Supplementary Material for:

Dianion Aggregates Derived from Lithiation of N-silyl allylamine

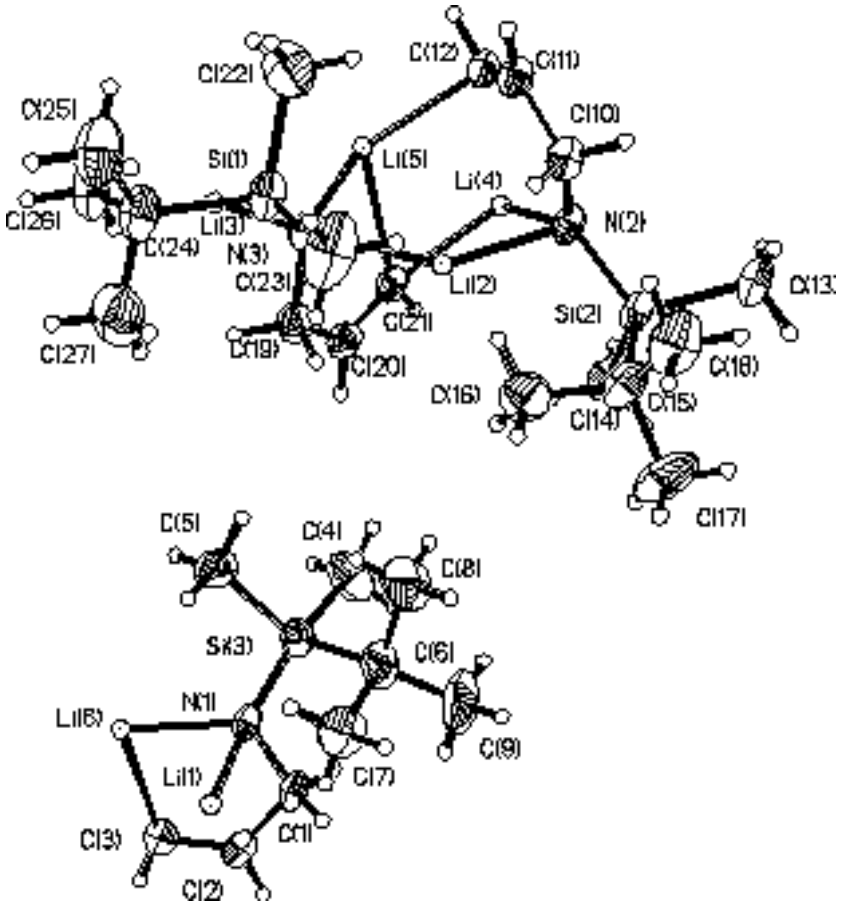
Paul G. Williard* and Madeleine A. Jacobson

Department of Chemistry, Brown University, Providence, Rhode Island 02912

e-mail:Paul_Williard@brown.edu

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

Identification code	mj20	
Empirical formula	C27 H57 Li6 N3 Si3	
Formula weight	549.67	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 14.203(10) Å	α = 90º.
	b = 12.651(9) Å	β= 100.32(3) º.
	c = 20.615(13) Å	γ = 90º.
Volume	3644(4) $Å^3$	
Z	4	
Density (calculated)	1.002 Mg/m^3	
Absorption coefficient	0.148 mm^{-1}	
F(000)	1200	
Crystal size	0.3 x 0.4 x 0.45 mm	
Theta range for data collection	1.61 to 23.37º.	
Index ranges	-13<=h<=15, -14<=k<=14, -22<=l<=22	
Reflections collected	16011	
Independent reflections	5155 [R(int) = 0.0866]	
Completeness to theta = 23.37º	97.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5155 / 0 / 355	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1580	
R indices (all data)	R1 = 0.0756, wR2 = 0.1697	
Largest diff. peak and hole	0.339 and -0.279 e. $Å^{-3}$	



Crystallographic Asymmetric Unit for Anion 1

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for anion 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	5730(1)	1797(1)	2437(1)	38(1)
Si(2)	1695(1)	670(1)	920(1)	33(1)
Si(3)	3125(1)	6290(1)	68(1)	34(1)
N(1)	3138(2)	7588(2)	-169(1)	30(1)
N(2)	2830(2)	164(2)	1033(1)	30(1)
N(3)	5274(2)	1867(2)	1610(1)	31(1)
C(1)	2259(2)	8088(3)	-516(2)	33(1)
C(2)	2455(2)	9159(3)	-786(2)	33(1)
C(3)	3338(2)	9567(3)	-739(1)	32(1)
C(4)	2950(3)	5324(3)	-630(2)	62(1)
C(5)	4311(3)	6018(3)	598(2)	48(1)
C(6)	2162(3)	6001(3)	584(2)	49(1)
C(7)	2174(3)	6882(3)	1091(2)	57(1)
C(8)	2379(3)	4947(3)	956(2)	70(1)
C(9)	1155(3)	5925(4)	161(3)	82(2)
C(10)	3226(2)	-406(3)	1642(1)	34(1)
C(11)	4136(2)	-984(3)	1590(2)	34(1)
C(12)	4525(2)	-1002(3)	1040(2)	32(1)
C(13)	744(2)	-371(3)	822(2)	51(1)
C(14)	1554(3)	1482(3)	152(2)	47(1)
C(15)	1451(2)	1577(3)	1615(2)	47(1)
C(16)	2309(3)	2304(3)	1832(2)	59(1)
C(17)	569(3)	2271(4)	1373(2)	78(2)
C(18)	1264(3)	936(4)	2213(2)	68(1)
C(19)	4888(2)	2873(3)	1326(2)	39(1)
C(20)	4358(2)	2736(3)	628(2)	35(1)
C(21)	4234(2)	1802(2)	318(2)	31(1)
C(22)	6189(3)	418(3)	2595(2)	65(1)
C(23)	4806(3)	2037(5)	2965(2)	76(2)
C(24)	6768(3)	2736(3)	2733(2)	47(1)
C(25)	7326(3)	2389(4)	3403(2)	71(1)
C(26)	7447(3)	2755(4)	2236(2)	60(1)
C(27)	6405(3)	3870(4)	2801(2)	74(1)
Li(1)	3013(4)	8563(5)	631(3)	39(1)
Li(2)	3813(4)	1371(5)	1284(3)	41(1)
Li(3)	6388(4)	2065(5)	1082(3)	40(1)
Li(4)	3616(4)	251(4)	290(2)	35(1)
Li(5)	5262(4)	570(4)	1003(3)	36(1)
Li(6)	4364(4)	8474(5)	28(2)	37(1)

Table 3. Bond lengths [Å] and angles [°] for anion 1.

Si(1)-N(3)	1.715(3)
Si(1)-C(22)	1.871(5)
Si(1)-C(23)	1.875(4)
Si(1)-C(24)	1.907(4)
Si(2)-N(2)	1.711(3)
Si(2)-C(13)	1.872(4)
Si(2)-C(14)	1.869(4)
Si(2)-C(15)	1.915(4)
Si(3)-N(1)	1.715(3)
Si(3)-C(5)	1.868(4)
Si(3)-C(4)	1.871(4)
Si(3)-C(6)	1.913(4)
N(1)-C(1)	1.467(4)
N(2)-C(10)	1.470(4)
N(3)-C(19)	1.465(4)
C(1)-C(2)	1.508(5)
C(2)-C(3)	1.344(4)
C(6)-C(7)	1.525(5)
C(6)-C(8)	1.541(6)
C(6)-C(9)	1.539(6)
C(10)-C(11)	1.506(4)
C(11)-C(12)	1.346(4)
C(15)-C(16)	1.529(5)
C(15)-C(17)	1.539(5)
C(15)-C(18)	1.538(6)
C(19)-C(20)	1.509(5)
C(20)-C(21)	1.340(5)
C(24)-C(27)	1.541(6)
C(24)-C(25)	1.528(5)
C(24)-C(26)	1.527(5)
N(3)-Si(1)-C(22)	106.25(15)
N(3)-Si(1)-C(23)	112.97(17)
C(22)-Si(1)-C(23)	107.9(2)
N(3)-Si(1)-C(24)	114.77(15)
C(22)-Si(1)-C(24)	107.46(19)
C(23)-Si(1)-C(24)	107.15(19)
N(2)-Si(2)-C(13)	113.28(16)
N(2)-Si(2)-C(14)	106.05(14)
C(13)-Si(2)-C(14)	109.19(18)
N(2)-Si(2)-C(15)	114.55(14)
C(13)-Si(2)-C(15)	106.17(17)
C(14)-Si(2)-C(15)	107.40(18)
N(1)-Si(3)-C(5)	106.78(15)
N(1)-Si(3)-C(4)	114.40(17)
C(5)-Si(3)-C(4)	108.2(2)
N(1)-Si(3)-C(6)	112.74(15)
C(5)-Si(3)-C(6)	107.39(18)
C(4)-Si(3)-C(6)	107.10(19)
C(1)-N(1)-Si(3)	120.0(2)
C(10)-N(2)-Si(2)	120.42(19)
C(19)-N(3)-Si(1)	119.3(2)
N(1)-C(1)-C(2)	111.7(2)
C(3)-C(2)-C(1)	123.4(3)
C(7)-C(6)-C(8)	108.4(3)

C(7)-C(6)-C(9)	109.2(4)
C(8)-C(6)-C(9)	108.1(4)
C(7)-C(6)-Si(3)	108.7(2)
C(8)-C(6)-Si(3)	110.0(3)
C(9)-C(6)-Si(3)	112.4(3)
N(2)-C(10)-C(11)	112.2(2)
C(12)-C(11)-C(10)	123.8(3)
C(16)-C(15)-C(17)	108.1(4)
C(16)-C(15)-C(18)	109.1(3)
C(17)-C(15)-C(18)	108.4(3)
C(16)-C(15)-Si(2)	109.7(2)
C(17)-C(15)-Si(2)	110.2(3)
C(18)-C(15)-Si(2)	111.4(3)
N(3)-C(19)-C(20)	111.6(3)
C(21)-C(20)-C(19)	123.8(3)
C(27)-C(24)-C(25)	108.2(3)
C(27)-C(24)-C(26)	108.0(4)
C(25)-C(24)-C(26)	108.9(3)
C(27)-C(24)-Si(1)	110.9(3)
C(25)-C(24)-Si(1)	110.9(3)
C(26)-C(24)-Si(1)	109.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (≈^{2}x 10^3)for anion 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	33(1)	57(1)	25(1)	-6(1)	10(1)	-8(1)
Si(2)	21(1)	50(1)	31(1)	-1(1)	8(1)	-2(1)
Si(3)	34(1)	38(1)	33(1)	-1(1)	11(1)	-6(1)
N(1)	21(1)	40(2)	30(1)	1(1)	8(1)	-4(1)
N(2)	23(1)	43(2)	26(1)	2(1)	8(1)	-2(1)
N(3)	26(1)	39(2)	29(1)	-3(1)	10(1)	0(1)
C(1)	22(2)	49(2)	30(2)	-2(1)	7(1)	-5(1)
C(2)	26(2)	46(2)	28(2)	4(1)	5(1)	4(1)
C(3)	34(2)	39(2)	22(2)	-1(1)	6(1)	-1(1)
C(4)	86(3)	52(2)	49(2)	-11(2)	19(2)	-13(2)
C(5)	45(2)	45(2)	54(2)	11(2)	12(2)	7(2)
C(6)	45(2)	51(2)	54(2)	6(2)	19(2)	-11(2)
C(7)	60(3)	65(3)	56(2)	6(2)	39(2)	-3(2)
C(8)	78(3)	61(3)	82(3)	19(2)	44(3)	-10(2)
C(9)	47(3)	97(4)	105(4)	15(3)	19(3)	-27(3)
C(10)	33(2)	48(2)	22(2)	1(1)	9(1)	-4(2)
C(11)	29(2)	44(2)	28(2)	6(1)	2(1)	-1(1)
C(12)	23(2)	38(2)	34(2)	2(1)	4(1)	-3(1)
C(13)	25(2)	70(3)	58(2)	-2(2)	8(2)	-6(2)
C(14)	40(2)	60(2)	42(2)	4(2)	7(2)	4(2)
C(15)	34(2)	69(2)	38(2)	-7(2)	7(2)	7(2)
C(16)	57(2)	61(3)	59(2)	-18(2)	8(2)	2(2)
C(17)	55(3)	103(4)	78(3)	-25(3)	14(2)	34(3)
C(18)	59(3)	104(4)	48(2)	-12(2)	29(2)	-5(3)
C(19)	34(2)	39(2)	45(2)	-8(2)	13(2)	-3(2)
C(20)	27(2)	40(2)	41(2)	9(2)	12(1)	2(1)
C(21)	23(2)	41(2)	31(2)	3(1)	10(1)	0(1)
C(22)	77(3)	65(3)	47(2)	6(2)	-8(2)	-12(2)
C(23)	56(3)	136(4)	40(2)	-22(2)	21(2)	-15(3)
C(24)	41(2)	68(2)	33(2)	-12(2)	7(2)	-10(2)
C(25)	64(3)	99(4)	44(2)	-11(2)	-5(2)	-21(3)
C(26)	44(2)	74(3)	62(2)	-14(2)	15(2)	-23(2)
C(27)	75(3)	75(3)	73(3)	-29(2)	11(2)	-11(3)
Li(1)	32(3)	51(3)	38(3)	-1(3)	15(2)	-7(3)
Li(2)	37(3)	56(3)	32(3)	-4(2)	16(2)	-4(3)
Li(3)	40(3)	48(3)	37(3)	-8(2)	20(2)	-9(3)
Li(4)	31(3)	46(3)	29(3)	-1(2)	11(2)	-4(2)
Li(5)	32(3)	43(3)	33(3)	0(2)	8(2)	-3(2)
Li(6)	32(3)	52(3)	29(3)	-1(2)	8(2)	-1(3)

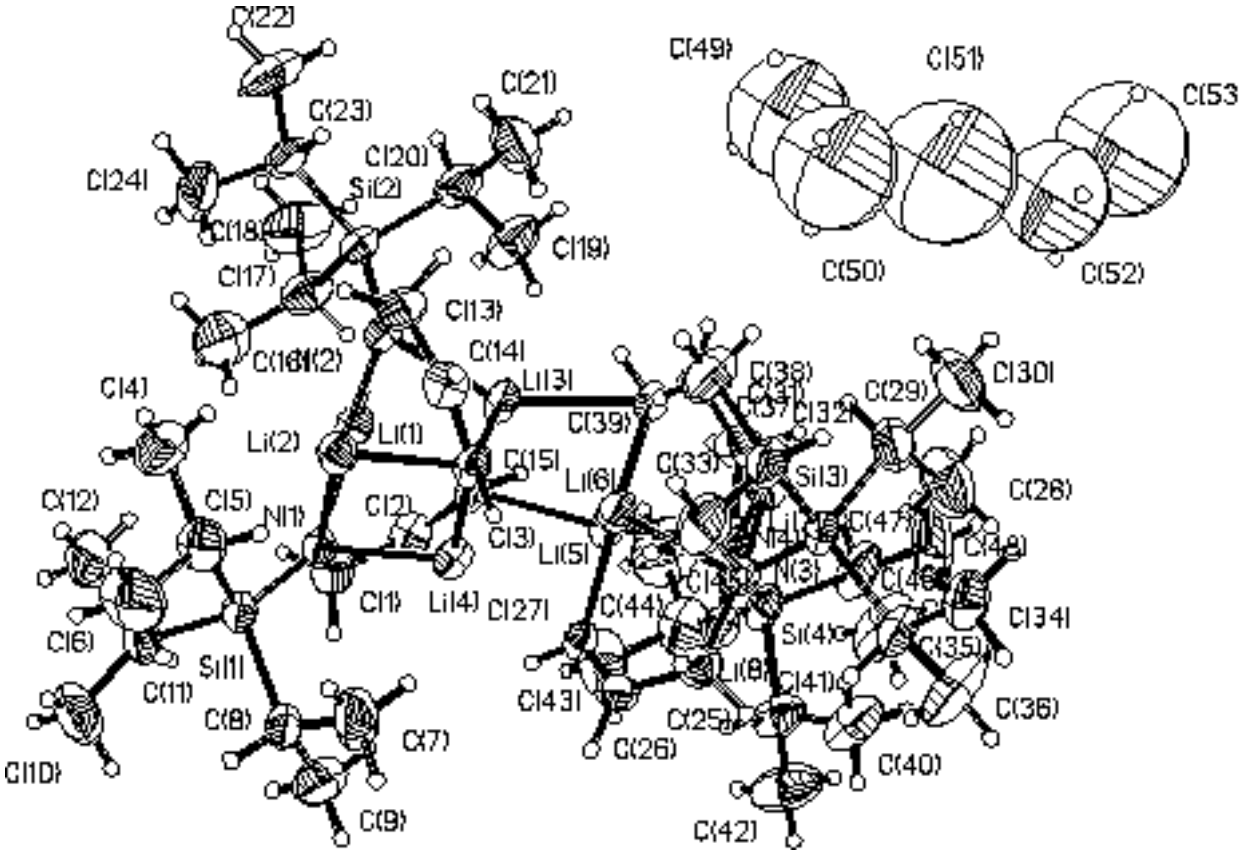
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (≈^{2}x 10^3) for anion 1.

	x	y	z	U(eq)
H(1B)	1811	8166	-215	40
H(1C)	1966	7636	-876	40
H(2A)	1938	9556	-995	40
H(3A)	3299	10252	-943	47
H(4A)	3420	5449	-904	92
H(4B)	2321	5409	-888	92
H(4C)	3020	4617	-459	92
H(5A)	4812	6151	352	72
H(5B)	4337	5292	737	72
H(5C)	4394	6470	978	72
H(7A)	1697	6743	1356	85
H(7B)	2039	7546	868	85
H(7C)	2793	6913	1368	85
H(8A)	1898	4813	1218	105
H(8B)	2995	4988	1237	105
H(8C)	2381	4384	644	105
H(9A)	697	5782	440	123
H(9B)	1142	5364	-154	123
H(9C)	999	6581	-67	123
H(10A)	2756	-910	1740	41
H(10B)	3352	93	2005	41
H(11A)	4448	-1349	1958	41
H(12A)	5112	-1395	1121	47
H(13A)	835	-849	477	76
H(13B)	126	-44	711	76
H(13C)	783	-755	1228	76
H(14A)	1668	1047	-208	71
H(14B)	2005	2054	213	71
H(14C)	915	1761	54	71
H(16A)	2184	2758	2180	89
H(16B)	2414	2726	1464	89
H(16C)	2867	1886	1987	89
H(17A)	455	2725	1724	117
H(17B)	20	1829	1236	117
H(17C)	681	2693	1007	117
H(18A)	1148	1410	2554	102
H(18B)	1813	506	2376	102
H(18C)	715	490	2083	102
H(19A)	5409	3370	1329	46
H(19B)	4457	3164	1595	46
H(20A)	4104	3334	400	42
H(21A)	3877	1911	-118	46
H(22A)	5681	-76	2451	98
H(22B)	6419	325	3059	98
H(22C)	6701	295	2358	98
H(23A)	4271	1573	2831	113
H(23B)	4594	2758	2917	113
H(23C)	5079	1902	3418	113
H(25A)	7842	2873	3543	106
H(25B)	7578	1692	3367	106
H(25C)	6906	2384	3720	106
H(26A)	7966	3231	2387	89

H(26B)	7106	2987	1816	89
H(26C)	7695	2057	2193	89
H(27A)	6938	4329	2950	112
H(27B)	5980	3879	3115	112
H(27C)	6069	4111	2381	112

Table 6. Crystal data and structure refinement for anion 2.

Identification code	mj3a	
Empirical formula	C53 H112 Li8 N4 Si4	
Formula weight	973.35	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.4678(2) Å	α = 111.9550(10)°.
	b = 15.6414(3) Å	β= 97.9480(10)°.
	c = 17.8961(2) Å	γ = 90.7640(10)°.
Volume	3454.23(9) $Å^3$	
Z	2	
Density (calculated)	0.936 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	1076	
Crystal size	0.2 x 0.2 x 0.15 mm^3	
Theta range for data collection	1.24 to 23.30°.	
Index ranges	-14<=h<=10, -17<=k<=15, -15<=l<=19	
Reflections collected	13380	
Independent reflections	9316 [R(int) = 0.0380]	
Completeness to theta = 23.30°	93.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9316 / 4 / 601	
Goodness-of-fit on F^2	1.134	
Final R indices [I>2sigma(I)]	R1 = 0.0901, wR2 = 0.2632	
R indices (all data)	R1 = 0.1126, wR2 = 0.2924	
Largest diff. peak and hole	1.479 and -0.397 $e.Å^{-3}$	



Crystallographic Asymmetric Unit for anion 2

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for anion 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	9241(1)	183(1)	2339(1)	40(1)
Si(2)	8231(1)	-3631(1)	-215(1)	38(1)
Si(3)	7941(1)	-3760(1)	4658(1)	39(1)
Si(4)	4138(1)	-2497(1)	3425(1)	46(1)
N(1)	8311(3)	-716(3)	1916(2)	36(1)
N(2)	8595(3)	-3023(3)	824(2)	35(1)
N(3)	7460(3)	-2914(3)	4330(2)	35(1)
N(4)	5191(3)	-3040(3)	3101(2)	39(1)
C(1)	7296(4)	-433(4)	1702(3)	48(1)
C(2)	6448(4)	-1152(4)	1539(3)	44(1)
C(3)	6537(3)	-1963(3)	1630(3)	40(1)
C(4)	10650(5)	-952(5)	1335(4)	79(2)
C(5)	10492(4)	-375(4)	2224(4)	57(2)
C(6)	11421(5)	313(5)	2659(5)	89(2)
C(7)	9613(6)	275(5)	4005(4)	80(2)
C(8)	9285(4)	850(4)	3484(3)	54(1)
C(9)	8311(5)	1290(5)	3694(4)	81(2)
C(10)	9687(7)	2004(5)	2302(5)	91(2)
C(11)	9075(5)	1072(4)	1843(3)	59(2)
C(12)	9190(7)	713(5)	937(4)	83(2)
C(13)	9449(4)	-3401(4)	1200(3)	45(1)
C(14)	9619(4)	-3019(3)	2125(3)	42(1)
C(15)	9046(3)	-2439(3)	2607(3)	37(1)
C(16)	8023(6)	-1922(5)	-532(4)	83(2)
C(17)	7458(5)	-2827(4)	-622(3)	58(2)
C(18)	6931(6)	-3324(6)	-1514(4)	91(2)
C(19)	6343(5)	-4488(5)	-184(4)	76(2)
C(20)	7359(4)	-4707(4)	-474(3)	55(1)
C(21)	7843(5)	-5409(4)	-148(5)	77(2)
C(22)	9098(6)	-4692(5)	-1668(4)	79(2)
C(23)	9357(4)	-4047(4)	-758(3)	49(1)
C(24)	10148(5)	-3280(5)	-649(5)	81(2)
C(25)	7850(4)	-1952(3)	4888(3)	43(1)
C(26)	7638(3)	-1217(3)	4529(3)	40(1)
C(27)	7199(3)	-1380(3)	3757(3)	37(1)
C(28)	5985(6)	-4800(5)	4266(6)	97(3)
C(29)	7068(5)	-4856(4)	4084(4)	59(2)
C(30)	7484(6)	-5740(4)	4166(5)	84(2)
C(31)	9233(5)	-4513(5)	3443(4)	68(2)
C(32)	9229(4)	-4106(4)	4377(3)	48(1)
C(33)	10058(4)	-3328(5)	4788(4)	69(2)
C(34)	8688(5)	-4014(4)	6169(4)	61(2)
C(35)	8107(4)	-3374(4)	5816(3)	48(1)
C(36)	7132(6)	-3136(7)	6195(4)	94(3)
C(37)	4981(4)	-3888(4)	2334(3)	56(1)
C(38)	5902(4)	-4271(4)	1973(3)	49(1)
C(39)	6842(4)	-3867(3)	2226(3)	40(1)
C(40)	4919(6)	-2074(6)	5147(4)	86(2)
C(41)	4562(4)	-1636(4)	4527(3)	57(2)
C(42)	3788(5)	-935(6)	4871(5)	94(3)
C(43)	4335(5)	-955(6)	2928(6)	91(2)
C(44)	3605(5)	-1756(5)	2852(4)	72(2)

C(45)	3191(8)	-2306(8)	1953(6)	125(3)
C(46)	2097(5)	-2914(7)	3606(5)	116(4)
C(47)	3074(4)	-3363(5)	3324(4)	74(2)
C(48)	3361(7)	-4081(7)	3683(6)	121(4)
Li(1)	7752(6)	-1945(5)	925(5)	38(2)
Li(2)	9223(6)	-1771(5)	1758(5)	40(2)
Li(3)	7658(6)	-3042(5)	1652(4)	38(2)
Li(4)	7879(6)	-1398(6)	2644(5)	40(2)
Li(5)	6212(6)	-2434(6)	2642(5)	39(2)
Li(6)	7867(6)	-2780(5)	3287(5)	40(2)
Li(7)	6418(6)	-3746(5)	3404(5)	43(2)
Li(8)	6196(6)	-2246(6)	4088(5)	42(2)
C(49)	6300(20)	-7180(20)	658(18)	370(16)
C(50)	6740(20)	-6950(20)	1545(18)	367(16)
C(51)	6120(30)	-7520(30)	1990(20)	490(30)
C(52)	5520(20)	-7908(18)	2581(16)	292(11)
C(53)	4740(30)	-8730(20)	2310(20)	440(20)

Table 8. Bond lengths [Å] and angles [°] for anion 2.

Si(1)-N(1)	1.735(4)
Si(1)-C(5)	1.909(6)
Si(1)-C(11)	1.911(6)
Si(1)-C(8)	1.912(5)
Si(2)-N(2)	1.736(4)
Si(2)-C(23)	1.905(5)
Si(2)-C(20)	1.907(6)
Si(2)-C(17)	1.925(6)
Si(3)-N(3)	1.735(4)
Si(3)-C(32)	1.902(5)
Si(3)-C(35)	1.909(5)
Si(3)-C(29)	1.916(6)
Si(4)-N(4)	1.720(4)
Si(4)-C(44)	1.902(7)
Si(4)-C(47)	1.902(6)
Si(4)-C(41)	1.926(6)
N(1)-C(1)	1.487(6)
N(2)-C(13)	1.492(6)
N(3)-C(25)	1.499(6)
N(4)-C(37)	1.498(6)
C(1)-C(2)	1.511(7)
C(2)-C(3)	1.343(7)
C(4)-C(5)	1.555(8)
C(5)-C(6)	1.548(8)
C(7)-C(8)	1.549(9)
C(8)-C(9)	1.517(9)
C(10)-C(11)	1.537(8)
C(11)-C(12)	1.536(8)
C(13)-C(14)	1.517(7)
C(14)-C(15)	1.333(7)
C(16)-C(17)	1.541(10)
C(17)-C(18)	1.550(8)
C(19)-C(20)	1.529(8)
C(20)-C(21)	1.537(9)
C(22)-C(23)	1.547(8)
C(23)-C(24)	1.532(8)
C(25)-C(26)	1.526(7)
C(26)-C(27)	1.354(7)
C(28)-C(29)	1.534(9)
C(29)-C(30)	1.549(9)
C(31)-C(32)	1.551(7)
C(32)-C(33)	1.529(8)
C(34)-C(35)	1.540(7)
C(35)-C(36)	1.546(8)
C(37)-C(38)	1.505(8)
C(38)-C(39)	1.346(7)
C(40)-C(41)	1.538(10)
C(41)-C(42)	1.540(8)
C(43)-C(44)	1.535(10)
C(44)-C(45)	1.531(11)
C(46)-C(47)	1.555(10)
C(47)-C(48)	1.519(11)
C(49)-C(50)	1.520(18)
C(50)-C(51)	1.674(18)
C(51)-C(52)	1.688(18)

C(52)-C(53)	1.532(18)

N(1)-Si(1)-C(5)	106.2(2)
N(1)-Si(1)-C(11)	111.9(2)
C(5)-Si(1)-C(11)	113.0(3)
N(1)-Si(1)-C(8)	113.8(2)
C(5)-Si(1)-C(8)	105.6(3)
C(11)-Si(1)-C(8)	106.3(3)
N(2)-Si(2)-C(23)	111.7(2)
N(2)-Si(2)-C(20)	113.9(2)
C(23)-Si(2)-C(20)	105.9(2)
N(2)-Si(2)-C(17)	106.7(2)
C(23)-Si(2)-C(17)	113.0(3)
C(20)-Si(2)-C(17)	105.6(3)
N(3)-Si(3)-C(32)	114.3(2)
N(3)-Si(3)-C(35)	112.2(2)
C(32)-Si(3)-C(35)	105.0(2)
N(3)-Si(3)-C(29)	106.7(2)
C(32)-Si(3)-C(29)	104.8(3)
C(35)-Si(3)-C(29)	113.9(3)
N(4)-Si(4)-C(44)	114.7(3)
N(4)-Si(4)-C(47)	111.5(3)
C(44)-Si(4)-C(47)	106.2(3)
N(4)-Si(4)-C(41)	106.1(2)
C(44)-Si(4)-C(41)	104.6(3)
C(47)-Si(4)-C(41)	113.6(3)
C(1)-N(1)-Si(1)	114.7(3)
C(13)-N(2)-Si(2)	114.5(3)
C(25)-N(3)-Si(3)	113.5(3)
C(37)-N(4)-Si(4)	114.5(3)
N(1)-C(1)-C(2)	114.5(4)
C(3)-C(2)-C(1)	125.8(4)
C(6)-C(5)-C(4)	108.8(5)
C(6)-C(5)-Si(1)	113.8(4)
C(4)-C(5)-Si(1)	115.6(4)
C(9)-C(8)-C(7)	110.8(5)
C(9)-C(8)-Si(1)	112.8(4)
C(7)-C(8)-Si(1)	113.6(4)
C(10)-C(11)-C(12)	109.8(5)
C(10)-C(11)-Si(1)	115.9(4)
C(12)-C(11)-Si(1)	115.1(4)
N(2)-C(13)-C(14)	114.8(4)
C(15)-C(14)-C(13)	126.1(4)
C(16)-C(17)-C(18)	109.5(6)
C(16)-C(17)-Si(2)	115.7(4)
C(18)-C(17)-Si(2)	112.9(4)
C(19)-C(20)-C(21)	109.6(5)
C(19)-C(20)-Si(2)	113.2(4)
C(21)-C(20)-Si(2)	112.6(4)
C(24)-C(23)-C(22)	110.4(5)
C(24)-C(23)-Si(2)	114.6(4)
C(22)-C(23)-Si(2)	115.3(4)
N(3)-C(25)-C(26)	114.7(4)
C(27)-C(26)-C(25)	125.4(4)
C(28)-C(29)-C(30)	108.4(5)
C(28)-C(29)-Si(3)	116.0(5)
C(30)-C(29)-Si(3)	114.3(5)
C(33)-C(32)-C(31)	109.6(5)

C(33)-C(32)-Si(3)	113.7(4)
C(31)-C(32)-Si(3)	113.0(4)
C(34)-C(35)-C(36)	109.2(5)
C(34)-C(35)-Si(3)	115.6(4)
C(36)-C(35)-Si(3)	115.3(4)
N(4)-C(37)-C(38)	114.4(4)
C(39)-C(38)-C(37)	125.9(4)
C(40)-C(41)-C(42)	108.8(6)
C(40)-C(41)-Si(4)	115.3(5)
C(42)-C(41)-Si(4)	114.4(4)
C(45)-C(44)-C(43)	109.8(7)
C(45)-C(44)-Si(4)	114.0(6)
C(43)-C(44)-Si(4)	113.8(5)
C(48)-C(47)-C(46)	111.5(7)
C(48)-C(47)-Si(4)	115.0(5)
C(46)-C(47)-Si(4)	114.0(6)
C(49)-C(50)-C(51)	113(3)
C(50)-C(51)-C(52)	170(3)
C(53)-C(52)-C(51)	128(3)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for anion 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	44(1)	41(1)	38(1)	17(1)	12(1)	-4(1)
Si(2)	42(1)	47(1)	28(1)	14(1)	13(1)	8(1)
Si(3)	47(1)	42(1)	35(1)	20(1)	15(1)	4(1)
Si(4)	28(1)	68(1)	45(1)	22(1)	11(1)	-4(1)
N(1)	38(2)	39(2)	37(2)	19(2)	11(2)	4(2)
N(2)	32(2)	44(2)	30(2)	15(2)	9(2)	9(2)
N(3)	40(2)	36(2)	30(2)	11(2)	10(2)	-1(2)
N(4)	35(2)	46(2)	37(2)	14(2)	9(2)	-7(2)
C(1)	41(3)	50(3)	58(3)	25(3)	10(2)	10(2)
C(2)	34(3)	57(3)	47(3)	25(3)	6(2)	10(2)
C(3)	32(2)	52(3)	38(3)	19(2)	11(2)	-3(2)
C(4)	65(4)	83(5)	84(5)	16(4)	40(4)	6(3)
C(5)	40(3)	61(3)	68(4)	21(3)	9(3)	-5(3)
C(6)	50(4)	82(5)	115(6)	15(4)	9(4)	-13(3)
C(7)	109(6)	85(5)	49(4)	33(3)	-2(4)	-39(4)
C(8)	66(4)	53(3)	42(3)	14(3)	17(3)	-19(3)
C(9)	87(5)	81(5)	63(4)	7(4)	35(4)	-3(4)
C(10)	136(7)	62(4)	81(5)	37(4)	10(5)	-29(4)
C(11)	76(4)	53(3)	55(3)	30(3)	11(3)	-8(3)
C(12)	133(7)	73(4)	55(4)	36(3)	19(4)	-13(4)
C(13)	41(3)	49(3)	45(3)	16(2)	11(2)	15(2)
C(14)	35(3)	49(3)	43(3)	20(2)	0(2)	4(2)
C(15)	36(2)	49(3)	29(2)	18(2)	5(2)	-2(2)
C(16)	109(6)	81(5)	76(5)	47(4)	19(4)	33(4)
C(17)	65(4)	68(4)	40(3)	19(3)	10(3)	20(3)
C(18)	118(6)	103(6)	44(4)	22(4)	-7(4)	33(5)
C(19)	57(4)	107(5)	43(3)	5(3)	11(3)	-22(4)
C(20)	57(3)	65(4)	32(3)	5(3)	10(2)	-7(3)
C(21)	83(5)	60(4)	89(5)	32(4)	11(4)	-13(3)
C(22)	97(5)	96(5)	46(4)	18(3)	35(3)	35(4)
C(23)	58(3)	53(3)	43(3)	20(2)	27(3)	18(3)
C(24)	75(4)	82(5)	109(6)	47(4)	55(4)	10(4)
C(25)	48(3)	43(3)	35(3)	13(2)	6(2)	5(2)
C(26)	40(3)	34(2)	38(3)	6(2)	9(2)	0(2)
C(27)	38(2)	39(3)	40(3)	17(2)	16(2)	3(2)
C(28)	82(5)	82(5)	139(8)	53(5)	23(5)	-19(4)
C(29)	71(4)	52(3)	58(3)	28(3)	9(3)	-9(3)
C(30)	116(6)	50(4)	93(5)	36(4)	11(4)	-5(4)
C(31)	86(4)	81(4)	57(4)	39(3)	37(3)	39(4)
C(32)	57(3)	53(3)	49(3)	31(3)	23(3)	20(3)
C(33)	52(3)	80(4)	83(5)	32(4)	35(3)	8(3)
C(34)	76(4)	69(4)	51(3)	37(3)	11(3)	7(3)
C(35)	54(3)	63(3)	39(3)	28(3)	17(2)	8(3)
C(36)	87(5)	161(8)	63(4)	63(5)	40(4)	48(5)
C(37)	42(3)	54(3)	55(3)	6(3)	0(3)	-13(2)
C(38)	60(3)	43(3)	34(3)	4(2)	8(2)	-1(2)
C(39)	46(3)	41(3)	36(3)	15(2)	16(2)	-1(2)
C(40)	87(5)	116(6)	49(4)	21(4)	21(4)	4(4)
C(41)	36(3)	75(4)	52(3)	10(3)	16(2)	6(3)
C(42)	59(4)	113(6)	80(5)	-4(4)	24(4)	13(4)
C(43)	66(4)	108(6)	137(7)	81(6)	34(5)	24(4)
C(44)	47(3)	98(5)	81(5)	44(4)	14(3)	12(3)

C(45)	134(8)	157(9)	94(7)	65(7)	-9(6)	25(7)
C(46)	49(4)	194(10)	88(6)	33(6)	20(4)	-43(5)
C(47)	44(3)	118(6)	55(4)	28(4)	11(3)	-31(3)
C(48)	104(7)	151(8)	135(8)	94(7)	-3(6)	-67(6)
Li(1)	35(4)	46(4)	35(4)	18(4)	7(3)	3(3)
Li(2)	37(4)	43(4)	40(4)	16(4)	5(3)	0(3)
Li(3)	37(4)	50(5)	33(4)	19(4)	9(3)	-1(3)
Li(4)	39(4)	47(5)	37(4)	17(4)	12(3)	5(3)
Li(5)	34(4)	51(5)	37(4)	22(4)	8(3)	0(3)
Li(6)	42(4)	46(4)	33(4)	16(4)	8(3)	-1(3)
Li(7)	47(5)	40(4)	44(5)	17(4)	9(4)	-3(4)
Li(8)	38(4)	48(5)	43(4)	17(4)	16(4)	4(4)

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

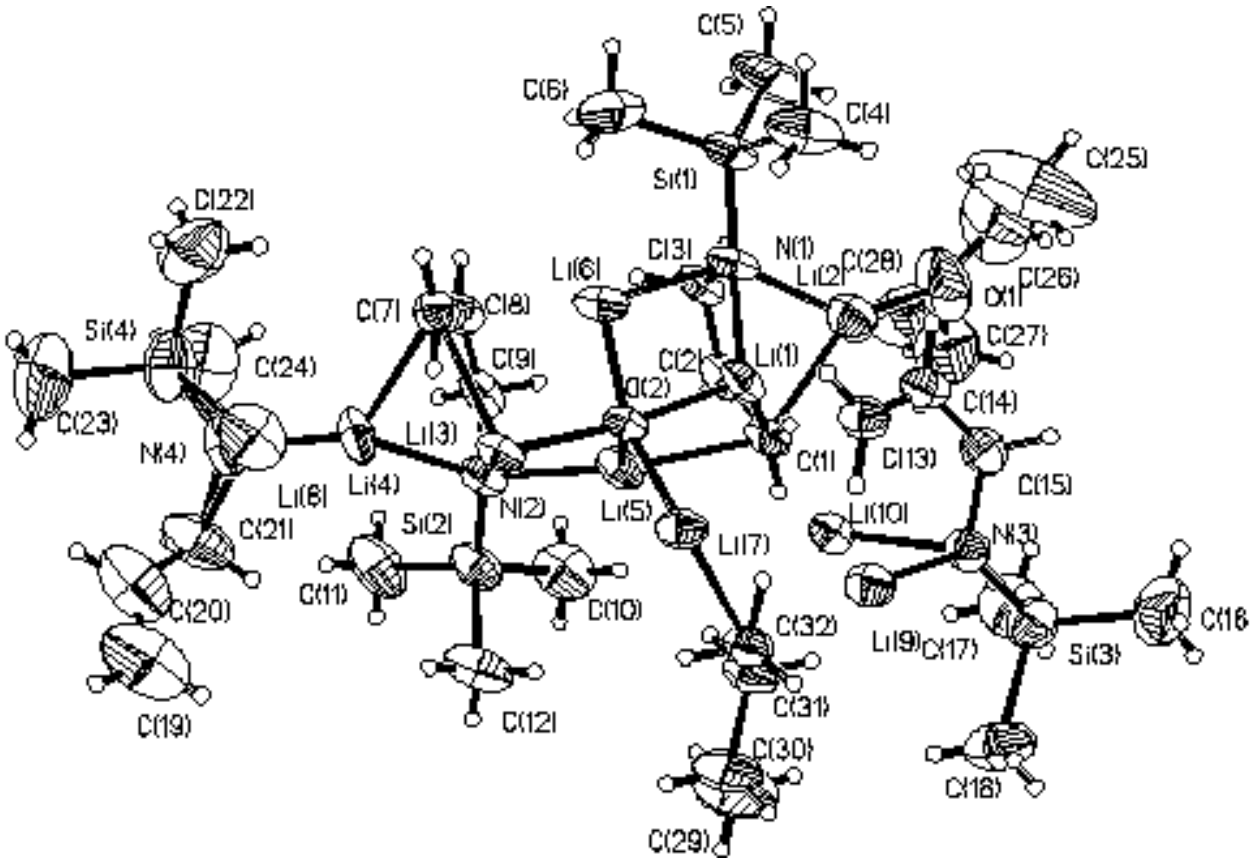
	x	y	z	U(eq)
H(1B)	7289	-286	1220	58
H(1C)	7173	127	2144	58
H(2B)	5808	-1021	1361	53
H(3A)	5950	-2368	1535	47
H(4B)	11294	-1207	1340	118
H(4C)	10622	-561	1029	118
H(4D)	10131	-1443	1087	118
H(5A)	10498	-811	2500	69
H(6A)	12022	-11	2582	134
H(6B)	11387	597	3231	134
H(6C)	11431	781	2432	134
H(7A)	9628	650	4571	121
H(7B)	10270	69	3914	121
H(7C)	9143	-251	3851	121
H(8A)	9802	1360	3644	65
H(9A)	8374	1617	4274	121
H(9B)	7771	818	3517	121
H(9C)	8173	1714	3426	121
H(10A)	9541	2404	2011	136
H(10B)	10391	1906	2345	136
H(10C)	9510	2284	2839	136
H(11A)	8371	1220	1855	70
H(12A)	9086	1200	736	125
H(12B)	8703	205	633	125
H(12C)	9854	509	875	125
H(13A)	10059	-3272	1018	54
H(13B)	9328	-4067	1002	54
H(14A)	10174	-3207	2380	50
H(15A)	9256	-2172	3186	45
H(16A)	7577	-1571	-751	124
H(16B)	8584	-2064	-824	124
H(16C)	8259	-1568	34	124
H(17A)	6918	-2642	-291	70
H(18A)	6556	-2893	-1685	137
H(18B)	6484	-3824	-1549	137
H(18C)	7428	-3561	-1862	137
H(19A)	5934	-5053	-336	114
H(19B)	6011	-4099	-432	114
H(19C)	6444	-4176	399	114
H(20A)	7227	-5009	-1069	66
H(21A)	7380	-5939	-297	116
H(21B)	8007	-5130	435	116
H(21C)	8444	-5598	-379	116
H(22A)	9708	-4867	-1890	119
H(22B)	8714	-4374	-1963	119
H(22C)	8712	-5235	-1715	119
H(23A)	9696	-4429	-488	58
H(24A)	10688	-3545	-939	121
H(24B)	10404	-2967	-80	121
H(24C)	9846	-2847	-861	121
H(25A)	8570	-1947	5039	51

H(25B)	7552	-1788	5383	51
H(26A)	7827	-605	4869	48
H(27A)	7082	-876	3580	45
H(28A)	5610	-5379	3948	146
H(28B)	5677	-4317	4128	146
H(28C)	5990	-4669	4835	146
H(29A)	7018	-4959	3505	70
H(30A)	7009	-6258	3863	126
H(30B)	7593	-5661	4731	126
H(30C)	8109	-5849	3956	126
H(31A)	9897	-4680	3336	102
H(31B)	9030	-4060	3220	102
H(31C)	8773	-5052	3194	102
H(32A)	9407	-4599	4573	57
H(33A)	10687	-3548	4624	103
H(33B)	10110	-3130	5370	103
H(33C)	9899	-2818	4629	103
H(34A)	8734	-3764	6752	91
H(34B)	9351	-4061	6025	91
H(34C)	8340	-4616	5951	91
H(35A)	8526	-2792	6028	58
H(36A)	7287	-2949	6776	141
H(36B)	6664	-3670	5977	141
H(36C)	6841	-2641	6067	141
H(37A)	4532	-3742	1932	67
H(37B)	4635	-4362	2448	67
H(38A)	5813	-4838	1536	58
H(39A)	7371	-4127	1920	48
H(40A)	5118	-1596	5676	129
H(40B)	5481	-2431	4983	129
H(40C)	4382	-2469	5170	129
H(41A)	5148	-1271	4507	69
H(42A)	4053	-530	5418	142
H(42B)	3178	-1259	4872	142
H(42C)	3650	-579	4537	142
H(43A)	4019	-610	2627	137
H(43B)	4931	-1197	2713	137
H(43C)	4510	-557	3492	137
H(44A)	3031	-1472	3109	87
H(45A)	2928	-1891	1705	188
H(45B)	2665	-2748	1912	188
H(45C)	3721	-2622	1678	188
H(46A)	1592	-3389	3531	174
H(46B)	1861	-2560	3289	174
H(46C)	2237	-2516	4172	174
H(47A)	2892	-3714	2737	88
H(48A)	2788	-4499	3592	182
H(48B)	3587	-3779	4259	182
H(48C)	3891	-4421	3426	182
H(49A)	6306	-6625	547	555
H(49B)	5621	-7439	555	555
H(49C)	6696	-7618	311	555
H(50A)	6728	-6295	1846	440
H(50B)	7434	-7107	1576	440
H(51A)	6568	-8017	1874	584
H(51B)	5577	-7752	1532	584
H(52A)	6046	-8022	2952	350
H(52B)	5189	-7383	2912	350

H(53A)	4427	-8713	2766	665
H(53B)	5073	-9298	2115	665
H(53C)	4244	-8708	1883	665

Table 11. Crystal data and structure refinement for anion 3 .

Identification code	mj4	
Empirical formula	C32 H72 Li10 N4 O2 Si4	
Formula weight	726.70	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.4625(3) Å	α = 92.64°.
	b = 13.7336(2) Å	β= 110.9320(10)°.
	c = 16.30260(10) Å	γ = 105.8650(10)°.
Volume	2673.14(7) $Å^3$	
Z	2	
Density (calculated)	0.903 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	788	
Crystal size	0.2 x 0.2 x 0.15 mm^3	
Theta range for data collection	1.72 to 23.26°.	
Index ranges	-14<=h<=14, -14<=k<=15, -17<=l<=17	
Reflections collected	11331	
Independent reflections	7095 [R(int) = 0.3703]	
Completeness to theta = 23.26°	92.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7095 / 0 / 469	
Goodness-of-fit on F^2	1.200	
Final R indices [I>2sigma(I)]	R1 = 0.1383, wR2 = 0.3417	
R indices (all data)	R1 = 0.1901, wR2 = 0.3868	
Largest diff. peak and hole	1.389 and -0.619 $e.Å^{-3}$	



Crystallographic asymmetric unit for anion 3

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for anion 3 . U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	13102(6)	2119(5)	2451(5)	107(3)
O(2)	9688(3)	3863(3)	-4(2)	33(1)
Si(1)	11732(2)	2139(1)	-420(1)	50(1)
Si(2)	6562(2)	2324(2)	344(1)	53(1)
Si(3)	13024(2)	5639(2)	4218(1)	59(1)
Si(4)	4510(2)	1218(2)	-3362(2)	81(1)
N(1)	11180(4)	2422(4)	302(3)	45(1)
N(2)	7322(4)	2408(4)	-293(3)	42(1)
N(3)	12769(4)	5480(4)	3120(3)	43(1)
N(4)	5066(4)	2325(5)	-2654(4)	58(2)
C(1)	10575(5)	2815(5)	1765(4)	43(1)
C(2)	10173(5)	1891(5)	1289(4)	47(2)
C(3)	10425(5)	1573(5)	501(4)	47(2)
C(4)	12905(8)	3245(6)	-348(6)	75(2)
C(5)	12201(7)	994(6)	-225(8)	83(3)
C(6)	10719(10)	1870(10)	-1594(6)	102(4)
C(7)	7931(5)	2268(5)	-1794(4)	47(2)
C(8)	7793(5)	1484(5)	-1362(5)	50(2)
C(9)	7444(5)	1441(5)	-590(5)	51(2)
C(10)	7165(8)	1827(7)	1389(6)	78(2)
C(11)	5117(7)	1438(8)	-222(7)	85(3)
C(12)	6507(8)	3628(7)	624(7)	80(2)
C(13)	12486(5)	5288(4)	1336(4)	41(1)
C(14)	13079(5)	4772(5)	1867(4)	45(1)
C(15)	13300(6)	4810(5)	2836(4)	51(2)
C(16)	14542(9)	6228(9)	4928(6)	97(3)
C(17)	12540(9)	4414(8)	4604(6)	91(3)
C(18)	12270(9)	6524(8)	4422(6)	87(3)
C(19)	3931(12)	4294(12)	-2458(13)	138(5)
C(20)	3852(9)	3404(11)	-2797(10)	113(4)
C(21)	4278(8)	2649(7)	-2342(7)	82(3)
C(22)	5504(10)	1084(9)	-3866(8)	116(4)
C(23)	3174(10)	1076(11)	-4293(8)	132(5)
C(24)	4219(11)	68(8)	-2818(9)	120(4)
C(25)	14700(20)	2671(19)	2242(18)	216(13)
C(26)	13969(17)	1858(16)	2544(15)	214(13)
C(27)	12629(12)	1708(11)	3215(8)	113(4)
C(28)	12131(14)	721(13)	2999(11)	144(5)
C(29)	8523(12)	4408(12)	3571(9)	126(5)
C(30)	8897(8)	5096(8)	2987(6)	79(2)
C(31)	9618(6)	4725(6)	2591(5)	56(2)
C(32)	10063(6)	5402(5)	2009(4)	49(2)
Li(1)	11013(7)	3718(7)	734(7)	42(2)
Li(2)	12128(10)	2709(9)	1622(8)	58(3)
Li(3)	8185(8)	3541(7)	-727(6)	38(2)
Li(4)	6350(9)	2307(10)	-1627(8)	61(3)
Li(5)	8996(8)	3029(8)	605(7)	44(2)
Li(6)	9798(9)	2823(8)	-676(7)	48(2)
Li(7)	10069(9)	5113(7)	703(6)	43(2)
Li(8)	6032(12)	3533(11)	-2838(11)	79(4)
Li(9)	11877(9)	6177(7)	2191(6)	45(2)
Li(10)	11194(8)	4453(8)	2320(6)	45(2)

Table 13. Bond lengths [Å] and angles [º] for anion 3 .

O(1)-C(26)	1.273(17)
O(1)-C(27)	1.645(16)
Si(1)-N(1)	1.683(5)
Si(1)-C(4)	1.832(8)
Si(1)-C(5)	1.849(7)
Si(1)-C(6)	1.858(9)
Si(2)-N(2)	1.686(5)
Si(2)-C(11)	1.854(9)
Si(2)-C(12)	1.855(8)
Si(2)-C(10)	1.857(8)
Si(3)-N(3)	1.688(5)
Si(3)-C(17)	1.856(10)
Si(3)-C(16)	1.869(10)
Si(3)-C(18)	1.870(9)
Si(4)-N(4)	1.674(7)
Si(4)-C(22)	1.845(13)
Si(4)-C(23)	1.846(11)
Si(4)-C(24)	1.864(11)
N(1)-C(3)	1.456(8)
N(2)-C(9)	1.463(8)
N(3)-C(15)	1.460(8)
N(4)-C(21)	1.484(10)
C(1)-C(2)	1.318(9)
C(2)-C(3)	1.514(9)
C(7)-C(8)	1.320(10)
C(8)-C(9)	1.491(10)
C(13)-C(14)	1.327(9)
C(14)-C(15)	1.495(9)
C(19)-C(20)	1.280(18)
C(20)-C(21)	1.431(14)
C(25)-C(26)	1.50(3)
C(27)-C(28)	1.305(18)
C(29)-C(30)	1.489(15)
C(30)-C(31)	1.518(9)
C(31)-C(32)	1.519(10)
C(26)-O(1)-C(27)	109.5(15)
N(1)-Si(1)-C(4)	109.3(3)
N(1)-Si(1)-C(5)	112.6(4)
C(4)-Si(1)-C(5)	110.0(4)
N(1)-Si(1)-C(6)	112.4(4)
C(4)-Si(1)-C(6)	106.0(5)
C(5)-Si(1)-C(6)	106.2(5)
N(2)-Si(2)-C(11)	112.7(4)
N(2)-Si(2)-C(12)	107.8(3)
C(11)-Si(2)-C(12)	109.2(4)
N(2)-Si(2)-C(10)	112.9(3)
C(11)-Si(2)-C(10)	105.1(4)
C(12)-Si(2)-C(10)	109.1(4)
N(3)-Si(3)-C(17)	112.6(4)
N(3)-Si(3)-C(16)	112.9(4)
C(17)-Si(3)-C(16)	106.8(5)
N(3)-Si(3)-C(18)	107.8(3)
C(17)-Si(3)-C(18)	109.0(5)
C(16)-Si(3)-C(18)	107.7(5)

N(4)-Si(4)-C(22)	109.1(4)
N(4)-Si(4)-C(23)	115.8(5)
C(22)-Si(4)-C(23)	106.4(6)
N(4)-Si(4)-C(24)	113.4(5)
C(22)-Si(4)-C(24)	106.9(7)
C(23)-Si(4)-C(24)	104.7(6)
C(3)-N(1)-Si(1)	117.3(4)
C(9)-N(2)-Si(2)	115.4(4)
C(15)-N(3)-Si(3)	115.5(4)
C(21)-N(4)-Si(4)	115.3(5)
C(1)-C(2)-C(3)	126.1(6)
N(1)-C(3)-C(2)	112.2(5)
C(7)-C(8)-C(9)	126.3(6)
N(2)-C(9)-C(8)	113.0(5)
C(13)-C(14)-C(15)	124.4(6)
N(3)-C(15)-C(14)	111.2(5)
C(19)-C(20)-C(21)	127.5(14)
C(20)-C(21)-N(4)	114.4(8)
O(1)-C(26)-C(25)	106.6(16)
C(28)-C(27)-O(1)	109.1(12)
C(29)-C(30)-C(31)	113.2(8)
C(30)-C(31)-C(32)	116.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for anion 3 . The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	80(4)	85(4)	140(6)	21(4)	5(4)	51(4)
O(2)	35(2)	31(2)	43(2)	9(2)	21(2)	16(2)
Si(1)	52(1)	46(1)	72(1)	8(1)	36(1)	28(1)
Si(2)	47(1)	58(1)	73(1)	27(1)	38(1)	21(1)
Si(3)	67(1)	72(1)	42(1)	11(1)	23(1)	25(1)
Si(4)	66(2)	68(2)	79(2)	10(1)	9(1)	1(1)
N(1)	48(3)	39(3)	66(3)	10(2)	37(3)	23(2)
N(2)	37(3)	39(3)	59(3)	13(2)	26(2)	15(2)
N(3)	47(3)	47(3)	42(3)	12(2)	18(2)	22(2)
N(4)	38(3)	64(4)	67(3)	21(3)	13(3)	13(3)
C(1)	44(3)	48(4)	50(3)	15(3)	24(3)	27(3)
C(2)	41(3)	48(4)	63(4)	27(3)	28(3)	19(3)
C(3)	37(3)	46(3)	71(4)	12(3)	29(3)	21(3)
C(4)	93(6)	61(5)	109(6)	22(4)	75(5)	31(4)
C(5)	81(5)	43(4)	161(9)	24(5)	75(6)	37(4)
C(6)	118(8)	138(9)	75(6)	-11(6)	41(6)	74(7)
C(7)	40(3)	45(4)	54(4)	-2(3)	18(3)	10(3)
C(8)	48(4)	35(3)	72(4)	1(3)	27(3)	16(3)
C(9)	37(3)	44(3)	77(4)	19(3)	22(3)	18(3)
C(10)	85(6)	89(6)	85(5)	43(5)	55(5)	32(5)
C(11)	46(4)	102(7)	121(7)	39(6)	46(5)	22(4)
C(12)	86(6)	80(6)	114(7)	28(5)	68(5)	48(5)
C(13)	50(4)	38(3)	44(3)	12(2)	23(3)	20(3)
C(14)	44(3)	45(3)	56(4)	7(3)	27(3)	16(3)
C(15)	48(4)	56(4)	53(4)	12(3)	13(3)	29(3)
C(16)	93(7)	108(8)	67(5)	2(5)	5(5)	33(6)
C(17)	106(7)	106(7)	83(6)	44(5)	53(5)	41(6)
C(18)	120(8)	93(6)	69(5)	8(4)	48(5)	52(6)
C(19)	123(11)	121(11)	202(15)	40(10)	77(10)	64(9)
C(20)	83(7)	122(10)	154(10)	45(8)	52(7)	49(7)
C(21)	75(5)	74(5)	133(8)	40(5)	68(6)	35(4)
C(22)	115(9)	100(8)	104(8)	-33(6)	29(7)	16(6)
C(23)	91(8)	147(12)	99(8)	-1(8)	-3(7)	2(7)
C(24)	136(10)	67(6)	131(9)	31(6)	34(8)	14(6)
C(25)	270(30)	220(20)	360(30)	180(20)	260(30)	170(20)
C(26)	180(18)	185(18)	230(20)	-48(16)	-39(16)	152(17)
C(27)	130(10)	119(10)	93(7)	34(7)	35(7)	52(8)
C(28)	156(13)	130(13)	143(12)	-20(9)	62(10)	42(10)
C(29)	144(11)	172(12)	137(9)	49(8)	120(9)	72(9)
C(30)	93(6)	95(6)	93(6)	23(5)	72(5)	48(5)
C(31)	60(4)	72(4)	61(4)	16(3)	40(3)	35(3)
C(32)	50(4)	59(4)	50(3)	11(3)	27(3)	27(3)
Li(1)	25(5)	45(5)	60(6)	10(4)	20(4)	14(4)
Li(2)	55(7)	60(7)	64(7)	13(5)	23(5)	27(5)
Li(3)	42(5)	41(5)	51(5)	20(4)	29(4)	24(4)
Li(4)	31(6)	78(8)	62(6)	11(6)	2(5)	21(5)
Li(5)	38(5)	50(6)	56(6)	17(4)	30(5)	17(4)
Li(6)	61(6)	46(6)	58(6)	8(4)	37(5)	29(5)
Li(7)	57(6)	37(5)	48(5)	13(4)	28(5)	23(4)
Li(8)	68(8)	64(8)	108(10)	24(7)	43(8)	12(6)
Li(9)	51(6)	45(5)	46(5)	10(4)	22(5)	21(4)
Li(10)	42(5)	49(6)	47(5)	6(4)	16(4)	22(4)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for anion 3 .

	x	y	z	U(eq)
H(1A)	11061	3342	1626	51
H(1B)	10372	2939	2239	51
H(2A)	9691	1388	1452	56
H(3A)	10760	1027	627	56
H(3B)	9731	1308	-16	56
H(4A)	13456	3419	249	112
H(4B)	12639	3819	-508	112
H(4C)	13234	3079	-748	112
H(5A)	12737	1099	374	124
H(5B)	12539	882	-634	124
H(5C)	11569	406	-313	124
H(6A)	10446	2444	-1729	154
H(6B)	10103	1269	-1676	154
H(6C)	11084	1757	-1982	154
H(7A)	7807	2865	-1623	57
H(7B)	8152	2223	-2270	57
H(8A)	7927	904	-1557	60
H(9A)	6736	902	-754	61
H(9B)	7995	1264	-99	61
H(10A)	7925	2247	1713	117
H(10B)	7147	1135	1249	117
H(10C)	6734	1843	1746	117
H(11A)	4749	1660	-768	128
H(11B)	4712	1439	157	128
H(11C)	5141	758	-349	128
H(12A)	6186	3884	86	119
H(12B)	7251	4076	962	119
H(12C)	6056	3598	970	119
H(13A)	12176	5708	1562	50
H(13B)	12381	5230	738	50
H(14A)	13378	4360	1620	54
H(15A)	13015	4124	2951	61
H(15B)	14100	5058	3178	61
H(16A)	14951	5788	4837	145
H(16B)	14639	6315	5542	145
H(16C)	14817	6884	4770	145
H(17A)	11756	4091	4261	136
H(17B)	12662	4548	5221	136
H(17C)	12951	3968	4529	136
H(18A)	11484	6234	4072	130
H(18B)	12549	7175	4257	130
H(18C)	12391	6618	5041	130
H(19A)	4300	4512	-1847	166
H(19B)	3619	4723	-2822	166
H(20A)	3475	3227	-3411	136
H(21A)	3653	2050	-2413	99
H(21B)	4657	2920	-1712	99
H(22A)	5298	384	-4134	174
H(22B)	6246	1280	-3414	174
H(22C)	5485	1519	-4312	174
H(23A)	2724	368	-4447	198

H(23B)	3321	1304	-4798	198
H(23C)	2783	1481	-4118	198
H(24A)	3676	-502	-3258	179
H(24B)	3933	210	-2379	179
H(24C)	4898	-98	-2536	179
H(25A)	15350	2491	2278	324
H(25B)	14918	3315	2618	324
H(25C)	14288	2728	1639	324
H(26A)	13763	1197	2185	257
H(26B)	14361	1811	3161	257
H(27A)	13244	1859	3789	135
H(27B)	12105	2054	3255	135
H(28A)	11861	475	3446	215
H(28B)	12653	383	2957	215
H(28C)	11514	577	2435	215
H(29A)	8086	4687	3811	189
H(29B)	9165	4350	4048	189
H(29C)	8077	3741	3229	189
H(30A)	9319	5775	3331	95
H(30B)	8244	5152	2508	95
H(31A)	9183	4052	2241	67
H(31B)	10251	4644	3076	67
H(32A)	10490	5089	1785	73
H(32B)	10532	6061	2355	73
H(32C)	9447	5485	1521	73