indices of R1 = 0.0513 and wR^2 = 0.1171 (GOF = 1.114) were obtained. The largest peak in a difference Fourier map was 0.347eÅ^{-3}.

Table S3. Selected bond lengths [Å] and angles [°] for **4**.

O(1)-Si(1)	1.6405(16)	O(11)-Si(1)-C(11)	110.40(8)
O(1)-Si(2)	1.6419(14)	O(1)-Si(1)-C(11)	111.75(8)
Si(1)-O(12)	1.6161(15)	O(22)-Si(2)-O(21)	107.04(10)
Si(1)-O(11)	1.6250(14)	O(22)-Si(2)-O(1)	110.53(8)
Si(1)-C(11)	1.8982(17)	O(21)-Si(2)-O(1)	104.76(8)
Si(2)-O(22)	1.6161(18)	O(22)-Si(2)-C(41)	110.27(8)
Si(2)-O(21)	1.6209(16)	O(21)-Si(2)-C(41)	114.49(8)
Si(2)-C(41)	1.8946(17)	O(1)-Si(2)-C(41)	109.60(8)

Si(1)-O(1)-Si(2)	137.58(9)	O(12)-Si(1)-C(11)-C(12)	3.42(18)
O(12)-Si(1)-O(11)	108.29(9)	O(12)-Si(1)-C(11)-C(16)	-176.91(14)
O(12)-Si(1)-O(1)	106.00(8)	O(21)-Si(2)-C(41)-C(46)	4.15(19)
O(11)-Si(1)-O(1)	108.19(8)	O(21)-Si(2)-C(41)-C(42)	-179.91(14)
O(12)-Si(1)-C(11)	112.01(8)		

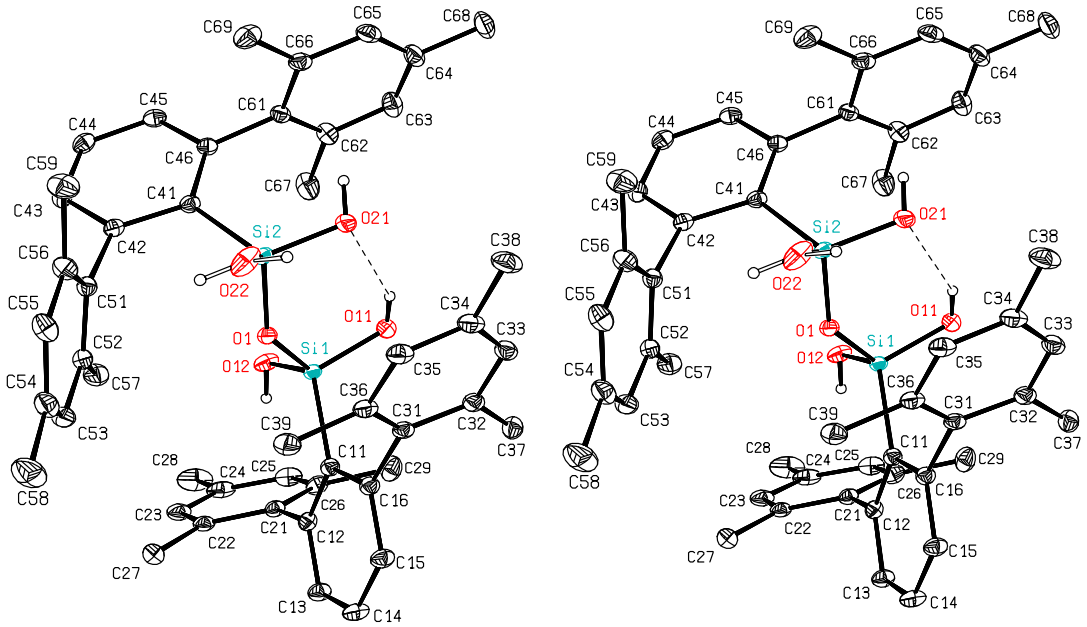


Figure S3. Stereoscopic ORTEP plot of **4** showing the atomic numbering scheme. The probability ellipsoids are drawn at the 30% probability level and the H atoms of the phenyl rings and of the methyl groups as well as the I atoms [s.o.f. of 0.0512(7)] were omitted for clarity reasons. The disordered H atoms are plotted with open bonds and the hydrogen bond with a dashed line.

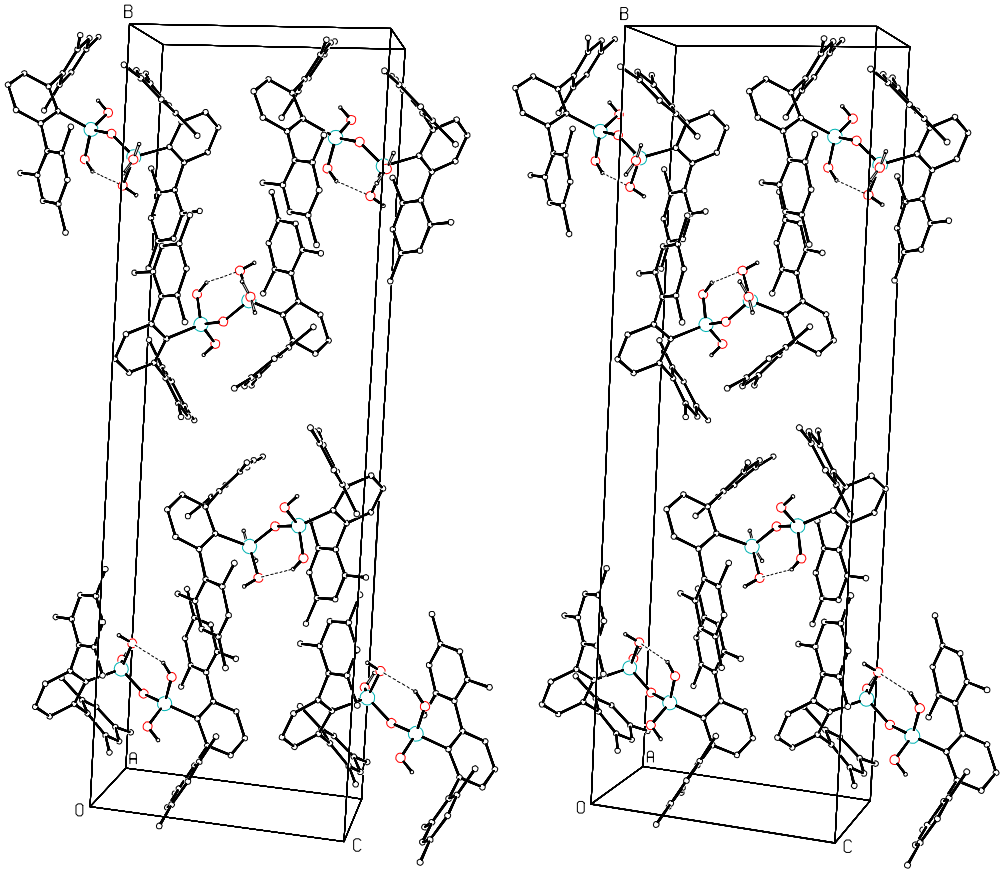


Figure S4. Stereoscopic ORTEP plot of the packing of **4**. The atoms and bonds are drawn as in Fig. S3 but with arbitrary atomic radii.

X-ray diffraction data of 4·THF. All the measurements were performed using graphite-monochromatized Mo K_α radiation at 100 K: $C_{48}H_{54}O_5Si_2 \cdot C_4H_8O$, M_r 839.19, triclinic, space group P -1, a = 10.6900(4)Å, b = 10.9103(4)Å, c = 21.4916(7)Å, α = 91.6194(15)°, β = 101.2382(15)°, γ = 113.3622(13)°, V = 2241.41(14)Å^3, Z = 2, d_{calc} = 1.243g cm^{-3}, μ = 0.130mm^{-1}. A total of 34198 reflections were collected (Θ_{max} = 30.0°), from which 13054 were unique (R_{int} = 0.0218), with 10988 having I > 2σ(I). The structure was solved by direct methods (SHELXS-97)[2] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/6)[2]. The non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints. The H atoms of the OH groups could be localized in a difference Fourier map and were refined with individual isotropic displacement parameters. Only the O–H bond lengths were fixed to 0.84Å, no angular or conformational constraints were applied. The H atoms of the phenyl rings were put at the external bisectors of the C–C–C angles at C–H distances of 0.95Å and common isotropic displacement parameters were refined for the H atoms of the same phenyl group. The H atoms of the methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometries with tetrahedral angles, enabling rotation around the C–C bond, and C–H distances of 0.98Å. The H atoms of the CH_2 groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometry with approximately tetrahedral angles and C–H distances of 0.99Å. For 591 parameters final *R* indices of R1 = 0.0377 and wR^2 = 0.1073 (GOF = 1.031) were obtained. The largest peak in a difference Fourier map was 0.597eÅ^{-3}.

Table S4. Selected bond lengths [Å] and angles [°] for **4•THF**.

O(1)-Si(2)	1.6298(8)
O(1)-Si(1)	1.6333(8)
Si(1)-O(11)	1.6070(9)
Si(1)-O(12)	1.6344(10)
Si(1)-C(11)	1.8852(11)
Si(2)-O(21)	1.6228(9)
Si(2)-O(22)	1.6331(9)
Si(2)-C(41)	1.8918(10)
Si(2)-O(1)-Si(1)	136.22(5)
O(11)-Si(1)-O(1)	110.72(5)
O(11)-Si(1)-O(12)	110.88(6)
O(1)-Si(1)-O(12)	102.90(5)
O(11)-Si(1)-C(11)	109.62(5)
O(1)-Si(1)-C(11)	110.53(4)
O(12)-Si(1)-C(11)	112.04(5)
O(21)-Si(2)-O(1)	110.60(4)
O(21)-Si(2)-O(22)	101.56(5)
O(1)-Si(2)-O(22)	109.53(4)
O(21)-Si(2)-C(41)	114.46(4)
O(1)-Si(2)-C(41)	109.09(4)
O(22)-Si(2)-C(41)	111.37(4)

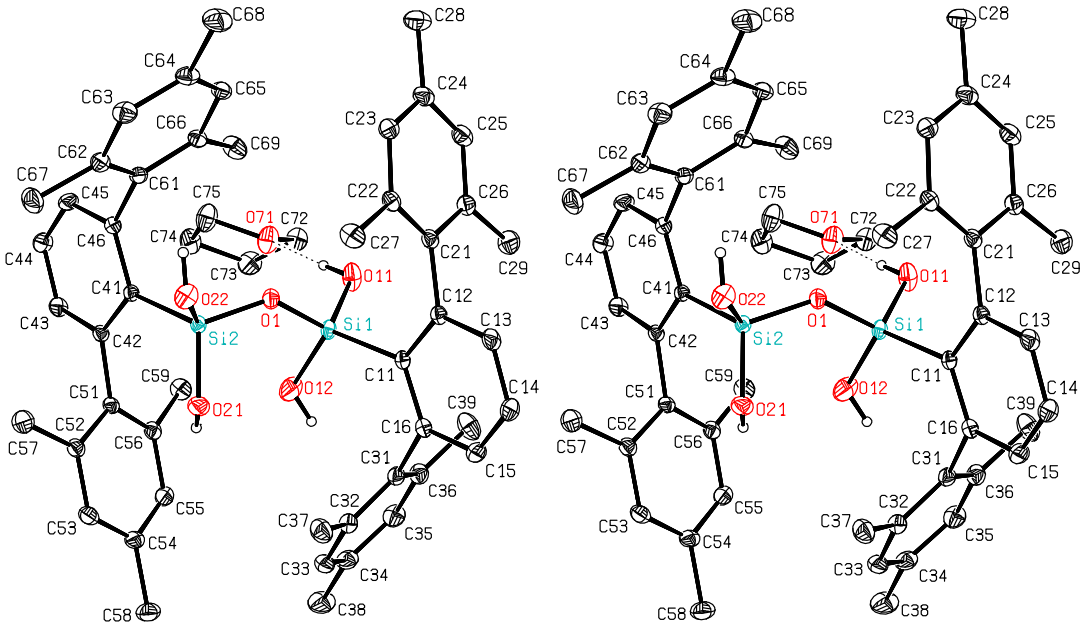


Figure S5. Stereoscopic ORTEP plot of **4•THF** showing the atomic numbering scheme. The probability ellipsoids are drawn at the 50% probability level. The H atoms of the phenyl rings and of the methyl groups were omitted for clarity reasons, the other H atoms were drawn with arbitrary radii. The hydrogen bond is indicated by a dashed line.

X-ray diffraction data of 4•DMF. All the measurements were performed using graphite-monochromatized MoK_α radiation at 100K: $C_{48}H_{54}O_5Si_2 \cdot C_3H_7NO$, M_r 840.18, triclinic, space group P 1, a = 11.0238(6)Å, b = 11.3839(6)Å, c = 11.6765(6)Å, α = 61.913(2)°, β = 66.372(2)°, γ = 65.614(2)°, V = 1137.92(11)Å^3, Z = 1, d_{calc} = 1.226g cm^{-3}, μ = 0.128mm^{-1}. A total of 14622 reflections were collected (Θ_{max} = 27.0°), from which 8431 were unique (R_{int} = 0.0278), with 7511 having I > 2σ(I). The structure was solved by direct methods (SHELXS-97)[2] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/6)[2]. The non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints. The H atoms of OH groups could be localized in a difference Fourier map and were refined with a common isotropic displacement parameter. The O–H distances were fixed to a bond length of 0.84Å but no further constraints were applied to these H atoms. The H atoms of the phenyl rings were put at the external bisectors of the C–C–C angles at C–H distances of 0.95Å and common isotropic displacement parameters were refined for the H atoms of the same ring. The H atoms of the methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometries with tetrahedral angles, enabling rotation around the C–C bond, and C–H distances of 0.98Å. For 589 parameters final *R* indices of R1 = 0.0456 and wR^2 = 0.1237 (GOF = 1.023) were obtained. The largest peak in a difference Fourier map was 0.645eÅ^{-3}.

Table S5. Selected bond lengths [Å] and angles [°] for **4•DMF**.

Si(1)-O(11)	1.590(3)
Si(1)-O(1)	1.622(3)
Si(1)-O(12)	1.646(3)
Si(1)-C(11)	1.882(3)
Si(2)-O(21)	1.606(3)
Si(2)-O(22)	1.628(3)
Si(2)-O(1)	1.641(3)
Si(2)-C(41)	1.886(4)
O(71)-C(71)	1.231(5)

O(11)-Si(1)-O(1)	113.74(15)
O(11)-Si(1)-O(12)	112.51(18)
O(1)-Si(1)-O(12)	99.72(15)
O(11)-Si(1)-C(11)	108.50(16)
O(1)-Si(1)-C(11)	110.44(14)
O(12)-Si(1)-C(11)	111.79(16)
O(21)-Si(2)-O(22)	101.25(17)
O(21)-Si(2)-O(1)	111.82(16)
O(22)-Si(2)-O(1)	107.15(16)
O(21)-Si(2)-C(41)	115.17(17)
O(22)-Si(2)-C(41)	112.15(16)
O(1)-Si(2)-C(41)	108.89(15)

Si(1)-O(1)-Si(2)	132.35(17)
O(11)-Si(1)-O(1)-Si(2)	131.8(2)
O(12)-Si(1)-O(1)-Si(2)	11.8(3)
C(11)-Si(1)-O(1)-Si(2)	-106.0(2)
O(21)-Si(2)-O(1)-Si(1)	37.9(3)
O(22)-Si(2)-O(1)-Si(1)	148.0(2)
C(41)-Si(2)-O(1)-Si(1)	-90.5(2)
O(11)-Si(1)-C(11)-C(12)	71.7(3)
O(11)-Si(1)-C(11)-C(16)	-110.8(3)
O(12)-Si(1)-C(11)-C(12)	-163.7(3)
O(12)-Si(1)-C(11)-C(16)	13.8(3)
O(1)-Si(1)-C(11)-C(12)	-53.6(3)
O(1)-Si(1)-C(11)-C(16)	123.9(3)
O(21)-Si(2)-C(41)-C(42)	-21.0(4)
O(21)-Si(2)-C(41)-C(46)	162.2(3)
O(22)-Si(2)-C(41)-C(42)	-136.1(3)
O(22)-Si(2)-C(41)-C(46)	47.1(3)
O(1)-Si(2)-C(41)-C(42)	105.5(3)
O(1)-Si(2)-C(41)-C(46)	-71.3(3)
C(72)-N(71)-C(71)-O(71)	-173.8(5)
C(73)-N(71)-C(71)-O(71)	-2.2(8)

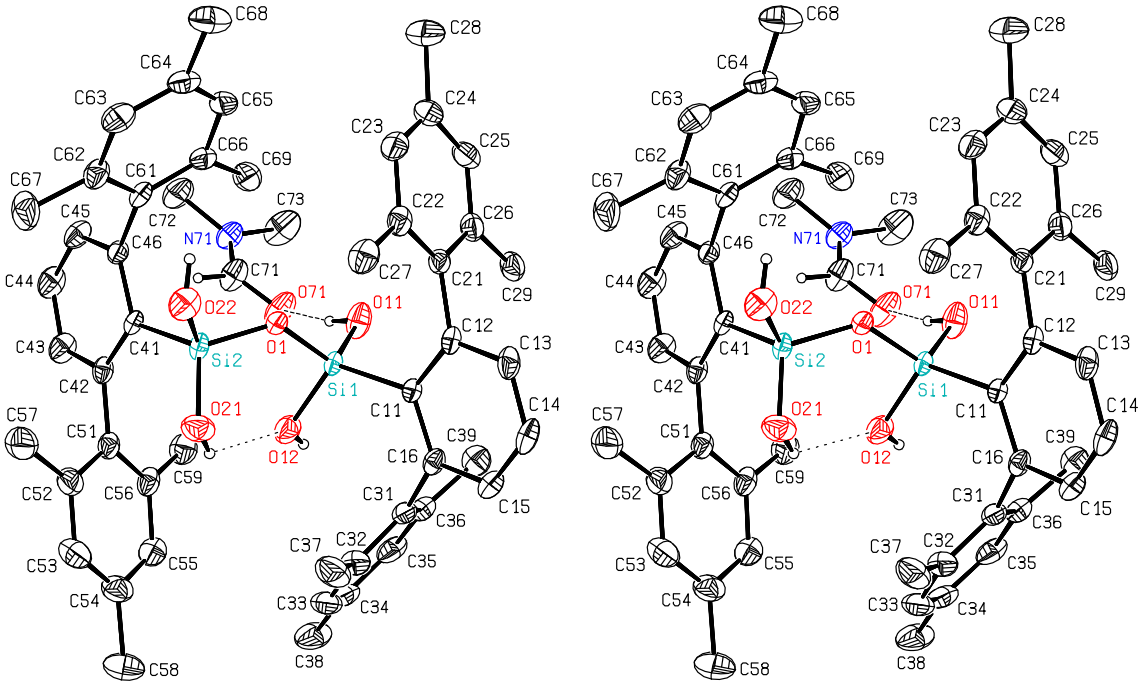


Figure S6. Stereoscopic ORTEP plot of **4•DMF** showing the atomic numbering scheme. The probability ellipsoids are drawn at the 50% probability level. The H atoms of the phenyl rings and of the methyl groups were omitted for clarity reasons, the other H atoms were drawn with arbitrary radii. The hydrogen bonds are indicated by dashed lines.

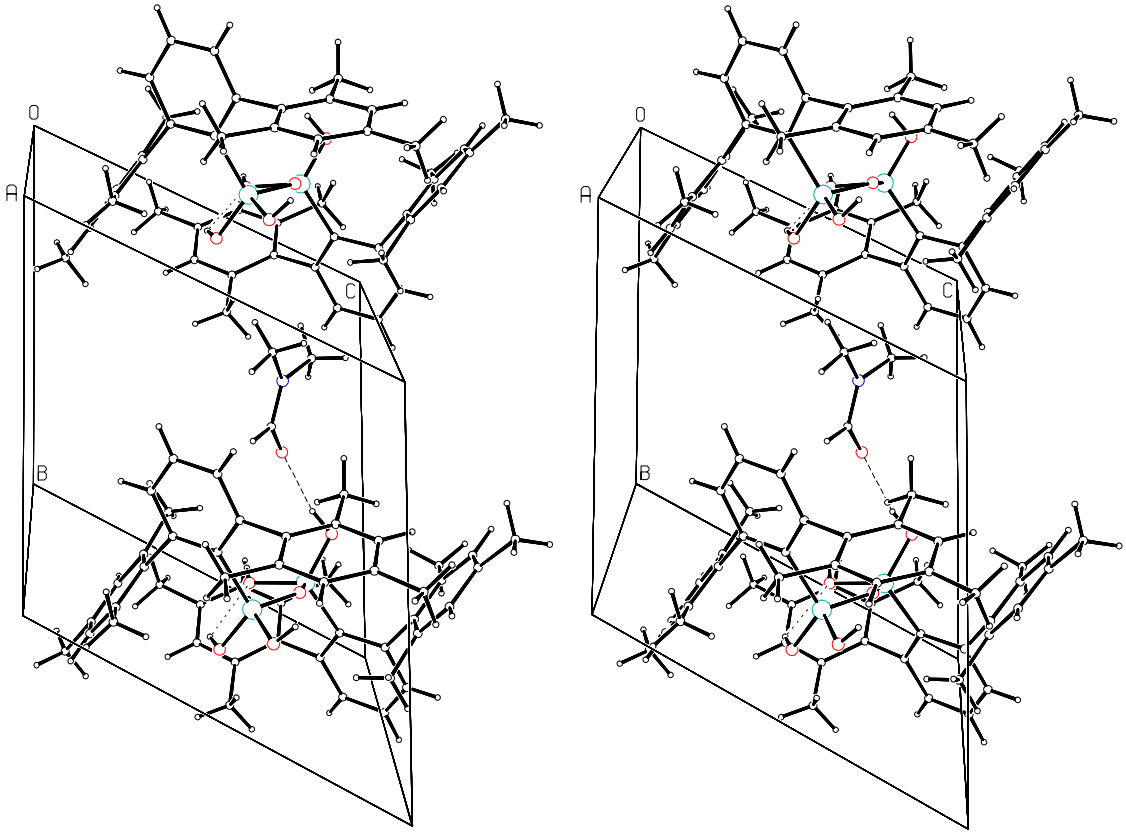


Figure S7. Stereoscopic ORTEP plot of the packing of **4•DMF**. The atoms are drawn with arbitrary radii. The hydrogen bonds are indicated by dashed lines.

X-ray diffraction data of 7

The measurements were performed using graded multilayer mirror monochromatized CuK_α radiation at 100 K: $C_{96}H_{106}Na_2O_{10}Si_4 \cdot 0.5(C_6H_6)$, M_r 1617.20, monoclinic, space group C2/c, a = 22.4147(11) Å, b = 16.9077(11) Å, c = 46.234(2) Å, α = 90°, β = 99.496(4)°, γ = 90°, V =17281.7(16) Å^3, Z = 8, d_{calc} = 1.243 g cm^{-3}, μ = 1.212 mm^{-1}. A total of 35065 reflections were collected (Θ_{max} = 69.0°), from which 14942 were unique (R_{int} = 0.157), with 4841 having I > 2σ(I). The structure was solved by direct methods (SHELXS-97) and refined by full-matrix least-squares techniques against F^2 (SHELXL-2014/6). The non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints. The H atoms of OH groups could be localized in a difference Fourier map and were refined with a common isotropic displacement parameter. For 1079 parameters final *R* indices of R1 = 0.0606 and wR^2 = 0.1912 (GOF = 0.781) were obtained. The largest peak in a difference Fourier map was 0.23 eÅ^{-3}.

Table S8. Selected bond lengths [Å] and angles [°] for **7**.

Si1	-O1	1.666(4)	O9	-H9	0.97(3)		
Si1	-O2	1.592(4)	O10	-H10	0.97(4)		
Si1	-O3	1.639(4)	C1	-C2	1.430(8)		
Si1	-C1	1.889(5)	C1	-C6	1.417(8)		
Si2	-O1	1.636(4)	C2	-C3	1.406(8)		
Si2	-O4	1.596(4)	C2	-C7	1.478(8)		
Si2	-O5	1.650(4)	C3	-C4	1.370(9)		
Si2	-C25	1.867(5)	C4	-C5	1.365(9)		
Si3	-O6	1.655(4)	C5	-C6	1.411(10)		
Si3	-O7	1.596(4)	C6	-C16	1.480(8)		
Si3	-O8	1.647(4)	C7	-C12	1.396(8)		
Si3	-C49	1.882(5)	C7	-C8	1.428(9)		
Si4	-O6	1.646(4)	C8	-C9	1.363(9)		
Si4	-O9	1.645(4)	C8	-C13	1.514(9)		
Si4	-O10	1.583(4)	C9	-C10	1.393(9)		
Si4	-C73	1.865(5)	C10	-C14	1.491(8)		
Na1	-O2	2.307(4)	C10	-C11	1.394(9)		
Na1	-O5	2.501(4)	C11	-C12	1.370(9)		
Na1	-O7	2.287(4)	C12	-C15	1.534(7)		
Na1	-O9	2.491(4)	C16	-C21	1.417(7)		
Na2	-O3	2.530(4)	C16	-C17	1.429(8)		
Na2	-O4	2.264(4)	C17	-C18	1.381(8)		
Na2	-O8	2.513(4)	C17	-C22	1.508(8)		
Na2	-O10	2.280(4)	C18	-C19	1.398(9)		
O3	-H3	0.94(4)	C19	-C20	1.398(9)		
O4	-H4	0.98(4)	C19	-C23	1.487(9)		
O5	-H5	0.99(3)	C20	-C21	1.391(8)		
O8	-H8	0.98(4)	C21	-C24	1.513(7)		

O1	-Si1	-O2	112.15(18)	O5	-Na1	-O9	168.09(15)
O1	-Si1	-O3	106.76(19)	O7	-Na1	-O9	89.44(14)
O1	-Si1	-C1	110.1(2)	O3	-Na2	-O4	87.58(14)
O2	-Si1	-O3	105.20(19)	O3	-Na2	-O8	167.05(14)
O2	-Si1	-C1	109.2(2)	O3	-Na2	-O10	83.93(14)
O3	-Si1	-C1	113.4(2)	O4	-Na2	-O8	83.79(14)
O1	-Si2	-O4	111.57(19)	O4	-Na2	-O10	103.20(14)
O1	-Si2	-O5	106.77(19)	O8	-Na2	-O10	88.65(14)

O1	-Si2	-C25	110.7(2)	Si1	-O1	-Si2	122.1(2)
O4	-Si2	-O5	106.23(19)	Si1	-O2	-Na1	132.6(2)
O4	-Si2	-C25	109.1(2)	Si1	-O3	-Na2	105.89(18)
O5	-Si2	-C25	112.4(2)	Si2	-O4	-Na2	135.2(2)
O6	-Si3	-O7	112.32(19)	Si2	-O5	-Na1	104.65(18)
O6	-Si3	-O8	105.58(19)	Si3	-O6	-Si4	123.7(2)
O6	-Si3	-C49	109.4(2)	Si3	-O7	-Na1	132.2(2)
O7	-Si3	-O8	106.43(19)	Si3	-O8	-Na2	106.36(18)
O7	-Si3	-C49	108.9(2)	Si4	-O9	-Na1	106.39(17)
O8	-Si3	-C49	114.3(2)	Si4	-O10	-Na2	133.2(2)
O6	-Si4	-O9	106.47(18)	Na2	-O3	-H3	115(3)
O6	-Si4	-O10	112.20(19)	Si1	-O3	-H3	130(3)
O6	-Si4	-C73	106.9(2)	Si2	-O4	-H4	114(3)
O9	-Si4	-O10	105.42(19)	Na2	-O4	-H4	99(2)
O9	-Si4	-C73	114.4(2)	Na1	-O5	-H5	98(3)
O10	-Si4	-C73	111.5(2)	Si2	-O5	-H5	117(3)
O2	-Na1	-O5	88.90(14)	Si3	-O8	-H8	139(3)
O2	-Na1	-O7	105.65(15)	Na2	-O8	-H8	101(3)
O2	-Na1	-O9	83.03(13)	Si4	-O9	-H9	132(3)
O5	-Na1	-O7	84.29(13)	Na1	-O9	-H9	105(3)
Na2	-O10	-H10	99(3)	C6	-C16	-C17	120.5(4)
Si4	-O10	-H10	114(3)	C6	-C16	-C21	121.4(4)
Si1	-C1	-C6	117.2(4)	C17	-C16	-C21	118.0(5)
Si1	-C1	-C2	124.8(4)	C18	-C17	-C22	121.2(6)

Table S9 - Hydrogen Bonds (Angstrom, Deg) for **7**

O4	-- H4 ..	O7	0.98(4)	1.49(4)	2.428(5)	158(4) .
O10	-- H10 ..	O2	0.97(4)	1.52(4)	2.431(5)	155(4) .
C24	-- H24A ..	O2	0.9800	2.5800	3.155(7)	117.00 .
C48	-- H48C ..	O4	0.9800	2.4800	3.118(7)	123.00 .
C70	-- H70C ..	O7	0.9800	2.5800	3.230(7)	124.00 .
C72	-- H72A ..	O6	0.9800	2.5000	3.261(6)	134.00 .
C85	-- H85A ..	O10	0.9800	2.5600	3.155(6)	119.00 .

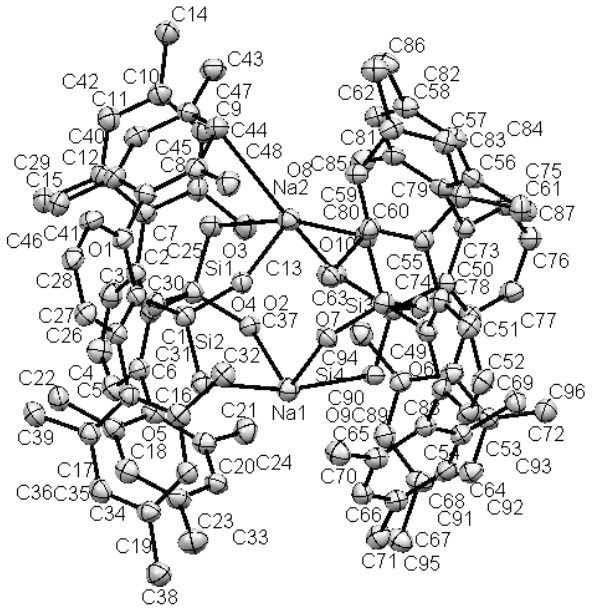


Figure S8. ORTEP plot of **7** showing the atomic numbering scheme. The probability ellipsoids are drawn at the 30% probability level. The H atoms were omitted for clarity reasons.

MS Spectra

HiREs-ESI-MSMS spectrum of **2**:

Elements Used:
C: 20-30 H: 0-200 Li: 0-5 O: 0-20 Na: 0-2 Si: 0-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		1.0	30.0	50.0			
399.1995	399.1995	0.0	0.0	7.5	166.0	1.5	C21 H28 Li O7
	399.1992	0.3	0.8	9.5	170.0	5.6	C23 H31 O4 Si
	399.1999	-0.4	-1.0	6.5	165.9	1.5	C20 H32 Li O4 Si2
	399.2004	-0.9	-2.3	13.5	192.3	27.8	C25 H18 Li5 Na2
	399.1975	2.0	5.0	8.5	169.2	4.8	C21 H29 Li2 O3 Si2
	399.1971	2.4	6.0	9.5	169.3	4.8	C22 H25 Li2 O6
	399.2019	-2.4	-6.0	5.5	168.6	4.2	C20 H31 O8
	399.1968	2.7	6.8	11.5	166.3	1.9	C24 H28 Li O3 Si
	399.1968	2.7	6.8	6.5	169.8	5.4	C21 H32 O4 Na Si
	399.1964	3.1	7.8	13.5	170.8	6.4	C26 H31 Si2
	399.2028	-3.3	-8.3	11.5	192.3	27.8	C24 H21 Li4 O Na2
	399.2028	-3.3	-8.3	16.5	192.3	27.8	C27 H17 Li5 Na
	399.1960	3.5	8.8	14.5	169.7	5.2	C27 H27 O3
	399.1955	4.0	10.0	8.5	192.3	27.8	C20 H23 Li4 O5 Si
	399.2036	-4.1	-10.3	8.5	192.3	27.8	C21 H22 Li5 O Na2 Si
	399.1952	4.3	10.8	10.5	192.3	27.8	C22 H26 Li3 O2 Si2
	399.1947	4.8	12.0	11.5	192.3	27.8	C23 H22 Li3 O5
	399.1947	4.8	12.0	6.5	169.7	5.2	C20 H26 Li2 O6 Na
	399.1944	5.1	12.8	8.5	166.6	2.2	C22 H29 Li O3 Na Si
	399.1944	5.1	12.8	13.5	169.7	5.3	C25 H25 Li2 O2 Si
	399.1940	5.5	13.8	10.5	170.7	6.3	C24 H32 Na Si2
	399.2052	-5.7	-14.3	14.5	192.3	27.8	C26 H20 Li4 O Na
	399.2052	-5.7	-14.3	9.5	192.3	27.8	C23 H24 Li3 O2 Na2
	399.2052	-5.7	-14.3	19.5	192.3	27.8	C29 H16 Li5
	399.1936	5.9	14.8	16.5	167.4	3.0	C28 H24 Li O2
	399.1936	5.9	14.8	11.5	169.4	5.0	C25 H28 O3 Na
	399.1931	6.4	16.0	10.5	192.3	27.8	C21 H20 Li5 O4 Si
	399.2059	-6.4	-16.0	6.5	192.3	27.8	C20 H25 Li4 O2 Na2 Si
	399.2060	-6.5	-16.3	11.5	192.3	27.8	C23 H21 Li5 O Na Si
	399.1928	6.7	16.8	12.5	192.3	27.8	C23 H23 Li4 O Si2
	399.1927	6.8	17.0	7.5	192.3	27.8	C20 H27 Li3 O2 Na Si2
	399.2065	-7.0	-17.5	12.5	169.6	5.2	C27 H29 Na2
	399.1924	7.1	17.8	13.5	192.3	27.8	C24 H19 Li4 O4
	399.1923	7.2	18.0	8.5	192.3	27.8	C21 H23 Li3 O5 Na
	399.1920	7.5	18.8	5.5	167.1	2.6	C20 H30 Li O3 Na2 Si
	399.1920	7.5	18.8	10.5	170.3	5.8	C23 H26 Li2 O2 Na Si
	399.1920	7.5	18.8	15.5	192.3	27.8	C26 H22 Li3 O Si

	399.2072		-7.7	-19.3	9.5	167.7
3.2	C24	H30	Li	Na2	Si	
	399.1916		7.9	19.8	7.5	170.6
6.1	C22	H33	Na2	Si2		
	399.2076		-8.1	-20.3	12.5	192.3
27.8	C25	H23	Li3	O2	Na	
	399.2076		-8.1	-20.3	17.5	192.3
27.8	C28	H19	Li4	O		
	399.2076		-8.1	-20.3	7.5	170.4
6.0	C22	H27	Li2	O3	Na2	
	399.1912		8.3	20.8	18.5	170.4
6.0	C29	H21	Li2	O		
	399.1912		8.3	20.8	13.5	167.8
3.3	C26	H25	Li	O2	Na	
	399.1912		8.3	20.8	8.5	169.1
4.7	C23	H29	O3	Na2		
	399.2080		-8.5	-21.3	6.5	170.5
6.1	C21	H31	Li2	Na2	Si2	
	399.2083		-8.8	-22.0	9.5	192.3
27.8	C22	H24	Li4	O2	Na	Si
	399.2084		-8.9	-22.3	14.5	192.3
27.8	C25	H20	Li5	O	Si	
	399.1904		9.1	22.8	9.5	192.3
27.8	C21	H24	Li4	O	Na	Si2
	399.1904		9.1	22.8	14.5	192.2
27.8	C24	H20	Li5	Si2		

HiREs-ESI-MSMS spectrum of **3**:

Elemental Composition Report

Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2047 formula(e) evaluated with 68 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 20-30 H: 0-200 Li: 0-5 O: 0-20 Na: 0-2 Si: 0-2

Minimum:					-1.5	
Maximum:			1.0	30.0	50.0	
Mass	Calc. Mass		mDa	PPM	DBE	i-FIT
i-FIT (Norm)	Formula					
405.2049	405.2049		0.0	0.0	6.5	67.8
3.8	C21	H31	Li	O4	Na	Si
	405.2050		-0.1	-0.2	11.5	65.9
1.9	C24	H27	Li2	O3	Si	
	405.2046		0.3	0.7	13.5	68.4
4.4	C26	H30	Li	Si2		
	405.2046		0.3	0.7	8.5	76.0
12.0	C23	H34	O	Na	Si2	
	405.2053		-0.4	-1.0	9.5	88.2
24.2	C22	H24	Li3	O6		
	405.2042		0.7	1.7	14.5	68.2
4.2	C27	H26	Li	O3		
	405.2042		0.7	1.7	9.5	75.3
11.3	C24	H30	O4	Na		
	405.2057		-0.8	-2.0	8.5	88.2
24.2	C21	H28	Li3	O3	Si2	
	405.2039		1.0	2.5	16.5	76.0
12.0	C29	H29	Si			
	405.2037		1.2	3.0	8.5	88.2
24.2	C20	H22	Li5	O5	Si	
	405.2033		1.6	3.9	10.5	88.2
24.2	C22	H25	Li4	O2	Si2	
	405.2066		-1.7	-4.2	12.5	75.5
11.5	C26	H29	O4			
	405.2029		2.0	4.9	11.5	88.2
24.2	C23	H21	Li4	O5		
	405.2029		2.0	4.9	6.5	88.2
24.2	C20	H25	Li3	O6	Na	
	405.2070		-2.1	-5.2	11.5	76.1
12.1	C25	H33	O	Si2		
	405.2026		2.3	5.7	8.5	66.1
2.0	C22	H28	Li2	O3	Na	Si
	405.2026		2.3	5.7	13.5	88.2
24.2	C25	H24	Li3	O2	Si	
	405.2073		-2.4	-5.9	4.5	75.8
11.8	C20	H34	O5	Na	Si	
	405.2073		-2.4	-5.9	9.5	68.0
4.0	C23	H30	Li	O4	Si	
	405.2022		2.7	6.7	10.5	68.2

4.2		C24	H31	Li	Na	Si2		
	405.2022			2.7		6.7	5.5	76.0
12.0		C21	H35	O	Na2	Si2		
	405.2077			-2.8		-6.9	7.5	66.1
2.1		C21	H27	Li2	O7			
	405.2018			3.1		7.7	6.5	75.2
11.2		C22	H31	O4	Na2			
	405.2018			3.1		7.7	16.5	66.2
2.1		C28	H23	Li2	O2			
	405.2018			3.1		7.7	11.5	68.0
4.0		C25	H27	Li	O3	Na		
	405.2081			-3.2		-7.9	6.5	66.2
2.2		C20	H31	Li2	O4	Si2		
	405.2014			3.5		8.6	13.5	75.9
11.9		C27	H30	Na	Si			
	405.2009			4.0		9.9	12.5	88.1
24.1		C23	H22	Li5	O	Si2		
	405.2009			4.0		9.9	7.5	88.2
24.2		C20	H26	Li4	O2	Na	Si2	
	405.2005			4.4		10.9	13.5	88.2
24.2		C24	H18	Li5	O4			
	405.2005			4.4		10.9	8.5	88.2
24.2		C21	H22	Li4	O5	Na		
	405.2002			4.7		11.6	15.5	88.2
24.2		C26	H21	Li4	O	Si		
	405.2002			4.7		11.6	10.5	88.2
24.2		C23	H25	Li3	O2	Na	Si	
	405.2097			-4.8		-11.8	7.5	75.9
11.9		C22	H33	O5	Si			
	405.2001			4.8		11.8	5.5	66.5
2.4		C20	H29	Li2	O3	Na2	Si	
	405.1998			5.1		12.6	7.5	68.1
4.1		C22	H32	Li	Na2	Si2		
	405.2101			-5.2		-12.8	5.5	67.5
3.5		C20	H30	Li	O8			
	405.1994			5.5		13.6	8.5	67.8
3.8		C23	H28	Li	O3	Na2		
	405.1994			5.5		13.6	18.5	88.2
24.2		C29	H20	Li3	O			
	405.1994			5.5		13.6	13.5	66.6
2.6		C26	H24	Li2	O2	Na		
	405.1990			5.9		14.6	10.5	75.9
11.9		C25	H31	Na2	Si			
	405.2110			-6.1		-15.1	11.5	88.2
24.2		C24	H20	Li5	O	Na2		
	405.1985			6.4		15.8	9.5	88.1
24.1		C21	H23	Li5	O	Na	Si2	
	405.1981			6.8		16.8	10.5	88.2
24.2		C22	H19	Li5	O4	Na		
	405.1978			7.1		17.5	12.5	88.2
24.2		C24	H22	Li4	O	Na	Si	
	405.1978			7.1		17.5	17.5	88.2
24.2		C27	H18	Li5	Si			
	405.1978			7.1		17.5	7.5	88.2
24.2		C21	H26	Li3	O2	Na2	Si	
	405.1970			7.9		19.5	15.5	88.2
24.2		C27	H21	Li3	O	Na		
	405.1970			7.9		19.5	20.5	88.2
24.2		C30	H17	Li4				
	405.1970			7.9		19.5	10.5	67.1
3.1		C24	H25	Li2	O2	Na2		

HiREs-ESI-MSMS spectrum of **4**:

Elemental Composition Report

Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
474 formula(e) evaluated with 29 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-200 O: 0-20 Na: 0-2 Si: 2-2

Minimum:							-1.5	
Maximum:				1.0		30.0	50.0	
Mass	Calc. Mass			mDa		PPM	DBE	i-FIT
i-FIT (Norm)	Formula							
767.3606	767.3599			0.7		0.9	8.5	56.5
5.5		C37	H61	O10	Na2	Si2		
	767.3623			-1.7		-2.2	11.5	55.3
4.3		C39	H60	O10	Na	Si2		

767.3588	1.8	2.3	23.5	52.7	1.7 C48 H55 O5 Si2
767.3647	-4.1	-5.3	14.5	54.0	3.1 C41 H59 O10 Si2
767.3564	4.2	5.5	20.5	52.6	1.6 C46 H56 O5 Na Si2
767.3657	-5.1	-6.6	-0.5	59.1	8.2 C30 H65 O15 Na2 Si2
767.3553	5.3	6.9	1.5	59.2	8.2 C30 H63 O18 Si2
767.3540	6.6	8.6	17.5	53.2	2.3 C44 H57 O5 Na2 Si2
767.3681	-7.5	-9.8	2.5	58.5	7.6 C32 H64 O15 Na Si2
767.3529	7.7	10.0	32.5	56.0	5.0 C55 H51 Si2
767.3529	7.7	10.0	-1.5	60.0	9.0 C28 H64 O18 Na Si2
767.3693	-8.7	-11.3	21.5	52.8	1.8 C48 H57 O2 Na2 Si2
767.3706	-10.0	-13.0	5.5	57.9	6.9 C34 H63 O15 Si2
767.3505	10.1	13.2	29.5	55.3	4.3 C53 H52 Na Si2
767.3717	-11.1	-14.5	24.5	53.7	2.7 C50 H56 O2 Na Si2
767.3494	11.2	14.6	10.5	57.0	6.1 C37 H59 O13 Si2
767.3481	12.5	16.3	26.5	54.5	3.6 C51 H53 Na2 Si2
767.3741	-13.5	-17.6	27.5	55.0	4.0 C52 H55 O2 Si2
767.3470	13.6	17.7	7.5	58.3	7.3 C35 H60 O13 Na Si2
767.3751	-14.5	-18.9	12.5	55.1	4.1 C41 H61 O7 Na2 Si2
767.3446	16.0	20.9	4.5	59.4	8.4 C33 H61 O13 Na2 Si2
767.3775	-16.9	-22.0	15.5	54.2	3.2 C43 H60 O7 Na Si2
767.3436	17.0	22.2	19.5	54.2	3.3 C44 H55 O8 Si2
767.3799	-19.3	-25.2	18.5	53.9	2.9 C45 H59 O7 Si2
767.3411	19.5	25.4	16.5	55.4	4.4 C42 H56 O8 Na Si2
767.3810	-20.4	-26.6	3.5	59.1	8.1 C34 H65 O12 Na2 Si2
767.3387	21.9	28.5	13.5	56.9	5.9 C40 H57 O8 Na2 Si2
767.3834	-22.8	-29.7	6.5	58.5	7.5 C36 H64 O12 Na Si2
767.3377	22.9	29.8	28.5	56.0	5.1 C51 H51 O3 Si2

HiRes-ESI-MSMS spectrum of **5:**

Elemental Composition Report

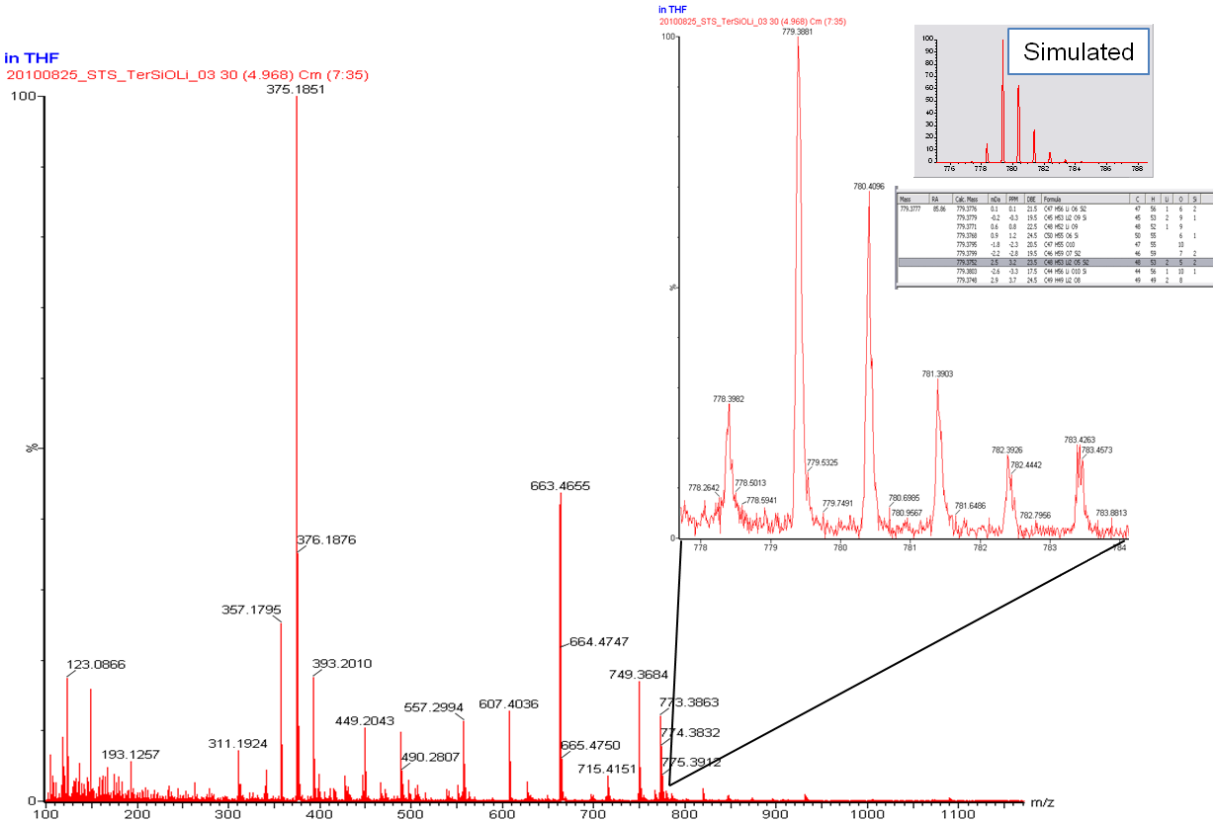
Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2712 formula(e) evaluated with 161 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-200 Li: 0-5 O: 0-20 Na: 0-2 Si: 2-2

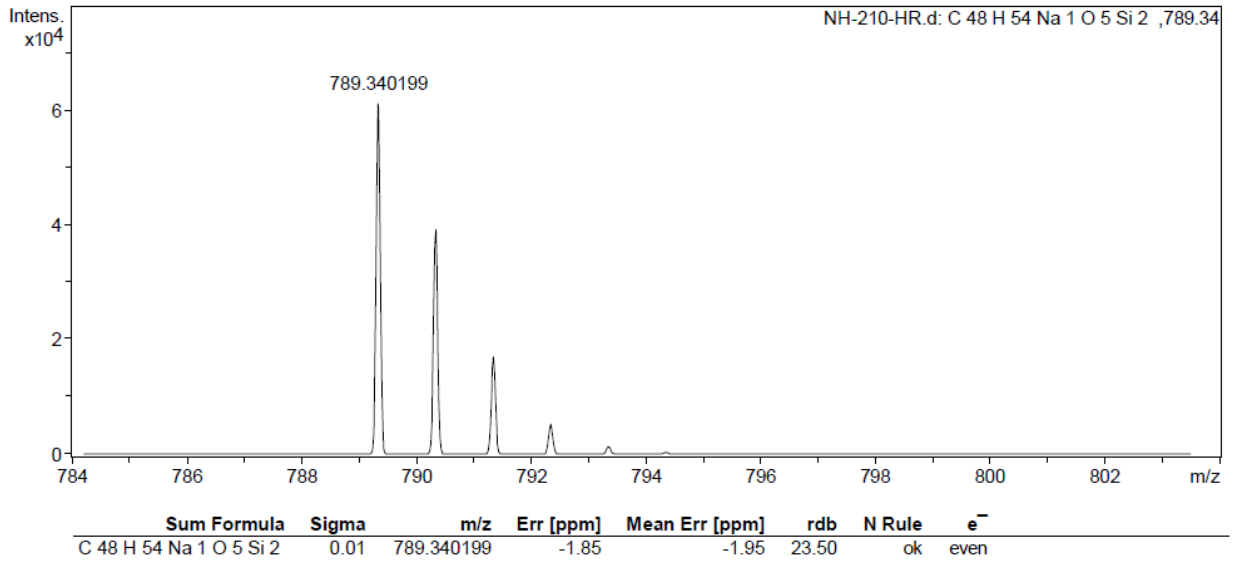
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		1.0	30.0	50.0			
773.3680	773.3680	0.0	0.0	8.5	110.1	17.8	C37 H60 Li O10 Na2 Si2
	773.3681	-0.1	-0.1	13.5	121.4	29.1	C40 H56 Li2 O9 Na Si2
	773.3681	-0.1	-0.1	18.5	145.1	52.7	C43 H52 Li3 O8 Si2
	773.3670	1.0	1.3	23.5	106.9	14.6	C48 H54 Li O5 Si2
	773.3670	1.0	1.3	18.5	93.6	1.3	C45 H58 O6 Na Si2
	773.3668	1.2	1.6	10.5	145.0		

52.7 C36 H51 Li5 O11 Na Si2
773.3692 -1.2 -1.6 8.5 145.0
52.7 C35 H54 Li4 O12 Na Si2
773.3668 1.2 1.6 5.5 145.0
52.7 C33 H55 Li4 O12 Na2 Si2
773.3692 -1.2 -1.6 13.5 145.0
52.7 C38 H50 Li5 O11 Si2
773.3692 -1.2 -1.6 3.5 145.1
52.7 C32 H58 Li3 O13 Na2 Si2
773.3694 -1.4 -1.8 21.5 96.7
4.4 C47 H57 O6 Si2
773.3659 2.1 2.7 -0.5 103.0
10.7 C29 H65 O19 Si2
773.3657 2.3 3.0 10.5 121.5
29.1 C38 H57 Li2 O9 Na2 Si2
773.3657 2.3 3.0 15.5 145.1
52.7 C41 H53 Li3 O8 Na Si2
773.3657 2.3 3.0 20.5 145.0
52.7 C44 H49 Li4 O7 Si2
773.3703 -2.3 -3.0 -1.5 145.0
52.7 C27 H56 Li5 O16 Na2 Si2
773.3704 -2.4 -3.1 6.5 100.2
7.9 C36 H63 O11 Na2 Si2
773.3705 -2.5 -3.2 16.5 121.5
29.2 C42 H55 Li2 O9 Si2
773.3705 -2.5 -3.2 11.5 109.2
16.9 C39 H59 Li O10 Na Si2
773.3646 3.4 4.4 20.5 104.7
12.4 C46 H55 Li O5 Na Si2
773.3646 3.4 4.4 15.5 92.7
0.4 C43 H59 O6 Na2 Si2
773.3646 3.4 4.4 25.5 121.5
29.2 C49 H51 Li2 O4 Si2
773.3715 -3.5 -4.5 1.5 121.5
29.2 C31 H61 Li2 O14 Na2 Si2
773.3716 -3.6 -4.7 11.5 145.0
52.7 C37 H53 Li4 O12 Si2
773.3716 -3.6 -4.7 6.5 145.1
52.7 C34 H57 Li3 O13 Na Si2
773.3644 3.6 4.7 7.5 145.0
52.7 C34 H52 Li5 O11 Na2 Si2
773.3635 4.5 5.8 30.5 100.4
8.1 C54 H53 O Si2
773.3635 4.5 5.8 1.5 112.4
20.1 C30 H62 Li O18 Si2
773.3633 4.7 6.1 12.5 145.1
52.7 C39 H54 Li3 O8 Na2 Si2
773.3727 -4.7 -6.1 1.5 145.0
52.7 C29 H55 Li5 O16 Na Si2
773.3633 4.7 6.1 22.5 145.0
52.7 C45 H46 Li5 O6 Si2
773.3727 -4.7 -6.1 25.5 145.1
52.7 C50 H50 Li3 Na2 Si2
773.3633 4.7 6.1 17.5 145.0
52.7 C42 H50 Li4 O7 Na Si2
773.3728 -4.8 -6.2 9.5 98.8
6.5 C38 H62 O11 Na Si2
773.3729 -4.9 -6.3 14.5 108.0
15.7 C41 H58 Li O10 Si2
773.3738 -5.8 -7.5 20.5 145.0
52.7 C45 H48 Li5 O3 Na2 Si2
773.3622 5.8 7.5 17.5 105.0
12.7 C44 H56 Li O5 Na2 Si2
773.3622 5.8 7.5 -1.5 145.0
52.7 C26 H57 Li4 O20 Si2
773.3622 5.8 7.5 22.5 121.7
29.3 C47 H52 Li2 O4 Na Si2
773.3622 5.8 7.5 27.5 145.1
52.7 C50 H48 Li3 O3 Si2
773.3739 -5.9 -7.6 4.5 121.7
29.4 C33 H60 Li2 O14 Na Si2
773.3739 -5.9 -7.6 -0.5 112.4
20.1 C30 H64 Li O15 Na2 Si2
773.3740 -6.0 -7.8 9.5 145.1
52.7 C36 H56 Li3 O13 Si2
773.3611 6.9 8.9 3.5 121.8
29.4 C31 H59 Li2 O17 Si2
773.3611 6.9 8.9 27.5 99.6
7.3 C52 H54 O Na Si2
773.3611 6.9 8.9 32.5 110.6
18.3 C55 H50 Li Si2
773.3611 6.9 8.9 -1.5 113.1
20.7 C28 H63 Li O18 Na Si2
773.3750 -7.0 -9.1 23.5 121.8
29.5 C49 H53 Li2 O Na2 Si2

	773.3750				-7.0		-9.1		-0.5	145.0
52.7		C28	H58	Li4	O17	Na	Si2			
	773.3609				7.1		9.2		19.5	145.0
52.7		C43	H47	Li5	O6	Na	Si2			



HiREs-ESI-MS-spectrum of **6**.



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 48 H 54 Na 1 O 5 Si 2	0.01	789.340199	-1.85	-1.95	23.50	ok	even

HiREs-ESI-MS-spectrum of **7**.