Supporting Information for:

New Tris(*tert*-butoxy)siloxy Complexes of Aluminum and Their Transformation to Homogeneous Aluminosilicate Materials via Low Temperature Thermolytic Pathways

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Data for **1**: Anal. Calcd. for $C_{40}H_{89}AlO_{13}Si_3$: C, 54.02; H, 10.09. Found: C, 54.10; H, 10.00. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.50 (t, 4 H, $O(CH_2)_4$), 2.05 (m, 4 H, $O(CH_2)_4$), 1.29 (s, 81 H, $OSi(O^tBu)_3$). $^{13}C\{^1H\}$ NMR (100 MHz): δ 71.54 $(OCH_2)_4$), 31.95 ($OSi(O^tBu)_3$), 25.36 $(OCH_2)_4$). IR (CsI, Nujol, cm^{-1}): 1387 m, 1364 m, 1240 m, 1221 w sh, 1197 s, 1081 s, 1050 s, 1026 s, 983 m sh, 913 w, 876 m, 829 m, 809 w, 702 m, 657 w, 591 w, 547 vw, 508 m, 481 m, 430 w.

Data for **2**: Anal. Calcd. for $C_{57}H_{131}Al_3O_{19}Si_3$: C, 53.24; H, 10.27. Found: C, 53.41; H, 10.64. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.69 (m, 3 H, $OCH(CH_3)_2$), 4.41 (m, 3 H, $OCH(CH_3)_2$), 1.68 (d, 9 H, $OCH(CH_3)_2$), 1.51 (s, 81 H, $OSi(O^tBu)_3$), 1.38 (d, 9 H, $OCH(CH_3)_2$), 1.32 (d, 18 H, $OCH(CH_3)_2$). $^{13}C\{^1H\}$ NMR (100 MHz): δ 72.22 ($SiOC(CH_3)_3$), 66.54 ($OCH(CH_3)_2$), 63.71 ($OCH(CH_3)_2$), 32.05 ($SiOC(CH_3)_3$), 28.31 ($OCH(CH_3)_2$), 28.10 ($OCH(CH_3)_2$), 26.78 ($OCH(CH_3)_2$), 25.55 ($OCH(CH_2)_2$). IR (CsI, Nujol, cm^{-1}): 1387 m, 1364 m, 1240 m, 1193 s, 1135 w sh, 1119 m sh, 1052 s br, 1026 m sh, 982 m, 950 m, 913 w, 860 w, 829 m, 806 w, 700 s, 660 w sh, 612 w, 571 w, 535 w, 510 m, 484 m, 433 m.

Data for **3**: Anal. Calcd. for $C_{36}H_{82}Al_2O_{12}Si_2$: C, 52.91; H, 10.12. Found: C, 52.55; H, 10.16. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.41 (m, 1 H, $OCH(CH_3)_2$), 4.21 (m, 1 H, $OCH(CH_3)_2$), 1.39 (d, 3 H, $OCH(CH_3)_2$), 1.36 (d, 3 H, $OCH(CH_3)_2$), 1.31 (s, 27 H, $OSi(O^tBu)_3$), 1.11 (d, 6 H, $OCH(CH_3)_2$). $^{13}C\{^1H\}$ NMR (100 MHz): δ 71.76 ($SiOC(CH_3)_2$), 68.78 ($OCH(CH_3)_2$), 63.50 ($OCH(CH_3)_2$), 31.93 ($SiOC(CH_3)_3$), 27.92 ($OCH(CH_3)_2$), 25.27 ($OCH(CH_3)_2$), 25.05 ($OCH(CH_3)_2$). IR (CsI, Nujol, cm^{-1}): 1388 m, 1378 w sh, 1363 m, 1242 m, 1194 s, 1174 w sh, 1145 w, 1120 w, 1056 vs br, 1028 m sh, 864 w, 840 m, 829 m, 809 w, 718 m sh, 702 m, 639 w.

EXPERIMENTAL DETAILS FOR 2

A. Crystal Data

Empirical Formula	$Al_3Si_3O_{19}C_{51}H_{131}$
Formula Weight	408.59
Crystal Color, Habit	colorless, blocky
Crystal Dimensions	0.30 X 0.30 X 0.30 mm
Crystal System	monoclinic
Lattice Type	C-centered
No. of Reflections Used for Unit Cell Determination (2Θ range)	5960 (0.0 - 46.5°)
Lattice Parameters	a = 23.989(1)Å b = 13.9207(7) Å c = 23.902(1) Å β = 95.349(1)° V = 7953.2(6) Å^3
Space Group	C2 (#5)
Z value	4
D_{calc}	1.365 g/cm^3
F_{000}	3584.00
μ(MoKα)	1.94 cm^{-1}

B. Intensity Measurements

Diffractometer	Siemens SMART
Radiation	MoKα (λ = 0.71069 Å)

	graphite monochromated
Crystal to Detector Distance	60 mm
Temperature	-110 °C
Scan Type	ω (0.3° per frame)
Scan Rate	30 sec. per frame
No. of Reflections Measured	Total: 16870 Unique: 10992 (R_{int} = 0.022)
Corrections	Lorentz-polarization
	Absorption (trans. factors: 0.86 - 0.93)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.030
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00sigma(I))	9647
No. Variables	738
Reflection/Parameter Ratio	13.07
Residuals: R; Rw	0.039 ; 0.048
R(all): R; Rw	0.048 ; 0.049
Goodness of Fit Indicator	2.06
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.39 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.22 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} for 2

atom	x	y	z	B_{eq}
Si(1)	0.17064(4)	0.5012	0.29687(4)	2.60(2)
Si(2)	0.39106(3)	0.40510(8)	0.33988(4)	2.33(2)
Si(3)	0.33520(4)	0.7871	0.32912(4)	2.29(2)
Al(1)	0.29842(4)	0.56384(8)	0.33167(4)	2.12(2)
Al(2)	0.0000	0.0214(1)	0.0000	2.10(3)
Al(3)	0.10488(4)	0.11973(8)	0.02331(4)	2.40(2)
Al(4)	0.0000	-0.1846(1)	0.0000	3.08(3)
O(1)	0.23562(9)	0.5220(2)	0.3031(1)	3.33(6)
O(2)	0.14081(9)	0.5919(2)	0.3245(1)	3.89(6)
O(3)	0.1474(1)	0.4810(2)	0.2320(1)	4.00(6)
O(4)	0.15287(9)	0.4083(2)	0.33214(10)	3.41(5)
O(5)	0.35456(8)	0.4946(2)	0.31663(9)	2.53(5)
O(6)	0.37529(9)	0.3036(2)	0.30959(9)	2.86(5)
O(7)	0.45757(8)	0.4224(2)	0.33690(10)	2.54(5)
O(8)	0.37557(8)	0.3907(2)	0.40533(9)	2.84(5)
O(9)	0.30559(10)	0.6845(2)	0.3272(1)	3.45(6)
O(10)	0.38202(9)	0.7992(2)	0.28491(9)	3.24(5)
O(11)	0.36787(9)	0.7971(2)	0.39150(9)	3.19(5)
O(12)	0.29086(9)	0.8737(2)	0.31556(10)	3.08(5)
O(13)	0.30173(10)	0.5339(2)	0.40737(9)	3.41(6)
O(14)	0.07335(8)	0.0353(2)	-0.02682(8)	2.42(5)
O(15)	0.02356(8)	-0.0875(2)	0.04580(8)	2.49(5)
O(16)	-0.0477(1)	-0.2466(2)	0.0339(1)	4.50(7)
O(17)	0.03686(8)	0.1155(2)	0.04910(8)	2.11(5)
O(18)	0.15242(9)	0.0777(2)	0.07414(9)	3.39(6)
O(19)	0.12257(10)	0.2205(2)	-0.0111(1)	3.61(6)
C(1)	0.0852(1)	0.6035(3)	0.3424(2)	4.40(10)
C(2)	0.0424(2)	0.5478(3)	0.3054(2)	4.7(1)
C(3)	0.0737(2)	0.7104(3)	0.3383(2)	5.2(1)
C(4)	0.0871(2)	0.5707(4)	0.4026(2)	5.8(1)
C(5)	0.1616(2)	0.5235(3)	0.1797(2)	4.48(10)
C(6)	0.1109(2)	0.5096(5)	0.1384(2)	7.9(2)
C(7)	0.1733(2)	0.6299(4)	0.1868(2)	6.8(1)
C(8)	0.2113(3)	0.4731(4)	0.1616(2)	7.7(2)
C(9)	0.1570(2)	0.3061(3)	0.3232(2)	4.36(9)
C(10)	0.1089(2)	0.2762(4)	0.2825(2)	6.2(2)
C(11)	0.2101(2)	0.2828(4)	0.2997(3)	6.9(2)
C(12)	0.1505(3)	0.2603(4)	0.3783(2)	7.0(2)
C(13)	0.3794(1)	0.2693(3)	0.2534(1)	3.25(9)
C(14)	0.3521(5)	0.3374(5)	0.2128(2)	11.1(3)
C(15)	0.3494(3)	0.1773(4)	0.2486(2)	7.4(2)
C(16)	0.4386(3)	0.2526(7)	0.2460(3)	8.8(3)
C(17)	0.4916(1)	0.5080(3)	0.3461(2)	3.61(8)
C(18)	0.5513(2)	0.4723(3)	0.3471(2)	4.4(1)
C(19)	0.4820(2)	0.5520(3)	0.4020(2)	4.8(1)
C(20)	0.4784(2)	0.5775(3)	0.2990(2)	4.4(1)
C(21)	0.3883(1)	0.3090(3)	0.4440(1)	3.26(8)
C(22)	0.3381(2)	0.2418(3)	0.4369(2)	5.2(1)
C(23)	0.4417(2)	0.2595(3)	0.4312(2)	4.27(9)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued) for 2

atom	x	y	z	B_{eq}
C(24)	0.3948(2)	0.3539(3)	0.5020(2)	5.0(1)
C(25)	0.3768(2)	0.8189(3)	0.2253(1)	3.90(9)
C(26)	0.4290(2)	0.7812(4)	0.2041(2)	5.9(1)
C(27)	0.3263(2)	0.7637(4)	0.1967(2)	5.5(1)
C(28)	0.3694(2)	0.9237(3)	0.2165(2)	5.6(1)
C(29)	0.4088(2)	0.8664(3)	0.4139(2)	3.91(9)
C(30)	0.3935(2)	0.9665(3)	0.3945(2)	6.4(1)
C(31)	0.4087(2)	0.8579(5)	0.4775(2)	7.0(2)
C(32)	0.4658(2)	0.8400(3)	0.3951(2)	5.2(1)
C(33)	0.2339(1)	0.8918(3)	0.3287(2)	3.54(9)
C(34)	0.2237(2)	0.8492(4)	0.3838(2)	5.3(1)
C(35)	0.2284(2)	1.0000(3)	0.3295(3)	6.3(1)
C(36)	0.1956(2)	0.8479(4)	0.2823(2)	5.5(1)
C(37)	0.2674(2)	0.5710(3)	0.4498(2)	4.21(10)
C(38)	0.2332(2)	0.4919(4)	0.4701(2)	6.0(1)
C(39)	0.3024(2)	0.6224(4)	0.4925(2)	7.1(2)
C(40)	0.1028(1)	-0.0183(2)	-0.0678(1)	2.89(8)
C(41)	0.1579(2)	-0.0538(3)	-0.0413(2)	4.4(1)
C(42)	0.1118(2)	0.0462(3)	-0.1173(2)	5.0(1)
C(43)	0.0589(1)	-0.0966(3)	0.0985(1)	3.23(8)
C(44)	0.0236(2)	-0.1118(5)	0.1462(2)	7.3(2)
C(45)	0.0993(2)	-0.1778(3)	0.0953(2)	6.1(1)
C(46)	-0.0714(2)	-0.3395(3)	0.0345(2)	4.9(1)
C(47)	-0.1321(2)	-0.3313(4)	0.0426(3)	8.9(2)
C(48)	-0.0390(2)	-0.4008(4)	0.0779(3)	7.6(2)
C(49)	0.0174(1)	0.1775(3)	0.0922(1)	2.96(8)
C(50)	0.0232(3)	0.2793(4)	0.0767(2)	7.5(2)
C(51)	0.0481(2)	0.1567(5)	0.1471(2)	6.6(2)
C(52)	0.2069(2)	0.0810(4)	0.0968(2)	6.0(1)
C(53)	0.2277(3)	-0.0154(5)	0.1158(3)	7.4(2)
C(54)	0.2187(3)	0.1572(6)	0.1377(4)	10.2(3)
C(55)	0.1625(2)	0.2922(3)	0.0012(2)	5.7(1)
C(56)	0.1417(3)	0.3866(4)	-0.0193(3)	8.3(2)
C(57)	0.2168(2)	0.2651(4)	-0.0219(2)	6.3(2)
H(1)	0.0423	0.5700	0.2677	5.6945
H(2)	0.0064	0.5571	0.3178	5.6945
H(3)	0.0517	0.4816	0.3069	5.6945
H(4)	0.0763	0.7313	0.3007	6.2210
H(5)	0.0374	0.7236	0.3488	6.2210
H(6)	0.1007	0.7440	0.3626	6.2210
H(7)	0.0510	0.5777	0.4156	6.9443
H(8)	0.0980	0.5052	0.4051	6.9443
H(9)	0.1133	0.6087	0.4252	6.9443
H(10)	0.0796	0.5404	0.1524	9.4574
H(11)	0.1034	0.4430	0.1340	9.4574
H(12)	0.1177	0.5370	0.1035	9.4574
H(13)	0.2026	0.4076	0.1546	9.1998
H(14)	0.2219	0.5022	0.1281	9.1998
H(15)	0.2414	0.4781	0.1901	9.1998

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued) for 2

atom	x	y	z	B_{eq}
H(16)	0.1827	0.6559	0.1521	8.1922
H(17)	0.2035	0.6393	0.2147	8.1922
H(18)	0.1408	0.6614	0.1977	8.1922
H(19)	0.0746	0.2901	0.2977	7.4882
H(20)	0.1110	0.2091	0.2754	7.4882
H(21)	0.1103	0.3102	0.2481	7.4882
H(22)	0.2125	0.2156	0.2937	8.2225
H(23)	0.2118	0.3154	0.2649	8.2225
H(24)	0.2409	0.3028	0.3252	8.2225
H(25)	0.1538	0.1925	0.3750	8.3980
H(26)	0.1146	0.2755	0.3898	8.3980
H(27)	0.1786	0.2832	0.4056	8.3980
H(28)	0.3132	0.3425	0.2189	13.3792
H(29)	0.3551	0.3154	0.1759	13.3792
H(30)	0.3690	0.3988	0.2179	13.3792
H(31)	0.3114	0.1869	0.2549	8.8888
H(32)	0.3662	0.1336	0.2757	8.8888
H(33)	0.3516	0.1516	0.2120	8.8888
H(34)	0.4419	0.2305	0.2087	10.5052
H(35)	0.4533	0.2057	0.2720	10.5052
H(36)	0.4589	0.3109	0.2518	10.5052
H(37)	0.5564	0.4416	0.3125	5.2961
H(38)	0.5587	0.4279	0.3770	5.2961
H(39)	0.5763	0.5252	0.3523	5.2961
H(40)	0.4912	0.5067	0.4310	5.7664
H(41)	0.5045	0.6075	0.4081	5.7664
H(42)	0.4435	0.5694	0.4019	5.7664
H(43)	0.5013	0.6329	0.3049	5.3107
H(44)	0.4401	0.5956	0.2977	5.3107
H(45)	0.4854	0.5480	0.2645	5.3107
H(46)	0.3056	0.2750	0.4459	6.1906
H(47)	0.3329	0.2207	0.3988	6.1906
H(48)	0.3445	0.1880	0.4608	6.1906
H(49)	0.4378	0.2369	0.3936	5.1235
H(50)	0.4489	0.2069	0.4562	5.1235
H(51)	0.4718	0.3039	0.4360	5.1235
H(52)	0.4027	0.3052	0.5293	5.9634
H(53)	0.4244	0.3991	0.5040	5.9634
H(54)	0.3609	0.3855	0.5088	5.9634
H(55)	0.4279	0.7917	0.1649	7.1130
H(56)	0.4605	0.8134	0.2226	7.1130
H(57)	0.4321	0.7142	0.2117	7.1130
H(58)	0.2931	0.7838	0.2119	6.6008
H(59)	0.3233	0.7760	0.1575	6.6008
H(60)	0.3316	0.6967	0.2030	6.6008
H(61)	0.3368	0.9443	0.2326	6.7212
H(62)	0.3659	0.9372	0.1775	6.7212
H(63)	0.4012	0.9565	0.2341	6.7212
H(64)	0.3908	0.9690	0.3547	7.6258

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued) for 2

atom	x	y	z	Beq
H(65)	0.3581	0.9834	0.4071	7.6258
H(66)	0.4211	1.0103	0.4097	7.6258
H(67)	0.3726	0.8734	0.4882	8.3834
H(68)	0.4355	0.9009	0.4953	8.3834
H(69)	0.4180	0.7939	0.4888	8.3834
H(70)	0.4764	0.7781	0.4090	6.1943
H(71)	0.4638	0.8399	0.3553	6.1943
H(72)	0.4928	0.8860	0.4095	6.1943
H(73)	0.1862	0.8618	0.3913	6.3031
H(74)	0.2296	0.7817	0.3827	6.3031
H(75)	0.2488	0.8767	0.4124	6.3031
H(76)	0.1919	1.0169	0.3385	7.6140
H(77)	0.2343	1.0251	0.2935	7.6140
H(78)	0.2554	1.0261	0.3568	7.6140
H(79)	0.1578	0.8573	0.2898	6.5995
H(80)	0.2018	0.8775	0.2476	6.5995
H(81)	0.2031	0.7810	0.2802	6.5995
H(82)	0.2422	0.6163	0.4314	5.0484
H(83)	0.2106	0.5161	0.4975	7.1735
H(84)	0.2099	0.4659	0.4395	7.1735
H(85)	0.2572	0.4432	0.4863	7.1735
H(86)	0.3293	0.5799	0.5102	8.4950
H(87)	0.3211	0.6734	0.4751	8.4950
H(88)	0.2798	0.6483	0.5192	8.4950
H(89)	0.0806	-0.0719	-0.0808	3.4664
H(90)	0.1765	-0.0891	-0.0680	5.2602
H(91)	0.1805	-0.0006	-0.0285	5.2602
H(92)	0.1520	-0.0941	-0.0103	5.2602
H(93)	0.1302	0.0112	-0.1443	5.9764
H(94)	0.1344	0.0996	-0.1046	5.9764
H(95)	0.0767	0.0686	-0.1338	5.9764
H(96)	0.0794	-0.0387	0.1050	3.8788
H(97)	0.0470	-0.1155	0.1804	8.7053
H(98)	-0.0017	-0.0596	0.1479	8.7053
H(99)	0.0031	-0.1699	0.1405	8.7053
H(100)	0.0794	-0.2364	0.0895	7.2874
H(101)	0.1216	-0.1670	0.0652	7.2874
H(102)	0.1229	-0.1815	0.1296	7.2874
H(103)	-0.0683	-0.3678	-0.0011	5.8574
H(104)	-0.1486	-0.3934	0.0414	10.6415
H(105)	-0.1503	-0.2927	0.0135	10.6415
H(106)	-0.1365	-0.3024	0.0779	10.6415
H(107)	-0.0417	-0.3740	0.1142	9.1199
H(108)	-0.0008	-0.4026	0.0705	9.1199
H(109)	-0.0539	-0.4638	0.0767	9.1199
H(110)	-0.0212	0.1646	0.0948	3.5464
H(111)	0.0024	0.2915	0.0418	8.9484
H(112)	0.0097	0.3190	0.1049	8.9484
H(113)	0.0617	0.2936	0.0738	8.9484

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued) for 2

atom	x	y	z	B_{eq}
H(114)	0.0349	0.1970	0.1750	7.9466
H(115)	0.0871	0.1679	0.1451	7.9466
H(116)	0.0427	0.0912	0.1568	7.9466
H(117)	0.2279	0.0970	0.0664	7.1774
H(118)	0.2066	-0.0378	0.1445	8.9236
H(119)	0.2242	-0.0583	0.0849	8.9236
H(120)	0.2661	-0.0102	0.1297	8.9236
H(121)	0.2087	0.2175	0.1206	12.2630
H(122)	0.1978	0.1474	0.1688	12.2630
H(123)	0.2576	0.1577	0.1498	12.2630
H(124)	0.1697	0.2960	0.0409	6.8297
H(125)	0.1700	0.4340	-0.0097	10.0004
H(126)	0.1090	0.4025	-0.0025	10.0004
H(127)	0.1344	0.3845	-0.0589	10.0004
H(128)	0.2110	0.2600	-0.0616	7.5380
H(129)	0.2297	0.2054	-0.0065	7.5380
H(130)	0.2442	0.3133	-0.0122	7.5380
H(131)	0.3361	0.4837	0.4171	5.1426

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic Displacement Parameters for 2

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si(1)	0.0258(5)	0.0284(5)	0.0428(5)	-0.0004(4)	-0.0011(4)	-0.0023(4)
Si(2)	0.0268(4)	0.0282(5)	0.0348(5)	0.0027(4)	0.0047(4)	0.0034(4)
Si(3)	0.0291(5)	0.0240(5)	0.0345(5)	-0.0010(4)	0.0070(4)	-0.0033(4)
Al(1)	0.0247(5)	0.0239(5)	0.0320(5)	0.0011(4)	0.0035(4)	0.0011(4)
Al(2)	0.0262(7)	0.0296(8)	0.0240(7)	0.0000	0.0015(5)	0.0000
Al(3)	0.0264(5)	0.0336(6)	0.0335(5)	0.0001(4)	0.0019(4)	-0.0005(5)
Al(4)	0.0421(8)	0.0290(8)	0.0484(9)	0.0000	0.0017(7)	0.0000
O(1)	0.031(1)	0.037(1)	0.068(2)	-0.002(1)	-0.001(1)	-0.001(1)
O(2)	0.036(1)	0.033(1)	0.085(2)	-0.004(1)	0.018(1)	-0.008(1)
O(3)	0.056(2)	0.044(2)	0.050(2)	-0.001(1)	-0.006(1)	0.004(1)
O(4)	0.042(1)	0.029(1)	0.058(1)	-0.003(1)	0.005(1)	-0.002(1)
O(5)	0.033(1)	0.033(1)	0.039(1)	0.007(1)	0.0070(10)	0.004(1)
O(6)	0.040(1)	0.032(1)	0.039(1)	0.002(1)	0.006(1)	0.000(1)
O(7)	0.026(1)	0.031(1)	0.053(1)	0.003(1)	0.007(1)	0.003(1)
O(8)	0.034(1)	0.039(1)	0.036(1)	0.003(1)	0.0060(10)	0.006(1)
O(9)	0.045(1)	0.021(1)	0.062(2)	-0.001(1)	0.006(1)	-0.004(1)
O(10)	0.044(1)	0.042(1)	0.039(1)	0.008(1)	0.015(1)	0.001(1)
O(11)	0.042(1)	0.043(1)	0.038(1)	-0.008(1)	0.003(1)	-0.003(1)
O(12)	0.035(1)	0.026(1)	0.059(2)	0.002(1)	0.014(1)	-0.002(1)
O(13)	0.048(1)	0.050(2)	0.039(1)	0.014(1)	0.014(1)	0.002(1)
O(14)	0.028(1)	0.031(1)	0.029(1)	0.0031(9)	0.0046(9)	-0.0030(10)
O(15)	0.034(1)	0.029(1)	0.035(1)	0.001(1)	-0.0022(9)	0.005(1)
O(16)	0.055(2)	0.035(2)	0.077(2)	-0.011(1)	0.013(1)	0.004(1)
O(17)	0.029(1)	0.032(1)	0.028(1)	-0.0018(10)	0.0027(9)	-0.006(1)
O(18)	0.031(1)	0.056(2)	0.043(1)	0.002(1)	-0.006(1)	-0.004(1)
O(19)	0.045(1)	0.045(2)	0.054(2)	-0.011(1)	0.003(1)	0.009(1)
C(1)	0.034(2)	0.040(2)	0.088(3)	-0.001(2)	0.024(2)	-0.011(2)
C(2)	0.044(2)	0.043(2)	0.114(4)	0.000(2)	0.014(2)	-0.005(2)
C(3)	0.050(2)	0.042(2)	0.108(4)	0.002(2)	0.030(3)	-0.009(2)
C(4)	0.071(3)	0.071(3)	0.095(4)	0.005(3)	0.033(3)	0.004(3)
C(5)	0.070(3)	0.047(2)	0.046(2)	0.004(2)	-0.009(2)	0.006(2)
C(6)	0.109(4)	0.142(6)	0.075(4)	-0.019(4)	-0.038(3)	0.007(4)
C(7)	0.120(4)	0.067(3)	0.070(3)	0.013(3)	0.001(3)	0.025(3)
C(8)	0.156(5)	0.091(4)	0.074(4)	0.044(4)	0.046(4)	0.018(3)
C(9)	0.051(2)	0.029(2)	0.055(2)	0.000(2)	0.008(2)	0.001(2)
C(10)	0.124(4)	0.052(3)	0.109(4)	-0.026(3)	-0.029(3)	-0.004(3)
C(11)	0.105(4)	0.039(3)	0.167(6)	0.014(3)	0.056(4)	0.007(3)
C(12)	0.211(7)	0.047(3)	0.075(4)	-0.016(4)	0.041(4)	0.003(3)
C(13)	0.046(2)	0.039(2)	0.043(2)	0.000(2)	0.001(2)	-0.005(2)
C(14)	0.42(1)	0.081(4)	0.039(3)	0.099(7)	-0.042(5)	-0.009(3)
C(15)	0.192(7)	0.061(3)	0.080(4)	-0.042(4)	0.028(4)	-0.031(3)
C(16)	0.083(4)	0.26(1)	0.154(6)	-0.016(5)	0.050(4)	-0.144(7)
C(17)	0.030(2)	0.032(2)	0.065(2)	-0.002(2)	0.007(2)	0.003(2)
C(18)	0.037(2)	0.046(3)	0.113(4)	-0.002(2)	0.017(2)	0.008(2)
C(19)	0.061(3)	0.051(3)	0.091(3)	-0.013(2)	0.007(2)	-0.021(2)
C(20)	0.046(2)	0.054(3)	0.095(3)	0.001(2)	0.016(2)	0.028(3)
C(21)	0.041(2)	0.050(2)	0.040(2)	0.000(2)	0.006(2)	0.019(2)
C(22)	0.055(3)	0.064(3)	0.089(3)	-0.014(2)	0.001(2)	0.031(3)
C(23)	0.046(2)	0.047(2)	0.055(2)	0.009(2)	-0.003(2)	0.015(2)

Table 2. Anisotropic Displacement Parameters (continued) for 2

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(24)	0.075(3)	0.075(3)	0.039(2)	0.016(2)	0.008(2)	0.011(2)
C(25)	0.049(2)	0.050(2)	0.037(2)	0.012(2)	0.014(2)	0.008(2)
C(26)	0.087(3)	0.088(4)	0.068(3)	0.032(3)	0.040(3)	0.019(3)
C(27)	0.082(3)	0.106(4)	0.046(3)	0.002(3)	0.011(2)	-0.008(3)
C(28)	0.086(3)	0.067(3)	0.060(3)	0.019(3)	0.020(2)	0.021(2)
C(29)	0.047(2)	0.048(2)	0.048(2)	-0.005(2)	-0.005(2)	-0.011(2)
C(30)	0.066(3)	0.039(3)	0.119(4)	-0.007(2)	-0.017(3)	-0.021(3)
C(31)	0.101(4)	0.136(5)	0.055(3)	-0.035(4)	-0.005(3)	-0.027(3)
C(32)	0.049(2)	0.060(3)	0.092(3)	-0.008(2)	0.003(2)	-0.010(3)
C(33)	0.030(2)	0.038(2)	0.066(2)	0.005(2)	0.014(2)	-0.004(2)
C(34)	0.053(2)	0.097(4)	0.067(3)	0.008(2)	0.023(2)	-0.009(3)
C(35)	0.056(3)	0.045(3)	0.183(6)	0.011(2)	0.038(3)	-0.012(3)
C(36)	0.046(2)	0.087(3)	0.073(3)	-0.005(2)	0.009(2)	0.007(3)
C(37)	0.066(3)	0.049(2)	0.050(2)	0.012(2)	0.023(2)	0.000(2)
C(38)	0.072(3)	0.086(3)	0.065(3)	0.003(3)	0.025(2)	0.020(3)
C(39)	0.099(4)	0.099(4)	0.084(4)	-0.014(3)	0.013(3)	-0.041(3)
C(40)	0.037(2)	0.037(2)	0.036(2)	0.004(2)	0.007(2)	-0.007(2)
C(41)	0.054(2)	0.064(3)	0.061(3)	0.024(2)	0.006(2)	-0.009(2)
C(42)	0.070(3)	0.058(3)	0.048(2)	0.016(2)	0.026(2)	0.004(2)
C(43)	0.047(2)	0.049(2)	0.038(2)	-0.008(2)	-0.012(2)	0.016(2)
C(44)	0.074(3)	0.180(6)	0.041(3)	-0.012(4)	-0.006(2)	0.029(3)
C(45)	0.081(3)	0.062(3)	0.081(3)	0.018(3)	-0.024(3)	0.017(3)
C(46)	0.059(3)	0.033(2)	0.082(3)	-0.008(2)	0.001(2)	0.004(2)
C(47)	0.064(3)	0.046(3)	0.249(8)	-0.020(3)	0.039(4)	0.013(4)
C(48)	0.094(4)	0.064(3)	0.131(5)	-0.025(3)	-0.006(3)	0.032(3)
C(49)	0.030(2)	0.044(2)	0.033(2)	-0.002(2)	0.006(2)	-0.013(2)
C(50)	0.204(6)	0.051(3)	0.094(4)	-0.030(4)	0.076(4)	-0.040(3)
C(51)	0.112(4)	0.156(6)	0.043(3)	0.072(4)	-0.005(3)	-0.034(3)
C(52)	0.048(3)	0.100(4)	0.080(3)	0.008(3)	-0.026(2)	0.005(3)
C(53)	0.102(4)	0.135(6)	0.113(5)	0.061(4)	-0.038(4)	-0.013(4)
C(54)	0.131(6)	0.146(7)	0.173(7)	0.019(5)	-0.096(6)	-0.066(6)
C(55)	0.082(3)	0.059(3)	0.078(3)	-0.034(3)	0.007(3)	0.007(3)
C(56)	0.172(6)	0.045(3)	0.123(5)	-0.016(4)	0.036(4)	0.018(3)
C(57)	0.059(3)	0.099(4)	0.117(4)	-0.028(3)	0.003(3)	0.031(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å) for 2

atom	atom	distance	atom	atom	distance
Si(1)	O(1)	1.579(2)	Si(1)	O(2)	1.621(2)
Si(1)	O(3)	1.623(3)	Si(1)	O(4)	1.623(2)
Si(2)	O(5)	1.593(2)	Si(2)	O(6)	1.617(2)
Si(2)	O(7)	1.622(2)	Si(2)	O(8)	1.655(2)
Si(3)	O(9)	1.594(2)	Si(3)	O(10)	1.622(2)
Si(3)	O(11)	1.625(2)	Si(3)	O(12)	1.621(2)
Al(1)	O(1)	1.698(2)	Al(1)	O(5)	1.721(2)
Al(1)	O(9)	1.693(2)	Al(1)	O(13)	1.853(2)
Al(2)	O(14)	1.938(2)	Al(2)	O(14)	1.938(2)
Al(2)	O(15)	1.924(2)	Al(2)	O(15)	1.924(2)
Al(2)	O(17)	1.920(2)	Al(2)	O(17)	1.920(2)
Al(3)	O(14)	1.795(2)	Al(3)	O(17)	1.798(2)
Al(3)	O(18)	1.692(2)	Al(3)	O(19)	1.700(2)
Al(4)	O(15)	1.797(2)	Al(4)	O(15)	1.797(2)
Al(4)	O(16)	1.698(2)	Al(4)	O(16)	1.698(2)
O(2)	C(1)	1.449(4)	O(3)	C(5)	1.453(5)
O(4)	C(9)	1.444(4)	O(6)	C(13)	1.439(4)
O(7)	C(17)	1.450(4)	O(8)	C(21)	1.480(4)
O(10)	C(25)	1.446(4)	O(11)	C(29)	1.444(4)
O(12)	C(33)	1.452(4)	O(13)	C(37)	1.460(4)
O(13)	H(131)	1.09	O(14)	C(40)	1.465(4)
O(15)	C(43)	1.458(4)	O(16)	C(46)	1.413(4)
O(17)	C(49)	1.455(4)	O(18)	C(52)	1.368(4)
O(19)	C(55)	1.396(5)	C(1)	C(2)	1.506(6)
C(1)	C(3)	1.516(6)	C(1)	C(4)	1.506(6)
C(5)	C(6)	1.506(6)	C(5)	C(7)	1.515(6)
C(5)	C(8)	1.483(7)	C(9)	C(10)	1.499(6)
C(9)	C(11)	1.475(6)	C(9)	C(12)	1.485(6)
C(13)	C(14)	1.466(7)	C(13)	C(15)	1.468(6)
C(13)	C(16)	1.467(7)	C(17)	C(18)	1.515(5)
C(17)	C(19)	1.508(6)	C(17)	C(20)	1.496(5)
C(21)	C(22)	1.523(5)	C(21)	C(23)	1.511(5)
C(21)	C(24)	1.517(5)	C(25)	C(26)	1.49(5)
C(25)	C(27)	1.539(6)	C(25)	C(28)	1.82(6)
C(29)	C(30)	1.503(6)	C(29)	C(31)	1.527(6)
C(29)	C(32)	1.525(5)	C(33)	C(34)	1.486(6)
C(33)	C(35)	1.512(6)	C(33)	C(36)	1.504(6)
C(37)	C(38)	1.481(6)	C(37)	C(39)	1.450(6)
C(40)	C(41)	1.496(5)	C(40)	C(42)	1.519(5)
C(43)	C(44)	1.497(6)	C(43)	C(45)	1.496(6)
C(46)	C(47)	1.492(7)	C(46)	C(48)	1.503(7)
C(49)	C(50)	1.475(6)	C(49)	C(51)	1.475(6)
C(52)	C(53)	1.487(8)	C(52)	C(54)	1.453(8)
C(55)	C(56)	1.475(7)	C(55)	C(57)	1.510(7)
H(131)	O(8)	1.64			
O(8)	O(13)	2.670(3)			

Table 4. Bond Angles(°) for 2

atom atom atom	angle	atom atom atom	angle
O(1)-Si(1)-O(2)	106.8(1)	O(14)-Al(2)-O(15)	96.78(9)
O(1)-Si(1)-O(3)	111.7(1)	O(14)-Al(2)-O(17)	75.73(8)
O(1)-Si(1)-O(4)	113.7(1)	O(14)-Al(2)-O(17)	96.29(9)
O(2)-Si(1)-O(3)	113.5(1)	O(14)-Al(2)-O(15)	96.78(9)
O(2)-Si(1)-O(4)	105.1(1)	O(14)-Al(2)-O(15)	92.29(9)
O(3)-Si(1)-O(4)	106.0(1)	O(14)-Al(2)-O(17)	96.29(9)
O(5)-Si(2)-O(6)	115.4(1)	O(14)-Al(2)-O(17)	75.73(8)
O(5)-Si(2)-O(7)	112.3(1)	O(15)-Al(2)-O(15)	76.0(1)
O(5)-Si(2)-O(8)	105.1(1)	O(15)-Al(2)-O(17)	95.48(9)
O(6)-Si(2)-O(7)	107.4(1)	O(15)-Al(2)-O(17)	168.6(1)
O(6)-Si(2)-O(8)	104.7(1)	O(15)-Al(2)-O(17)	168.6(1)
O(7)-Si(2)-O(8)	111.6(1)	O(15)-Al(2)-O(17)	95.48(9)
O(9)-Si(3)-O(10)	114.1(1)	O(17)-Al(2)-O(17)	93.9(1)
O(9)-Si(3)-O(11)	106.2(1)	O(14)-Al(3)-O(17)	82.46(9)
O(9)-Si(3)-O(12)	112.2(1)	O(14)-Al(3)-O(18)	117.9(1)
O(10)-Si(3)-O(11)	106.6(1)	O(14)-Al(3)-O(19)	109.0(1)
O(10)-Si(3)-O(12)	105.9(1)	O(17)-Al(3)-O(18)	108.3(1)
O(11)-Si(3)-O(12)	111.8(1)	O(17)-Al(3)-O(19)	117.9(1)
O(1)-Al(1)-O(5)	113.9(1)	O(18)-Al(3)-O(19)	116.8(1)
O(1)-Al(1)-O(9)	113.9(1)	O(15)-Al(4)-O(15)	82.5(1)
O(1)-Al(1)-O(13)	105.8(1)	O(15)-Al(4)-O(16)	106.2(1)
O(5)-Al(1)-O(9)	117.2(1)	O(15)-Al(4)-O(16)	119.0(1)
O(5)-Al(1)-O(13)	96.6(1)	O(15)-Al(4)-O(16)	119.0(1)
O(9)-Al(1)-O(13)	106.9(1)	O(15)-Al(4)-O(16)	106.2(1)
O(14)-Al(2)-O(14)	168.5(1)	O(16)-Al(4)-O(16)	118.9(2)
O(14)-Al(2)-O(15)	92.29(9)	Si(1)-O(1)-Al(1)	158.7(2)
Si(1)-O(2)-C(1)	131.4(2)	O(2)-C(1)-C(4)	107.6(3)
Si(1)-O(3)-C(5)	131.7(2)	C(2)-C(1)-C(3)	111.0(4)
Si(1)-O(4)-C(9)	133.1(2)	C(2)-C(1)-C(4)	111.5(4)
Si(2)-O(5)-Al(1)	141.3(1)	C(3)-C(1)-C(4)	110.4(4)
Si(2)-O(6)-C(13)	132.5(2)	O(3)-C(5)-C(6)	105.8(4)
Si(2)-O(7)-C(17)	131.1(2)	O(3)-C(5)-C(7)	110.9(3)
Si(2)-O(8)-C(21)	129.2(2)	O(3)-C(5)-C(8)	108.6(3)
Si(3)-O(9)-Al(1)	159.2(2)	C(6)-C(5)-C(7)	109.3(4)
Si(3)-O(10)-C(25)	131.4(2)	C(6)-C(5)-C(8)	111.8(5)
Si(3)-O(11)-C(29)	130.6(2)	C(7)-C(5)-C(8)	110.4(4)
Si(3)-O(12)-C(33)	134.3(2)	O(4)-C(9)-C(10)	108.1(3)
Al(1)-O(13)-C(37)	128.6(2)	O(4)-C(9)-C(11)	110.3(3)
Al(2)-O(14)-Al(3)	100.6(1)	O(4)-C(9)-C(12)	106.1(3)
Al(2)-O(14)-C(40)	132.8(2)	C(10)-C(9)-C(11)	109.3(4)
Al(3)-O(14)-C(40)	125.6(2)	C(10)-C(9)-C(12)	108.6(4)
Al(2)-O(15)-Al(4)	100.7(1)	C(11)-C(9)-C(12)	114.2(4)
Al(2)-O(15)-C(43)	132.6(2)	O(6)-C(13)-C(14)	109.8(3)
Al(4)-O(15)-C(43)	125.9(2)	O(6)-C(13)-C(15)	106.7(3)
Al(4)-O(16)-C(46)	139.4(3)	O(6)-C(13)-C(16)	108.4(3)
Al(2)-O(17)-Al(3)	101.1(1)	C(14)-C(13)-C(15)	109.1(5)
Al(2)-O(17)-C(49)	132.7(2)	C(14)-C(13)-C(16)	113.7(6)
Al(3)-O(17)-C(49)	125.9(2)	C(15)-C(13)-C(16)	109.0(5)
Al(3)-O(18)-C(52)	145.9(3)	O(7)-C(17)-C(18)	104.5(3)

Table 4. Bond Angles(°) for 2

atom atom atom	angle	atom atom atom	angle
Al(3)-O(19)-C(55)	133.2(3)	O(7)-C(17)-C(19)	109.8(3)
O(2)-C(1)-C(2)	111.3(3)	O(7)-C(17)-C(20)	109.9(3)
O(2)-C(1)-C(3)	104.8(3)	C(18)-C(17)-C(19)	110.0(3)
C(18)-C(17)-C(20)	111.0(3)	O(13)-C(37)-C(38)	109.3(3)
C(19)-C(17)-C(20)	111.5(3)	O(13)-C(37)-C(39)	109.6(3)
O(8)-C(21)-C(22)	106.7(3)	C(38)-C(37)-C(39)	116.0(4)
O(8)-C(21)-C(23)	110.7(3)	O(14)-C(40)-C(41)	110.3(3)
O(8)-C(21)-C(24)	104.6(3)	O(14)-C(40)-C(42)	109.5(3)
C(22)-C(21)-C(23)	112.0(3)	C(41)-C(40)-C(42)	110.0(3)
C(22)-C(21)-C(24)	111.5(3)	O(15)-C(43)-C(44)	110.3(3)
C(23)-C(21)-C(24)	111.0(3)	O(15)-C(43)-C(45)	110.4(3)
O(10)-C(25)-C(26)	105.7(3)	C(44)-C(43)-C(45)	110.4(4)
O(10)-C(25)-C(27)	109.6(3)	O(16)-C(46)-C(47)	109.3(4)
O(10)-C(25)-C(28)	108.9(3)	O(16)-C(46)-C(48)	110.1(4)
C(26)-C(25)-C(27)	108.9(4)	C(47)-C(46)-C(48)	113.7(5)
C(26)-C(25)-C(28)	113.1(4)	O(17)-C(49)-C(50)	110.3(3)
C(27)-C(25)-C(28)	110.5(4)	O(17)-C(49)-C(51)	110.4(3)
O(11)-C(29)-C(30)	111.5(3)	C(50)-C(49)-C(51)	111.2(4)
O(11)-C(29)-C(31)	104.7(3)	O(18)-C(52)-C(53)	111.8(5)
O(11)-C(29)-C(32)	109.1(3)	O(18)-C(52)-C(54)	114.2(5)
C(30)-C(29)-C(31)	110.9(4)	C(53)-C(52)-C(54)	114.5(5)
C(30)-C(29)-C(32)	109.4(4)	O(19)-C(55)-C(56)	111.3(4)
C(31)-C(29)-C(32)	111.1(4)	O(19)-C(55)-C(57)	110.1(4)
O(12)-C(33)-C(34)	111.0(3)	C(56)-C(55)-C(57)	112.2(4)
O(12)-C(33)-C(35)	105.1(3)	O(12)-C(33)-C(36)	107.0(3)
C(34)-C(33)-C(35)	111.4(4)	C(34)-C(33)-C(36)	110.7(3)
C(35)-C(33)-C(36)	111.4(4)		

Experimental Details For **3**

D. Crystal Data

Empirical Formula (asymmetric unit)	$C_{54}H_{123}Al_3O_{18}Si_3$
Formula Weight	817.18
Crystal Color, Habit	colorless, plate-like
Crystal Dimensions	0.30 x 0.15 x 0.05 mm
Crystal System	monoclinic
Lattice Type	primitive
Lattice Parameters	a = 9.097(3) Å
	b = 24.530(7) Å
	c = 33.678(10) Å
	β = 90.205(6)°
	V = 7515.2(39) Å^3
Space Group	$P2_1/c$
Z value	4
D_{calc}	1.083 g cm^{-3}
F_{000}	2688
$\mu(MoK_\alpha)$	1.5 cm^{-1}

E. Intensity Measurements

Diffractometer	SMART CCD
Radiation	MoK_α ($\lambda = 0.71069$ Å)
	graphite monochromated
Detector Position	60.00 mm
Exposure Time	30 seconds per frame.
Scan Type	ω (0.3° per frame)
No. of Reflections Measured	Total: 34230
	Unique: 24139 (Rint = 0.124)
Corrections	Lorentz-polarization
	Absorption
	(Tmax = 0.9778, Tmin = 0.6571)

F. Structure Solution and Refinement

Structure Solution	direct: SHELXS-86 (Sheldrick, 1990)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w\ (\|Fo\|^2 - \|Fc\|^2)^2$
Least Squares Weights	$1/[\sigma^2(Fo^2) + (0.0338P)^2 + 0.00P]$
	where $P = (Fo^2 + 2Fc^2)/3$
p-factor	0.0338
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I>2.00\sigma(I)$)	3225
No. Variables	650
Observations/Parameter Ratio	5.0
Residuals: R; Rw; Rall	0.055; 0.089; 0.146
Goodness of Fit Indicator	0.843
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.27 e^- $Å^{-3}$
Minimum peak in Final Diff. Map	-0.26 e^- $Å^{-3}$

Table 5. Atomic coordinates and U_{iso}/U_{eq} for **3**

atom	x	y	z	Ueq
Si1	0.4453(3)	-0.1278(1)	0.2592(1)	.044(1)
Si2	0.4254(3)	0.1295(1)	0.4066(1)	.040(1)
Si3	-0.0102(4)	0.6310(1)	0.4292(1)	.043(1)
Al1	0.3858(4)	-0.0514(1)	0.3327(1)	.046(1)
Al2	0.4893(3)	0.0540(1)	0.3323(1)	.042(1)
Al3	0.0480(4)	0.5532(1)	0.5018(1)	.045(1)
O1	0.4532(7)	-0.0986(2)	0.3012(2)	.044(2)
O2	0.4222(7)	0.1008(2)	0.3640(2)	.048(2)
O3	0.3451(7)	0.0140(3)	0.3101(2)	.040(2)
O4	0.5320(7)	-0.0117(2)	0.3552(2)	.047(2)
O5	0.2587(8)	-0.0699(3)	0.3657(2)	.062(2)
O6	0.6158(7)	0.0726(2)	0.2997(2)	.056(2)
O11	0.4804(8)	-0.0865(2)	0.2223(2)	.055(2)
O12	0.2772(7)	-0.1475(3)	0.2531(2)	.048(2)
O13	0.5640(7)	-0.1769(2)	0.2555(2)	.045(2)
O21	0.3096(6)	0.1802(3)	0.4091(2)	.040(2)
O22	0.5942(7)	0.1464(2)	0.4139(2)	.047(2)
O23	0.3825(8)	0.0877(2)	0.4420(2)	.045(2)
O70	-0.0210(7)	0.6014(2)	0.4709(2)	.052(2)
O71	-0.0391(8)	0.5913(2)	0.3914(2)	.049(2)
O72	-0.1280(7)	0.6803(3)	0.4260(2)	.045(2)
O73	0.1526(8)	0.6506(3)	0.4253(2)	.052(2)
O74	0.1723(7)	0.5708(3)	0.5358(2)	.063(2)
O75	0.0976(8)	0.4890(2)	0.4786(2)	.046(2)
C1	0.6159(13)	-0.0647(4)	0.2076(3)	.042(3)
C2	0.7208(11)	-0.0508(5)	0.2404(3)	.062(4)
C3	0.5735(13)	-0.0149(4)	0.1841(3)	.093(4)
C4	0.6838(11)	-0.1060(5)	0.1796(3)	.065(4)
C5	0.1941(13)	-0.1686(6)	0.2199(4)	.057(4)
C6	0.1506(28)	-0.1141(9)	0.1943(7)	.046(8)
C6A	0.0973(33)	-0.1299(13)	0.2024(9)	.107(13)
C7	0.0569(26)	-0.1934(10)	0.2339(6)	.066(8)
C7A	0.1075(27)	-0.2174(8)	0.2429(6)	.063(8)
C8	0.2924(11)	-0.1999(4)	0.1918(3)	.065(4)

C9	0.6051(15)	-0.2191(4)	0.2833(3)	.049(3)
C10	0.6764(11)	-0.2622(5)	0.2580(3)	.075(4)
C11	0.4770(14)	-0.2403(4)	0.3048(3)	.103(5)
C12	0.7201(13)	-0.1958(5)	0.3114(4)	.076(4)
C13	0.2775(13)	0.2226(5)	0.3808(4)	.049(3)
C14	0.2184(12)	0.2700(4)	0.4051(3)	.074(4)
C15	0.4136(12)	0.2402(4)	0.3585(3)	.070(4)
C16	0.1619(11)	0.2005(5)	0.3524(4)	.072(4)
C17	0.6727(13)	0.1664(6)	0.4485(4)	.057(4)
C18	0.7320(14)	0.1170(5)	0.4703(4)	.108(5)
C19	0.5751(12)	0.2003(4)	0.4739(3)	.085(4)
C20	0.7988(13)	0.1991(6)	0.4320(4)	.100(5)
C21	0.2441(14)	0.0671(5)	0.4552(3)	.045(3)
C22	0.1758(11)	0.1093(4)	0.4836(3)	.070(4)
C23	0.2804(13)	0.0138(5)	0.4780(3)	.083(4)
C24	0.1365(11)	0.0558(4)	0.4213(3)	.065(4)
C30	0.2042(29)	0.0352(10)	0.2948(8)	.052(8)
C30A	0.2520(27)	0.0220(10)	0.2769(8)	.044(7)
C31	0.0877(25)	0.0005(9)	0.2895(7)	.071(9)
C31A	0.1406(29)	-0.0063(9)	0.2697(7)	.059(8)
C32	0.2786(24)	0.0784(8)	0.2610(6)	.052(7)
C32A	0.2134(20)	0.0841(7)	0.2734(6)	.029(6)
C40	0.6240(29)	-0.0192(11)	0.3927(9)	.073(10)
C40A	0.6662(29)	-0.0309(10)	0.3737(9)	.050(8)
C41	0.6198(15)	-0.0796(6)	0.4017(4)	.124(5)
C41A	0.6198(15)	-0.0796(6)	0.4017(4)	.124(5)
C42	0.7475(25)	0.0063(8)	0.3929(6)	.044(7)
C42A	0.7962(35)	-0.0065(14)	0.3662(10)	.162(16)
C50	0.1938(12)	-0.1199(5)	0.3763(4)	.067(4)
C50A	0.1938(12)	-0.1199(5)	0.3763(4)	.067(4)
C51	0.0696(14)	-0.1337(5)	0.3490(3)	.113(4)
C51A	0.0696(14)	-0.1337(5)	0.3490(3)	.113(4)
C52	0.1810(28)	-0.1259(11)	0.4180(8)	.093(10)
C52A	0.1018(25)	-0.1094(9)	0.4136(6)	.070(8)
C60	0.6841(11)	0.1231(5)	0.2884(3)	.058(3)
C60A	0.6841(11)	0.1231(5)	0.2884(3)	.058(3)
C61	0.7780(26)	0.1157(11)	0.2506(8)	.091(11)
C61A	0.7040(21)	0.1237(8)	0.2442(5)	.024(5)

C62	0.8009(11)	0.1376(4)	0.3176(3)	.076(4)
C62A	0.8009(11)	0.1376(4)	0.3176(3)	.076(4)
C70	-0.1707(15)	0.5711(5)	0.3743(4)	.061(4)
C71	-0.2402(12)	0.6143(4)	0.3466(3)	.081(4)
C72	-0.1214(13)	0.5218(5)	0.3493(4)	.098(5)
C73	-0.2778(11)	0.5523(5)	0.4059(3)	.075(4)
C74	-0.1755(14)	0.7201(5)	0.4550(4)	.051(4)
C75	-0.0420(13)	0.7403(4)	0.4787(3)	.076(4)
C76	-0.2432(11)	0.7659(4)	0.4295(3)	.067(4)
C77	-0.2894(12)	0.6938(5)	0.4802(3)	.082(4)
C78	0.2325(13)	0.6747(5)	0.3930(4)	.064(4)
C79	0.1370(12)	0.7054(5)	0.3643(3)	.084(4)
C80	0.3453(27)	0.6391(10)	0.3782(7)	.068(9)
C80A	0.2875(28)	0.6251(10)	0.3665(7)	.070(9)
C81	0.3198(26)	0.7266(8)	0.4144(7)	.062(8)
C81A	0.3647(31)	0.7000(12)	0.4085(8)	.095(11)
C82	0.2390(14)	0.6207(5)	0.5478(4)	.086(4)
C82A	0.2390(14)	0.6207(5)	0.5478(4)	.086(4)
C83	0.3678(20)	0.6308(7)	0.5265(5)	.203(8)
C83A	0.3678(20)	0.6308(7)	0.5265(5)	.203(8)
C84	0.3169(19)	0.6130(8)	0.5872(6)	.051(7)
C84A	0.1778(25)	0.6444(9)	0.5834(7)	.109(9)
C85	0.2435(25)	0.4686(8)	0.4641(7)	.032(7)
C85A	0.1973(28)	0.4811(12)	0.4443(10)	.070(9)
C86	0.3406(25)	0.5080(11)	0.4590(9)	.091(10)
C86A	0.2978(34)	0.5121(11)	0.4348(8)	.096(10)
C87	0.1971(13)	0.4243(6)	0.4325(4)	.113(5)
C87A	0.1971(13)	0.4243(6)	0.4325(4)	.113(5)
H2A	0.7458(11)	-0.0833(5)	0.2548(3)	.092
H2B	0.6755(11)	-0.0252(5)	0.2581(3)	.092
H2C	0.8083(11)	-0.0351(5)	0.2294(3)	.092
H3A	0.5064(13)	-0.0251(4)	0.1633(3)	.139
H3B	0.6599(13)	0.0011(4)	0.1727(3)	.139
H3C	0.5271(13)	0.0110(4)	0.2013(3)	.139
H4A	0.6152(11)	-0.1144(5)	0.1587(3)	.097
H4B	0.7073(11)	-0.1386(5)	0.1940(3)	.097
H4C	0.7718(11)	-0.0911(5)	0.1683(3)	.097

H6A	0.2385(28)	-0.0966(9)	0.1851(7)	.070
H6B	0.0966(28)	-0.0894(9)	0.2109(7)	.070
H6C	0.0910(28)	-0.1243(9)	0.1719(7)	.070
H6A1	0.1535(33)	-0.1029(13)	0.1884(9)	.160
H6A2	0.0405(33)	-0.1126(13)	0.2228(9)	.160
H6A3	0.0326(33)	-0.1481(13)	0.1841(9)	.160
H7A	0.0792(26)	-0.2254(10)	0.2491(6)	.099
H7B	-0.0030(26)	-0.2033(10)	0.2115(6)	.099
H7C	0.0049(26)	-0.1678(10)	0.2501(6)	.099
H7A1	0.1776(27)	-0.2423(8)	0.2541(6)	.095
H7A2	0.0455(27)	-0.2365(8)	0.2244(6)	.095
H7A3	0.0484(27)	-0.2022(8)	0.2637(6)	.095
H8A	0.3527(11)	-0.2247(4)	0.2067(3)	.097
H8B	0.3539(11)	-0.1749(4)	0.1776(3)	.097
H8C	0.2330(11)	-0.2200(4)	0.1733(3)	.097
H10A	0.7593(11)	-0.2468(5)	0.2444(3)	.113
H10B	0.6066(11)	-0.2754(5)	0.2388(3)	.113
H10C	0.7086(11)	-0.2918(5)	0.2745(3)	.113
H11A	0.4348(14)	-0.2117(4)	0.3206(3)	.155
H11B	0.5073(14)	-0.2697(4)	0.3218(3)	.155
H11C	0.4052(14)	-0.2534(4)	0.2862(3)	.155
H12A	0.8019(13)	-0.1824(5)	0.2963(4)	.114
H12B	0.7533(13)	-0.2239(5)	0.3292(4)	.114
H12C	0.6780(13)	-0.1665(5)	0.3264(4)	.114
H14A	0.1321(12)	0.2586(4)	0.4192(3)	.112
H14B	0.1938(12)	0.2997(4)	0.3877(3)	.112
H14C	0.2920(12)	0.2817(4)	0.4237(3)	.112
H15A	0.4852(12)	0.2539(4)	0.3770(3)	.105
H15B	0.3881(12)	0.2683(4)	0.3399(3)	.105
H15C	0.4538(12)	0.2095(4)	0.3445(3)	.105
H16A	0.0766(11)	0.1896(5)	0.3671(4)	.109
H16B	0.2009(11)	0.1697(5)	0.3384(4)	.109
H16C	0.1351(11)	0.2284(5)	0.3337(4)	.109
H18A	0.7941(14)	0.0964(5)	0.4528(4)	.162
H18B	0.6516(14)	0.0945(5)	0.4788(4)	.162
H18C	0.7878(14)	0.1286(5)	0.4930(4)	.162
H19A	0.4963(12)	0.1782(4)	0.4839(3)	.128
H19B	0.5352(12)	0.2297(4)	0.4584(3)	.128

H19C	0.6307(12)	0.2148(4)	0.4957(3)	.128
H20A	0.8593(13)	0.1761(6)	0.4158(4)	.150
H20B	0.8564(13)	0.2136(6)	0.4534(4)	.150
H20C	0.7609(13)	0.2285(6)	0.4161(4)	.150
H22A	0.2430(11)	0.1166(4)	0.5050(3)	.105
H22B	0.0855(11)	0.0952(4)	0.4941(3)	.105
H22C	0.1563(11)	0.1425(4)	0.4694(3)	.105
H23A	0.3480(13)	-0.0216(5)	0.4992(3)	.124
H23B	0.3239(13)	-0.0120(5)	0.4601(3)	.124
H23C	0.1916(13)	-0.0013(5)	0.4888(3)	.124
H24A	0.1785(11)	0.0296(4)	0.4035(3)	.098
H24B	0.1171(11)	0.0891(4)	0.4072(3)	.098
H24C	0.0463(11)	0.0418(4)	0.4319(3)	.098
H30	0.1385(29)	0.0517(10)	0.3144(8)	.063
H30A	0.2892(27)	0.0059(10)	0.2523(8)	.053
H31A	0.0899(25)	-0.0383(9)	0.2931(7)	.107
H31B	0.0187(25)	0.0095(9)	0.2688(7)	.107
H31C	0.0584(25)	0.0177(9)	0.3138(7)	.107
H31D	0.0945(29)	-0.0335(9)	0.2859(7)	.089
H31E	0.2165(29)	-0.0229(9)	0.2541(7)	.089
H31F	0.0686(29)	0.0098(9)	0.2524(7)	.089
H32A	0.3250(24)	0.1083(8)	0.2745(6)	.078
H32B	0.2026(24)	0.0921(8)	0.2438(6)	.078
H32C	0.3504(24)	0.0593(8)	0.2455(6)	.078
H32D	0.2997(20)	0.1041(7)	0.2659(6)	.044
H32E	0.1783(20)	0.0972(7)	0.2984(6)	.044
H32F	0.1385(20)	0.0890(7)	0.2535(6)	.044
H40	0.6020(29)	0.0054(11)	0.4149(9)	.088
H40A	0.7276(29)	-0.0462(10)	0.3526(9)	.060
H41A	0.5309(15)	-0.0881(6)	0.4157(4)	.186
H41B	0.7031(15)	-0.0892(6)	0.4178(4)	.186
H41C	0.6227(15)	-0.0997(6)	0.3773(4)	.186
H41D	0.5619(25)	-0.1052(8)	0.3869(6)	.186
H41E	0.5631(25)	-0.0657(8)	0.4235(6)	.186
H41F	0.7063(25)	-0.0973(8)	0.4118(6)	.186
H42A	0.7734(25)	0.0351(8)	0.3749(6)	.065
H42B	0.8353(25)	-0.0106(8)	0.4029(6)	.065
H42C	0.6921(25)	0.0211(8)	0.4146(6)	.065

H42D	0.8037(35)	0.0315(14)	0.3599(10)	.244
H42E	0.7975(35)	0.0275(14)	0.3422(10)	.244
H42F	0.8778(35)	-0.0170(14)	0.3827(10)	.244
H50	0.2693(12)	-0.1467(5)	0.3693(4)	.080
H50A	0.2650(14)	-0.1495(5)	0.3794(3)	.080
H51A	0.0985(14)	-0.1270(5)	0.3221(3)	.169
H51B	0.0141(14)	-0.1116(5)	0.3554(3)	.169
H51C	0.0445(14)	-0.1715(5)	0.3521(3)	.169
H51D	0.1074(28)	-0.1418(11)	0.3231(8)	.169
H51E	0.0034(28)	-0.1034(11)	0.3473(8)	.169
H51F	0.0182(28)	-0.1649(11)	0.3591(8)	.169
H52A	0.2713(28)	-0.1151(11)	0.4305(8)	.140
H52B	0.1608(28)	-0.1634(11)	0.4242(8)	.140
H52C	0.1022(28)	-0.1034(11)	0.4274(8)	.140
H52D	0.1656(25)	-0.0995(9)	0.4352(6)	.105
H52E	0.0485(25)	-0.1419(9)	0.4204(6)	.105
H52F	0.0337(25)	-0.0803(9)	0.4086(6)	.105
H60	0.6119(11)	0.1525(5)	0.2853(3)	.070
H60A	0.6074(26)	0.1504(11)	0.2930(8)	.070
H61A	0.7154(26)	0.1060(11)	0.2287(8)	.137
H61B	0.8489(26)	0.0874(11)	0.2550(8)	.137
H61C	0.8279(26)	0.1492(11)	0.2448(8)	.137
H61D	0.6139(21)	0.1129(8)	0.2315(5)	.037
H61E	0.7808(21)	0.0988(8)	0.2371(5)	.037
H61F	0.7300(21)	0.1598(8)	0.2358(5)	.037
H62A	0.7573(11)	0.1435(4)	0.3432(3)	.114
H62B	0.8498(11)	0.1702(4)	0.3092(3)	.114
H62C	0.8708(11)	0.1084(4)	0.3194(3)	.114
H62D	0.7628(15)	0.1342(5)	0.3441(4)	.114
H62E	0.8322(15)	0.1745(5)	0.3132(4)	.114
H62F	0.8830(15)	0.1134(5)	0.3145(4)	.114
H71A	-0.1697(12)	0.6252(4)	0.3270(3)	.122
H71B	-0.2694(12)	0.6454(4)	0.3619(3)	.122
H71C	-0.3248(12)	0.5990(4)	0.3336(3)	.122
H72A	-0.0536(13)	0.5336(5)	0.3293(4)	.147
H72B	-0.2056(13)	0.5054(5)	0.3369(4)	.147
H72C	-0.0742(13)	0.4955(5)	0.3662(4)	.147
H73A	-0.3086(11)	0.5830(5)	0.4215(3)	.112

H73B	-0.2306(11)	0.5260(5)	0.4228(3)	.112
H73C	-0.3620(11)	0.5359(5)	0.3935(3)	.112
H75A	0.0274(13)	0.7568(4)	0.4609(3)	.114
H75B	0.0035(13)	0.7101(4)	0.4921(3)	.114
H75C	-0.0733(13)	0.7667(4)	0.4979(3)	.114
H76A	-0.1680(11)	0.7822(4)	0.4135(3)	.100
H76B	-0.2856(11)	0.7930(4)	0.4465(3)	.100
H76C	-0.3182(11)	0.7509(4)	0.4125(3)	.100
H77A	-0.3699(12)	0.6820(5)	0.4638(3)	.123
H77B	-0.3244(12)	0.7195(5)	0.4994(3)	.123
H77C	-0.2475(12)	0.6629(5)	0.4936(3)	.123
H79A	0.0676(12)	0.7272(5)	0.3787(3)	.126
H79B	0.0852(12)	0.6800(5)	0.3476(3)	.126
H79C	0.1972(12)	0.7286(5)	0.3481(3)	.126
H80A	0.3011(27)	0.6103(10)	0.3630(7)	.102
H80B	0.3994(27)	0.6239(10)	0.4000(7)	.102
H80C	0.4109(27)	0.6595(10)	0.3615(7)	.102
H80D	0.2055(28)	0.6095(10)	0.3525(7)	.105
H80E	0.3316(28)	0.5979(10)	0.3832(7)	.105
H80F	0.3587(28)	0.6379(10)	0.3477(7)	.105
H81A	0.2492(26)	0.7518(8)	0.4250(7)	.094
H81B	0.3797(26)	0.7448(8)	0.3951(7)	.094
H81C	0.3810(26)	0.7132(8)	0.4356(7)	.094
H81D	0.3388(31)	0.7319(12)	0.4235(8)	.143
H81E	0.4272(31)	0.7103(12)	0.3869(8)	.143
H81F	0.4157(31)	0.6747(12)	0.4254(8)	.143
H82	0.1707(14)	0.6516(5)	0.5477(4)	.103
H82A	0.1779(20)	0.6428(7)	0.5300(5)	.103
H83A	0.3438(20)	0.6372(7)	0.4991(5)	.305
H83B	0.4320(20)	0.5999(7)	0.5285(5)	.305
H83C	0.4161(20)	0.6624(7)	0.5372(5)	.305
H83D	0.3724(19)	0.6068(8)	0.5040(6)	.305
H83E	0.4515(19)	0.6247(8)	0.5433(6)	.305
H83F	0.3680(19)	0.6680(8)	0.5175(6)	.305
H84A	0.2459(19)	0.6051(8)	0.6074(6)	.076
H84B	0.3692(19)	0.6457(8)	0.5940(6)	.076
H84C	0.3851(19)	0.5832(8)	0.5852(6)	.076
H84D	0.0861(25)	0.6270(9)	0.5894(7)	.164

H84E	0.1615(25)	0.6827(9)	0.5792(7)	.164
H84F	0.2451(25)	0.6394(9)	0.6051(7)	.164
H85	0.3137(25)	0.4569(8)	0.4846(7)	.038
H85A	0.1593(28)	0.5028(12)	0.4220(10)	.084
H86A	0.3219(25)	0.5454(11)	0.4657(9)	.137
H86B	0.4134(25)	0.5062(11)	0.4385(9)	.137
H86C	0.3758(25)	0.4890(11)	0.4821(9)	.137
H86D	0.3317(34)	0.5434(11)	0.4493(8)	.144
H86E	0.2186(34)	0.5226(11)	0.4175(8)	.144
H86F	0.3770(34)	0.4975(11)	0.4194(8)	.144
H87A	0.0999(13)	0.4140(6)	0.4242(4)	.169
H87B	0.2269(13)	0.4020(6)	0.4545(4)	.169
H87C	0.2643(13)	0.4191(6)	0.4109(4)	.169
H87D	0.1591	0.3927	0.4458(52)	.169
H87E	0.2813	0.4140	0.4170(52)	.169
H87F	0.1228	0.4390	0.4152(52)	.169

Ueq is defined as one third of the orthoganalized Uij tensor

Table 6. Anisotropic displacement parameters for **3**.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	0.058(3)	0.031(2)	0.042(2)	-0.005(2)	0.008(2)	-0.002(2)
Si2	0.053(3)	0.028(2)	0.039(2)	-0.004(2)	0.000(2)	-0.001(2)
Si3	0.058(3)	0.029(2)	0.041(2)	-0.001(2)	0.000(2)	-0.001(2)
Al1	0.070(3)	0.030(2)	0.037(2)	-0.001(2)	0.000(2)	0.002(2)
Al2	0.054(3)	0.033(2)	0.038(2)	-0.003(2)	-0.003(2)	-0.006(2)
Al3	0.071(3)	0.030(2)	0.035(2)	0.000(2)	0.003(2)	-0.006(2)
O1	0.069(6)	0.026(4)	0.038(4)	-0.013(3)	0.012(4)	-0.009(4)
O2	0.074(5)	0.030(4)	0.040(4)	-0.007(3)	0.006(4)	-0.003(4)
O3	0.050(6)	0.031(5)	0.038(5)	-0.003(4)	-0.014(4)	0.007(4)
O4	0.061(6)	0.047(5)	0.035(4)	-0.004(3)	-0.025(4)	-0.001(4)
O5	0.104(7)	0.027(5)	0.056(6)	-0.008(4)	0.024(5)	-0.024(5)
O6	0.067(5)	0.042(5)	0.058(5)	-0.014(4)	0.025(4)	-0.018(4)
O11	0.065(6)	0.044(5)	0.058(5)	-0.003(4)	0.011(4)	-0.006(4)
O12	0.035(6)	0.040(5)	0.071(7)	-0.015(4)	0.017(5)	-0.006(4)
O13	0.056(5)	0.041(4)	0.038(4)	-0.002(4)	0.003(4)	0.010(4)
O21	0.059(5)	0.028(5)	0.032(5)	-0.003(4)	0.004(4)	0.004(4)
O22	0.045(6)	0.044(5)	0.053(5)	0.001(4)	-0.019(4)	-0.003(4)
O23	0.053(6)	0.036(5)	0.045(5)	0.002(4)	0.000(4)	0.000(4)
O70	0.104(6)	0.023(4)	0.028(4)	0.010(4)	0.004(4)	0.002(4)
O71	0.072(6)	0.037(5)	0.038(5)	-0.014(4)	-0.021(4)	-0.007(4)
O72	0.068(6)	0.034(5)	0.034(5)	-0.001(4)	-0.001(4)	0.003(4)
O73	0.042(6)	0.067(6)	0.048(6)	0.017(4)	0.009(4)	-0.006(4)
O74	0.098(6)	0.033(5)	0.058(6)	-0.001(4)	-0.036(4)	-0.025(4)
O75	0.058(6)	0.041(5)	0.040(5)	-0.002(4)	0.018(4)	-0.002(4)
C1	0.042(9)	0.031(8)	0.053(8)	-0.001(7)	0.008(8)	-0.002(7)
C2	0.064(9)	0.070(10)	0.051(9)	0.006(8)	-0.018(7)	-0.034(7)
C3	0.100(11)	0.063(9)	0.115(11)	0.025(8)	-0.008(10)	-0.001(8)
C4	0.096(10)	0.066(10)	0.033(9)	0.015(8)	0.014(6)	0.011(7)
C5	0.038(10)	0.082(12)	0.053(10)	-0.031(9)	-0.015(8)	-0.024(8)
C8	0.062(10)	0.057(9)	0.074(10)	-0.021(8)	0.013(8)	-0.007(7)
C9	0.097(11)	0.027(7)	0.022(7)	0.006(6)	0.009(8)	0.003(8)
C10	0.113(11)	0.045(9)	0.068(10)	0.007(8)	-0.004(8)	0.026(7)
C11	0.124(13)	0.070(9)	0.115(11)	0.048(8)	0.039(10)	0.004(9)
C12	0.105(12)	0.064(11)	0.058(11)	-0.008(8)	-0.024(8)	0.034(8)

C13	0.061(10)	0.046(9)	0.039(9)	0.012(8)	-0.009(8)	0.010(8)
C14	0.147(13)	0.033(9)	0.044(9)	-0.008(7)	0.006(8)	0.029(7)
C15	0.073(10)	0.058(9)	0.079(10)	0.042(7)	0.017(8)	0.010(7)
C16	0.073(10)	0.064(10)	0.080(11)	0.007(8)	-0.037(8)	-0.001(7)
C17	0.058(11)	0.068(11)	0.045(10)	-0.014(9)	-0.017(8)	-0.010(8)
C18	0.154(14)	0.090(11)	0.079(11)	0.016(8)	-0.069(10)	0.023(10)
C19	0.069(10)	0.111(10)	0.076(9)	-0.056(8)	-0.017(8)	0.007(8)
C20	0.081(11)	0.141(14)	0.077(11)	-0.010(10)	-0.021(8)	-0.060(10)
C21	0.052(10)	0.045(9)	0.039(9)	0.009(8)	0.021(8)	0.001(7)
C22	0.083(10)	0.052(10)	0.075(10)	-0.018(8)	0.004(7)	-0.009(7)
C23	0.116(12)	0.058(9)	0.074(10)	0.017(8)	0.020(8)	0.005(8)
C24	0.064(10)	0.059(9)	0.072(10)	-0.005(7)	-0.012(8)	-0.016(7)
C70	0.098(12)	0.046(10)	0.039(9)	-0.010(8)	-0.017(8)	0.004(8)
C71	0.117(11)	0.057(8)	0.070(10)	0.000(7)	-0.042(8)	-0.006(8)
C72	0.136(13)	0.054(9)	0.104(11)	-0.039(8)	-0.044(9)	-0.010(9)
C73	0.072(10)	0.087(10)	0.065(10)	0.002(8)	-0.025(8)	-0.002(8)
C74	0.079(11)	0.037(9)	0.038(9)	0.000(8)	0.004(8)	0.015(7)
C75	0.113(11)	0.049(8)	0.065(9)	-0.020(6)	-0.014(9)	0.000(8)
C76	0.079(9)	0.042(8)	0.078(10)	-0.014(7)	-0.021(7)	0.025(7)
C77	0.089(11)	0.101(11)	0.055(9)	0.002(8)	0.020(8)	0.027(9)
C78	0.047(10)	0.080(10)	0.066(10)	-0.006(8)	-0.008(8)	0.002(8)
C79	0.093(11)	0.109(12)	0.049(9)	0.049(8)	-0.002(8)	-0.006(8)

The general temperature factor expression:

exp(-2p2(a*2U11h2 + b*2U22k2 + c*2U33l2 + 2a*b*U12hk + 2a*c*U13hl + 2b*c*U23kl))

Table 7. Bond Lengths (Å) for **3**.

atom	atom	distance			
			Si2	O21	1.633(7)
			Si3	O73	1.563(7)
Si1	O1	1.588(6)	Si3	O70	1.585(6)
Si1	O12	1.616(7)	Si3	O72	1.620(7)
Si1	O13	1.621(6)	Si3	O71	1.624(6)
Si1	O11	1.635(7)	Al1	O5	1.670(7)
Si2	O2	1.596(6)	Al1	O1	1.687(6)
Si2	O22	1.608(7)	Al1	O4	1.812(6)
Si2	O23	1.620(7)	Al1	O3	1.815(7)

Al1	Al2	2.753(4)	C5	C7A	1.63(2)
Al2	O6	1.658(6)	C5	C6	1.64(3)
Al2	O2	1.684(6)	C9	C11	1.470(13)
Al2	O3	1.799(7)	C9	C10	1.506(13)
Al2	O4	1.827(6)	C9	C12	1.518(13)
Al3	O74	1.664(7)	C13	C15	1.513(13)
Al3	O70	1.694(6)	C13	C16	1.520(13)
Al3	O75#1	1.807(7)	C13	C14	1.522(13)
Al3	O75	1.816(6)	C17	C19	1.489(13)
Al3	Al3#1	2.754(6)	C17	C20	1.509(14)
O3	C30A	1.41(2)	C17	C18	1.515(15)
O3	C30	1.47(3)	C21	C24	1.527(13)
O4	C40A	1.45(2)	C21	C22	1.540(13)
O4	C40	1.53(3)	C21	C23	1.552(13)
O5	C50A	1.406(12)	C30	C31A	1.44(3)
O5	C50	1.406(12)	C30	C32	1.70(3)
O6	C60A	1.438(11)	C30A	C32A	1.57(3)
O6	C60	1.438(11)	C30A	C31	1.64(3)
O11	C1	1.435(11)	C40	C41	1.51(3)
O12	C5	1.445(12)	C40	C42A	1.83(4)
O13	C9	1.445(10)	C40A	C42	1.34(3)
O21	C13	1.439(11)	C40A	C41A	1.58(3)
O22	C17	1.450(11)	C50	C52	1.42(3)
O23	C21	1.430(11)	C50	C51	1.492(14)
O71	C70	1.415(12)	C50A	C51A	1.492(14)
O72	C74	1.448(12)	C50A	C52A	1.54(2)
O73	C78	1.436(13)	C60	C62	1.489(13)
O74	C82A	1.424(12)	C60	C61	1.54(3)
O74	C82	1.424(12)	C60A	C62A	1.489(13)
O75	C85A	1.48(3)	C60A	C61A	1.50(2)
O75	C85	1.50(2)	C70	C73	1.519(14)
O75	Al3#1	1.807(7)	C70	C72	1.542(14)
C1	C2	1.498(12)	C70	C71	1.546(13)
C1	C3	1.505(12)	C74	C77	1.488(14)
C1	C4	1.517(12)	C74	C75	1.533(13)
C5	C6A	1.42(3)	C74	C76	1.543(13)
C5	C7	1.47(2)	C78	C80	1.44(2)
C5	C8	1.512(14)	C78	C81A	1.45(3)

C78	C79	1.502(14)	C82A	C84A	1.45(2)
C78	C80A	1.59(3)	C85	C86A	1.54(3)
C78	C81	1.66(2)	C85	C87A	1.58(2)
C82	C83	1.40(2)	C85A	C87	1.45(3)
C82	C84	1.52(2)	C85A	C86	1.54(3)
C82A	C83A	1.40(2)			

Table 8. Bond angles (°) for **3**.

atom	atom	atom	angle	O4	Al1	Al2	41.1(2)
				O3	Al1	Al2	40.2(2)
O1	Si1	O12	106.7(4)	O6	Al2	O2	119.1(3)
O1	Si1	O13	112.0(3)	O6	Al2	O3	112.3(3)
O12	Si1	O13	113.5(4)	O2	Al2	O3	111.8(3)
O1	Si1	O11	112.8(3)	O6	Al2	O4	112.0(3)
O12	Si1	O11	106.1(4)	O2	Al2	O4	114.3(3)
O13	Si1	O11	105.7(4)	O3	Al2	O4	81.3(3)
O2	Si2	O22	105.4(4)	O6	Al2	Al1	120.0(2)
O2	Si2	O23	112.3(3)	O2	Al2	Al1	120.9(2)
O22	Si2	O23	106.5(4)	O3	Al2	Al1	40.6(2)
O2	Si2	O21	111.8(4)	O4	Al2	Al1	40.6(2)
O22	Si2	O21	114.3(3)	O74	Al3	O70	119.4(4)
O23	Si2	O21	106.6(4)	O74	Al3	O75#1	113.2(3)
O73	Si3	O70	106.1(4)	O70	Al3	O75#1	110.7(3)
O73	Si3	O72	113.1(4)	O74	Al3	O75	110.6(4)
O70	Si3	O72	110.9(4)	O70	Al3	O75	115.7(3)
O73	Si3	O71	105.7(4)	O75#1	Al3	O75	81.1(3)
O70	Si3	O71	114.2(3)	O74	Al3	Al3#1	119.4(3)
O72	Si3	O71	106.9(4)	O70	Al3	Al3#1	121.2(3)
O5	Al1	O1	119.1(3)	O75#1	Al3	Al3#1	40.6(2)
O5	Al1	O4	112.1(4)	O75	Al3	Al3#1	40.4(2)
O1	Al1	O4	111.3(3)	Si1	O1	Al1	148.7(4)
O5	Al1	O3	112.3(4)	Si2	O2	Al2	149.8(4)
O1	Al1	O3	114.6(3)	C30A	O3	C30	32.5(12)
O4	Al1	O3	81.2(3)	C30A	O3	Al2	133.5(11)
O5	Al1	Al2	119.7(3)	C30	O3	Al2	125.8(11)
O1	Al1	Al2	121.1(2)	C30A	O3	Al1	125.2(11)

C30	O3	Al1	129.4(11)	C3	C1	C4	108.7(9)
Al2	O3	Al1	99.2(3)	C6A	C5	O12	113.8(16)
C40A	O4	C40	31.2(13)	C6A	C5	C7	83.3(15)
C40A	O4	Al1	128.5(11)	O12	C5	C7	110.0(12)
C40	O4	Al1	133.0(11)	C6A	C5	C8	116.6(16)
C40A	O4	Al2	130.2(11)	O12	C5	C8	110.9(10)
C40	O4	Al2	124.7(11)	C7	C5	C8	119.7(13)
Al1	O4	Al2	98.3(3)	C6A	C5	C7A	112.8(17)
C50A	O5	C50	0.0(14)	O12	C5	C7A	98.4(11)
C50A	O5	Al1	134.2(7)	C7	C5	C7A	29.6(11)
C50	O5	Al1	134.2(7)	C8	C5	C7A	102.3(12)
C60A	O6	C60	0.0(13)	C6A	C5	C6	24.3(15)
C60A	O6	Al2	135.6(6)	O12	C5	C6	103.9(12)
C60	O6	Al2	135.6(6)	C7	C5	C6	107.6(16)
C1	O11	Si1	131.6(6)	C8	C5	C6	103.2(12)
C5	O12	Si1	134.1(7)	C7A	C5	C6	137.1(16)
C9	O13	Si1	130.8(6)	O13	C9	C11	111.7(10)
C13	O21	Si2	130.2(6)	O13	C9	C10	104.3(8)
C17	O22	Si2	132.6(7)	C11	C9	C10	112.0(10)
C21	O23	Si2	131.9(7)	O13	C9	C12	108.0(9)
Si3	O70	Al3	147.1(4)	C11	C9	C12	111.8(9)
C70	O71	Si3	131.5(7)	C10	C9	C12	108.6(11)
C74	O72	Si3	131.1(6)	O21	C13	C15	111.8(9)
C78	O73	Si3	132.2(7)	O21	C13	C16	107.4(9)
C82A	O74	C82	0.0(14)	C15	C13	C16	110.8(10)
C82A	O74	Al3	134.9(7)	O21	C13	C14	105.5(9)
C82	O74	Al3	134.9(7)	C15	C13	C14	109.8(10)
C85A	O75	C85	32.9(12)	C16	C13	C14	111.4(10)
C85A	O75	Al3#1	131.4(11)	O22	C17	C19	110.9(9)
C85	O75	Al3#1	125.4(9)	O22	C17	C20	104.8(10)
C85A	O75	Al3	126.9(12)	C19	C17	C20	111.8(11)
C85	O75	Al3	130.5(9)	O22	C17	C18	107.0(10)
Al3#1	O75	Al3	98.9(3)	C19	C17	C18	112.4(11)
O11	C1	C2	112.0(9)	C20	C17	C18	109.6(11)
O11	C1	C3	105.4(9)	O23	C21	C24	113.2(9)
C2	C1	C3	111.4(9)	O23	C21	C22	108.3(9)
O11	C1	C4	108.6(8)	C24	C21	C22	109.1(10)
C2	C1	C4	110.6(10)	O23	C21	C23	105.4(9)

C24	C21	C23	110.6(10)	O72	C74	C75	109.4(9)
C22	C21	C23	110.2(9)	C77	C74	C75	113.3(11)
C31A	C30	O3	107.5(21)	O72	C74	C76	103.5(9)
C31A	C30	C32	102.1(21)	C77	C74	C76	110.8(10)
O3	C30	C32	96.1(17)	C75	C74	C76	111.6(10)
O3	C30A	C32A	109.3(19)	O73	C78	C80	112.2(14)
O3	C30A	C31	107.2(18)	O73	C78	C81A	109.0(14)
C32A	C30A	C31	97.4(17)	C80	C78	C81A	78.1(15)
C41	C40	O4	105.6(19)	O73	C78	C79	113.7(10)
C41	C40	C42A	106.6(19)	C80	C78	C79	119.4(14)
O4	C40	C42A	92.5(18)	C81A	C78	C79	119.6(15)
C42	C40A	O4	116.8(20)	O73	C78	C80A	105.8(13)
C42	C40A	C41A	112.0(21)	C80	C78	C80A	27.7(13)
O4	C40A	C41A	106.0(17)	C81A	C78	C80A	105.5(17)
O5	C50	C52	112.2(15)	C79	C78	C80A	101.7(12)
O5	C50	C51	111.2(10)	O73	C78	C81	103.3(11)
C52	C50	C51	121.4(15)	C80	C78	C81	105.9(15)
O5	C50A	C51A	111.2(10)	C81A	C78	C81	28.5(13)
O5	C50A	C52A	107.0(12)	C79	C78	C81	99.8(12)
C51A	C50A	C52A	97.4(12)	C80A	C78	C81	132.7(16)
O6	C60	C62	109.7(9)	C83	C82	O74	111.4(12)
O6	C60	C61	111.0(13)	C83	C82	C84	94.7(12)
C62	C60	C61	100.2(13)	O74	C82	C84	109.8(11)
O6	C60A	C62A	109.7(9)	C83A	C82A	O74	111.4(12)
O6	C60A	C61A	109.0(11)	C83A	C82A	C84A	132.8(16)
C62A	C60A	C61A	124.4(11)	O74	C82A	C84A	114.6(13)
O71	C70	C73	111.4(10)	O75	C85	C86A	105.3(18)
O71	C70	C72	104.4(10)	O75	C85	C87A	102.3(15)
C73	C70	C72	109.4(10)	C86A	C85	C87A	97.5(19)
O71	C70	C71	110.5(10)	C87	C85A	O75	109.7(21)
C73	C70	C71	111.7(10)	C87	C85A	C86	120.0(21)
C72	C70	C71	109.1(10)	O75	C85A	C86	102.3(21)
O72	C74	C77	107.7(9)				