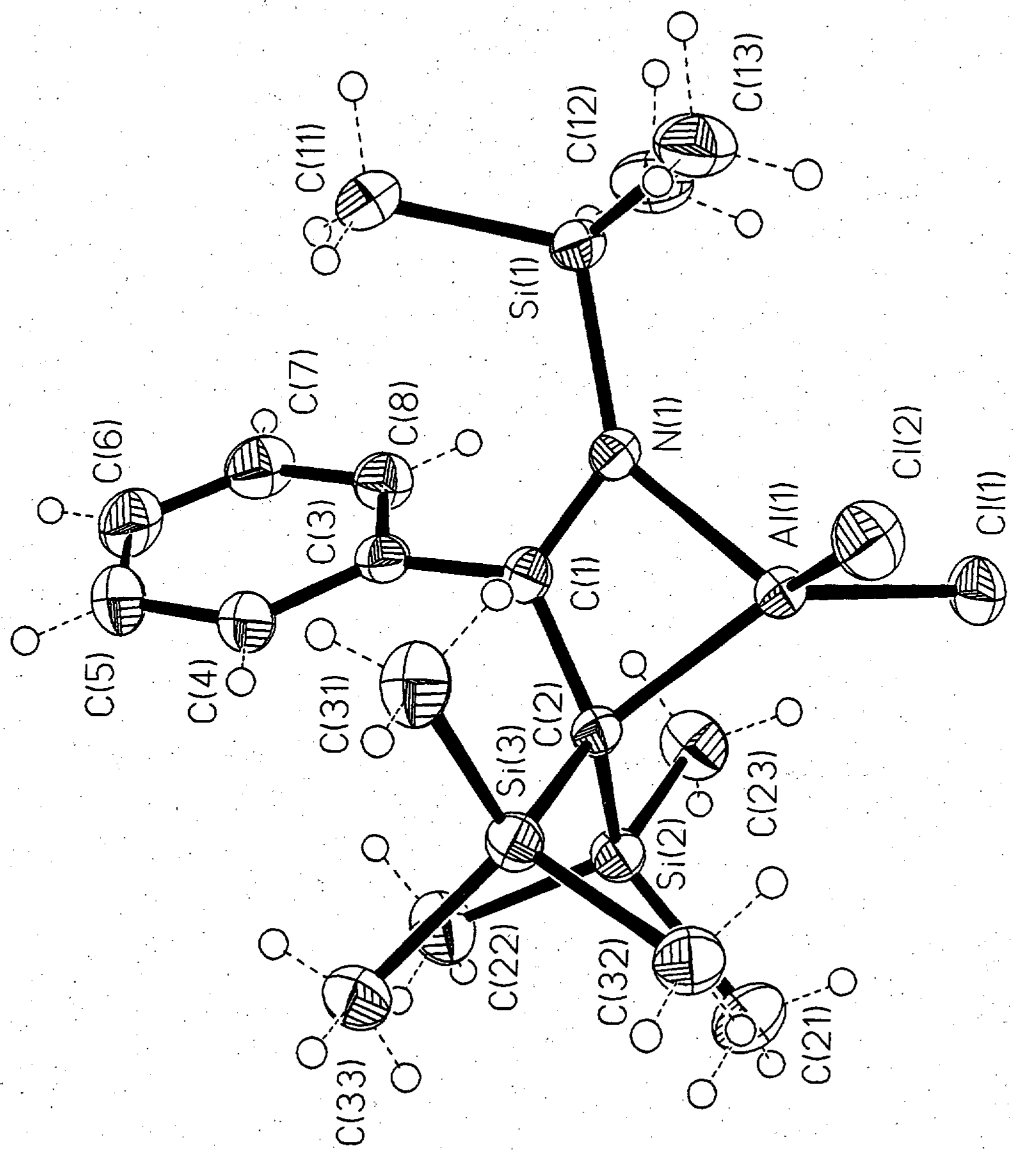
C(11)
C(12)
C(13)
Si(1)
C(7)
C(8)
C(6)
N(1)
Cl(2)
C(3)
Al(1)
Cl(1)
C(1)
C(5)
C(4)
C(31)
Si(3)
C(2)
C(23)
Si(2)
C(22)
C(32)
C(21)
C(33)

Table 1. Crystal data and structure refinement for 1.

Identification code	roe761x
Empirical formula	$C_{17}H_{32}AlCl_2NSi_3$
Formula weight	432.59
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 16.895(2) Å alpha = 90°
	b = 16.129(2) Å beta = 90°
	c = 17.769(2) Å gamma = 90°
Volume, Z	4842.3(10) $Å^3$, 8
Density (calculated)	1.187 Mg/m^3
Absorption coefficient	0.454 mm^{-1}
F(000)	1840
Crystal size	0.70 x 0.40 x 0.20 mm
θ range for data collection	3.56 to 25.05°
Limiting indices	$-18 \le h \le 20$, $-19 \le k \le 19$, $-21 \le l \le 19$
Reflections collected	10178
Independent reflections	4273 (R_{int} = 0.0502)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4266 / 0 / 226
Goodness-of-fit on F^2	1.091
Final R indices [$I>2\sigma(I)$]	R1 = 0.0380, wR2 = 0.0844
R indices (all data)	R1 = 0.0590, wR2 = 0.1007
Largest diff. peak and hole	0.361 and -0.231 $eÅ^{-3}$

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

	x	y	z	U(eq)
Al(1)	1219(1)	8822(1)	3747(1)	21(1)
Cl(1)	1969(1)	9118(1)	2820(1)	34(1)
Cl(2)	1125(1)	9918(1)	4407(1)	35(1)
N(1)	211(1)	8369(1)	3471(1)	21(1)
Si(1)	-699(1)	8751(1)	3073(1)	24(1)
Si(2)	1881(1)	6850(1)	3758(1)	24(1)
Si(3)	1198(1)	7726(1)	5238(1)	24(1)
C(1)	397(2)	7660(2)	3791(1)	21(1)
C(2)	1189(2)	7663(2)	4169(1)	21(1)
C(3)	-115(2)	6916(2)	3727(2)	24(1)
C(4)	-349(2)	6467(2)	4358(2)	32(1)
C(5)	-848(2)	5789(2)	4285(2)	39(1)
C(6)	-1100(2)	5537(2)	3580(2)	41(1)
C(7)	-858(2)	5962(2)	2948(2)	38(1)
C(8)	-373(2)	6653(2)	3018(2)	30(1)
C(11)	-1557(2)	8236(2)	3518(2)	43(1)
C(12)	-649(2)	8641(2)	2033(2)	41(1)
C(13)	-721(2)	9863(2)	3315(2)	40(1)
C(21)	2911(2)	7084(2)	4068(2)	40(1)
C(22)	1631(2)	5754(2)	4018(2)	39(1)
C(23)	1844(2)	6881(2)	2708(2)	38(1)
C(31)	256(2)	8216(2)	5574(2)	34(1)
C(32)	2062(2)	8362(2)	5543(2)	33(1)
C(33)	1303(2)	6707(2)	5734(2)	34(1)

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

Al(1)-N(1)	1.918(2)	Al(1)-C(2)	2.015(3)
Al(1)-Cl(2)	2.1276(10)	Al(1)-Cl(1)	2.1321(10)
Al(1)-C(1)	2.334(3)	N(1)-C(1)	1.314(3)
N(1)-Si(1)	1.800(2)	Si(1)-C(13)	1.846(3)
Si(1)-C(11)	1.849(3)	Si(1)-C(12)	1.858(3)
Si(2)-C(21)	1.864(3)	Si(2)-C(23)	1.867(3)
Si(2)-C(22)	1.875(3)	Si(2)-C(2)	1.902(3)
Si(3)-C(32)	1.864(3)	Si(3)-C(33)	1.873(3)
Si(3)-C(31)	1.874(3)	Si(3)-C(2)	1.903(3)
C(1)-C(3)	1.484(4)	C(1)-C(2)	1.498(3)
C(3)-C(4)	1.392(4)	C(3)-C(8)	1.399(4)
C(4)-C(5)	1.388(4)	C(5)-C(6)	1.382(4)
C(6)-C(7)	1.378(4)	C(7)-C(8)	1.388(4)
N(1)-Al(1)-C(2)	73.68(10)	N(1)-Al(1)-Cl(2)	113.05(7)
C(2)-Al(1)-Cl(2)	124.28(8)	N(1)-Al(1)-Cl(1)	114.57(7)
C(2)-Al(1)-Cl(1)	120.70(8)	Cl(2)-Al(1)-Cl(1)	106.53(4)
N(1)-Al(1)-C(1)	34.27(9)	C(2)-Al(1)-C(1)	39.44(9)
Cl(2)-Al(1)-C(1)	127.16(7)	Cl(1)-Al(1)-C(1)	124.01(7)
C(1)-N(1)-Si(1)	132.1(2)	C(1)-N(1)-Al(1)	90.5(2)
Si(1)-N(1)-Al(1)	136.76(12)	N(1)-Si(1)-C(13)	104.98(12)
N(1)-Si(1)-C(11)	110.38(12)	C(13)-Si(1)-C(11)	108.7(2)
N(1)-Si(1)-C(12)	108.62(12)	C(13)-Si(1)-C(12)	108.98(15)
C(11)-Si(1)-C(12)	114.8(2)	C(21)-Si(2)-C(23)	108.72(15)
C(21)-Si(2)-C(22)	109.15(15)	C(23)-Si(2)-C(22)	105.28(14)
C(21)-Si(2)-C(2)	108.69(12)	C(23)-Si(2)-C(2)	110.17(13)
C(22)-Si(2)-C(2)	114.66(12)	C(32)-Si(3)-C(33)	105.76(13)
C(32)-Si(3)-C(31)	109.87(13)	C(33)-Si(3)-C(31)	107.54(14)
C(32)-Si(3)-C(2)	109.01(12)	C(33)-Si(3)-C(2)	115.09(12)
C(31)-Si(3)-C(2)	109.45(12)	N(1)-C(1)-C(3)	122.1(2)
N(1)-C(1)-C(2)	113.9(2)	C(3)-C(1)-C(2)	123.9(2)
N(1)-C(1)-Al(1)	55.23(13)	C(3)-C(1)-Al(1)	173.6(2)
C(2)-C(1)-Al(1)	58.71(13)	C(1)-C(2)-Si(2)	112.0(2)
C(1)-C(2)-Si(3)	117.1(2)	Si(2)-C(2)-Si(3)	114.50(13)
C(1)-C(2)-Al(1)	81.85(14)	Si(2)-C(2)-Al(1)	118.75(13)
Si(3)-C(2)-Al(1)	108.84(12)	C(4)-C(3)-C(8)	118.6(3)
C(4)-C(3)-C(1)	121.7(2)	C(8)-C(3)-C(1)	119.7(2)
C(5)-C(4)-C(3)	120.5(3)	C(6)-C(5)-C(4)	120.2(3)
C(7)-C(6)-C(5)	120.1(3)	C(6)-C(7)-C(8)	120.1(3)
C(7)-C(8)-C(3)	120.5(3)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Al(1)	19(1)	22(1)	22(1)	1(1)	-1(1)	-1(1)
Cl(1)	32(1)	38(1)	32(1)	8(1)	8(1)	-2(1)
Cl(2)	40(1)	25(1)	39(1)	-6(1)	-1(1)	-1(1)
N(1)	18(1)	22(1)	23(1)	0(1)	0(1)	0(1)
Si(1)	19(1)	29(1)	25(1)	3(1)	-2(1)	1(1)
Si(2)	23(1)	24(1)	26(1)	0(1)	3(1)	3(1)
Si(3)	25(1)	28(1)	20(1)	0(1)	0(1)	-2(1)
C(1)	20(1)	24(1)	19(1)	-1(1)	5(1)	0(1)
C(2)	19(1)	23(1)	20(1)	1(1)	-3(1)	-2(1)
C(3)	20(1)	22(1)	29(1)	1(1)	-2(1)	3(1)
C(4)	29(2)	29(2)	37(2)	5(1)	-3(1)	-4(1)
C(5)	36(2)	33(2)	47(2)	9(1)	0(1)	-9(1)
C(6)	34(2)	29(2)	60(2)	-3(1)	-7(2)	-10(1)
C(7)	35(2)	32(2)	45(2)	-10(1)	-9(1)	-2(1)
C(8)	30(2)	29(2)	31(2)	-2(1)	-3(1)	-1(1)
C(11)	21(2)	53(2)	56(2)	17(2)	1(1)	3(1)
C(12)	44(2)	53(2)	28(2)	-1(1)	-9(1)	11(2)
C(13)	38(2)	33(2)	48(2)	0(1)	-7(2)	10(1)
C(21)	27(2)	47(2)	46(2)	-5(2)	4(1)	5(1)
C(22)	44(2)	27(2)	47(2)	0(1)	11(2)	6(1)
C(23)	45(2)	39(2)	30(2)	-2(1)	6(1)	3(1)
C(31)	38(2)	34(2)	32(2)	-6(1)	10(1)	-1(1)
C(32)	34(2)	40(2)	26(2)	1(1)	-8(1)	-6(1)
C(33)	36(2)	39(2)	27(2)	6(1)	-4(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(4A)	-165(2)	6626(2)	4842(2)	38
H(5A)	-1017(2)	5496(2)	4720(2)	47
H(6A)	-1440(2)	5072(2)	3532(2)	49
H(7A)	-1023(2)	5782(2)	2464(2)	45
H(8A)	-216(2)	6950(2)	2581(2)	36
H(11A)	-1475(6)	8207(12)	4064(2)	65
H(11B)	-1613(8)	7674(5)	3315(9)	65
H(11C)	-2039(3)	8554(8)	3412(10)	65
H(12A)	-135(5)	8843(12)	1853(2)	62
H(12B)	-1074(8)	8967(11)	1802(2)	62
H(12C)	-711(13)	8056(3)	1896(2)	62
H(13A)	-731(12)	9926(2)	3864(2)	60
H(13B)	-1196(7)	10118(3)	3099(10)	60
H(13C)	-249(6)	10135(3)	3113(10)	60
H(21A)	3283(2)	6736(9)	3788(8)	60
H(21B)	2962(4)	6970(12)	4608(3)	60
H(21C)	3028(4)	7670(4)	3973(11)	60
H(22A)	1972(8)	5373(2)	3736(9)	59
H(22B)	1076(4)	5643(4)	3896(11)	59
H(22C)	1716(12)	5674(4)	4559(3)	59
H(23A)	2191(9)	6449(8)	2503(2)	57
H(23B)	2022(11)	7425(5)	2532(2)	57
H(23C)	1300(3)	6783(12)	2539(2)	57
H(31A)	286(5)	8307(11)	6118(2)	52
H(31B)	-190(2)	7849(6)	5460(10)	52
H(31C)	181(6)	8748(6)	5318(8)	52
H(32A)	2098(7)	8354(10)	6094(2)	50
H(32B)	1993(6)	8934(3)	5369(9)	50
H(32C)	2548(2)	8131(7)	5328(9)	50
H(33A)	1280(12)	6795(2)	6279(2)	51
H(33B)	1812(5)	6455(6)	5601(9)	51
H(33C)	872(7)	6337(5)	5581(8)	51

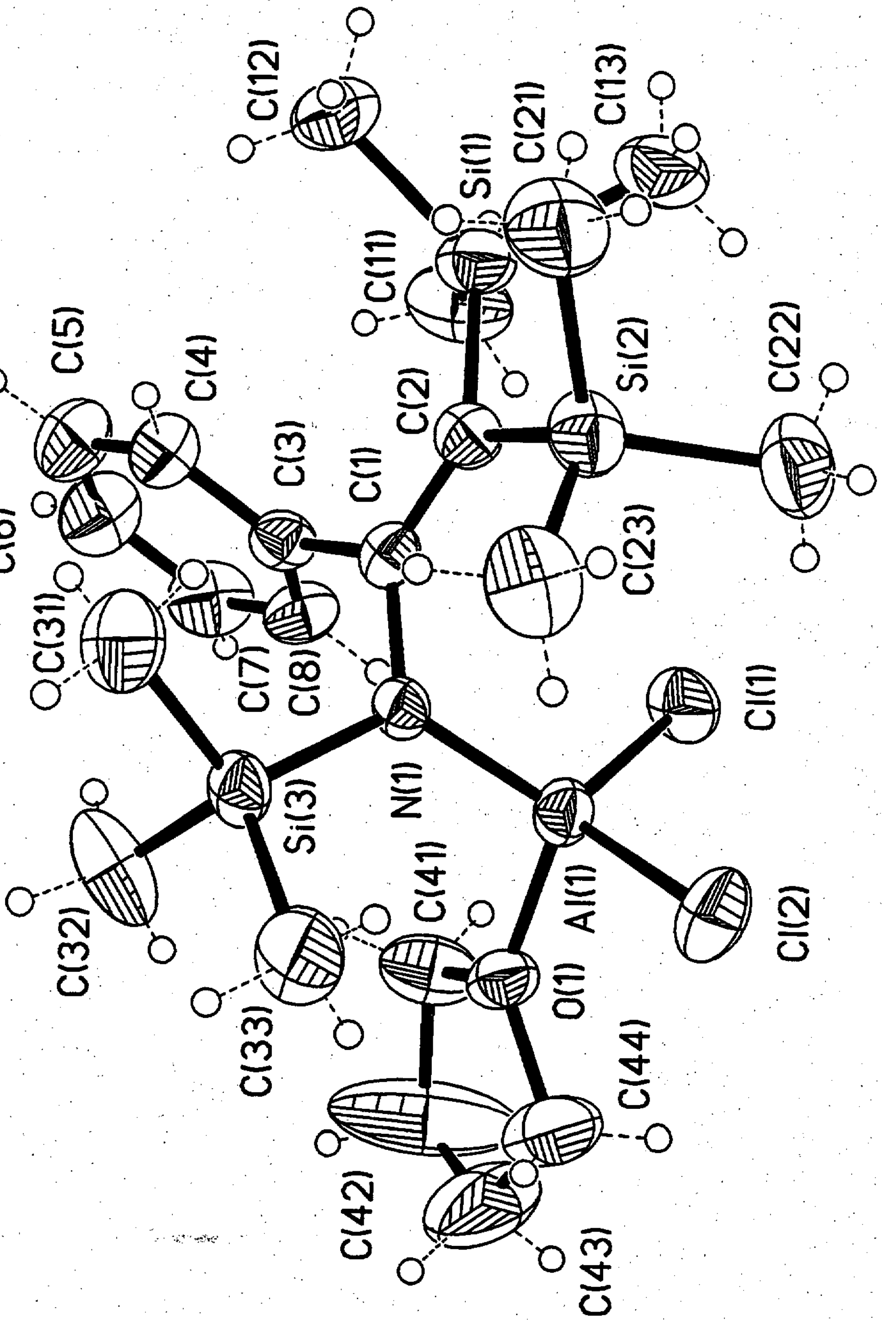
C(12)
C(13)
C(21)
Si(1)
C(11)
C(5)
C(4)
C(2)
Si(2)
C(22)
C(3)
C(1)
C(6)
C(23)
C(31)
C(7)
C(8)
Cl(1)
N(1)
Si(3)
C(41)
Al(1)
Cl(2)
C(32)
C(33)
O(1)
C(44)
C(42)
C(43)

Table 1. Crystal data and structure refinement for 1.

Identification code	roe754
Empirical formula	$C_{21}H_{40}AlCl_2NOSi_3$
Formula weight	504.69
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	*a* = 14.290(2) Å alpha = 90°
	b = 11.217(2) Å beta = 98.268(11)°
	c = 18.358(3) Å gamma = 90°
Volume, Z	2912.1(9) $Å^3$, 4
Density (calculated)	1.151 Mg/m^3
Absorption coefficient	0.389 mm^{-1}
F(000)	1080
Crystal size	0.60 x 0.60 x 0.50 mm
θ range for data collection	3.63 to 21.95°
Limiting indices	$-15 \le h \le 15$, $-8 \le k \le 11$, $-16 \le l \le 19$
Reflections collected	3809
Independent reflections	3519 (R_{int} = 0.1363)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3500 / 0 / 271
Goodness-of-fit on F^2	1.063
Final R indices [I>2σ(I)]	R1 = 0.0518, wR2 = 0.1100
R indices (all data)	R1 = 0.0748, wR2 = 0.1384
Largest diff. peak and hole	0.266 and -0.258 $eÅ^{-3}$

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

	x	y	z	U(eq)
Al(1)	973(1)	1880(1)	8416(1)	37(1)
Cl(1)	1087(1)	2506(1)	7334(1)	52(1)
Cl(2)	843(1)	-15(1)	8418(1)	60(1)
N(1)	1781(2)	2589(3)	9133(2)	31(1)
C(1)	2524(3)	3328(4)	8912(2)	32(1)
C(2)	3306(3)	2909(4)	8657(2)	36(1)
C(3)	2349(3)	4641(4)	9002(2)	36(1)
C(4)	2976(3)	5325(4)	9475(2)	43(1)
C(5)	2826(4)	6533(5)	9562(3)	60(2)
C(6)	2045(4)	7079(5)	9176(3)	62(2)
C(7)	1410(4)	6404(5)	8712(3)	57(1)
C(8)	1568(3)	5200(4)	8626(3)	45(1)
Si(1)	4070(1)	3932(1)	8175(1)	49(1)
C(11)	3399(4)	5193(5)	7671(3)	75(2)
C(12)	5098(4)	4556(6)	8813(3)	72(2)
C(13)	4559(4)	3104(6)	7423(3)	70(2)
Si(2)	3684(1)	1293(1)	8729(1)	49(1)
C(21)	5005(3)	1264(5)	8998(3)	73(2)
C(22)	3344(4)	476(5)	7838(3)	67(2)
C(23)	3265(4)	361(5)	9460(3)	64(2)
Si(3)	1623(1)	2634(1)	10064(1)	39(1)
C(31)	2770(4)	2812(5)	10674(3)	68(2)
C(32)	845(4)	3849(5)	10292(3)	79(2)
C(33)	1061(5)	1210(5)	10291(3)	79(2)
O(1)	-266(2)	2300(3)	8528(2)	42(1)
C(41)	-629(3)	3520(5)	8425(3)	63(2)
C(42)	-1659(5)	3387(9)	8471(6)	160(5)
C(43)	-1876(5)	2284(8)	8577(7)	164(5)
C(44)	-1071(4)	1494(6)	8544(4)	88(2)

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

Al(1)-N(1)	1.806(3)	Al(1)-O(1)	1.872(3)
Al(1)-Cl(2)	2.134(2)	Al(1)-Cl(1)	2.135(2)
N(1)-C(1)	1.450(5)	N(1)-Si(3)	1.757(3)
C(1)-C(2)	1.356(6)	C(1)-C(3)	1.507(6)
C(2)-Si(1)	1.888(4)	C(2)-Si(2)	1.891(5)
C(3)-C(8)	1.377(6)	C(3)-C(4)	1.386(6)
C(4)-C(5)	1.386(6)	C(5)-C(6)	1.377(7)
C(6)-C(7)	1.378(7)	C(7)-C(8)	1.382(6)
Si(1)-C(11)	1.877(5)	Si(1)-C(12)	1.877(5)
Si(1)-C(13)	1.881(5)	Si(2)-C(23)	1.867(5)
Si(2)-C(22)	1.877(5)	Si(2)-C(21)	1.881(5)
Si(3)-C(32)	1.845(5)	Si(3)-C(31)	1.857(5)
Si(3)-C(33)	1.862(5)	O(1)-C(41)	1.466(6)
O(1)-C(44)	1.467(6)	C(41)-C(42)	1.493(8)
C(42)-C(43)	1.298(10)	C(43)-C(44)	1.460(9)
N(1)-Al(1)-O(1)	109.0(2)	N(1)-Al(1)-Cl(2)	118.98(13)
O(1)-Al(1)-Cl(2)	99.61(11)	N(1)-Al(1)-Cl(1)	114.00(12)
O(1)-Al(1)-Cl(1)	102.64(11)	Cl(2)-Al(1)-Cl(1)	110.34(8)
C(1)-N(1)-Si(3)	117.3(3)	C(1)-N(1)-Al(1)	117.7(2)
Si(3)-N(1)-Al(1)	124.3(2)	C(2)-C(1)-N(1)	124.9(4)
C(2)-C(1)-C(3)	122.3(4)	N(1)-C(1)-C(3)	112.8(4)
C(1)-C(2)-Si(1)	120.8(3)	C(1)-C(2)-Si(2)	123.3(3)
Si(1)-C(2)-Si(2)	115.9(2)	C(8)-C(3)-C(4)	117.8(4)
C(8)-C(3)-C(1)	121.7(4)	C(4)-C(3)-C(1)	120.5(4)
C(5)-C(4)-C(3)	121.2(5)	C(6)-C(5)-C(4)	120.2(5)
C(5)-C(6)-C(7)	119.2(5)	C(6)-C(7)-C(8)	120.2(5)
C(3)-C(8)-C(7)	121.4(5)	C(11)-Si(1)-C(12)	108.9(3)
C(11)-Si(1)-C(13)	103.1(3)	C(12)-Si(1)-C(13)	107.6(2)
C(11)-Si(1)-C(2)	113.6(2)	C(12)-Si(1)-C(2)	112.8(2)
C(13)-Si(1)-C(2)	110.2(2)	C(23)-Si(2)-C(22)	106.5(3)
C(23)-Si(2)-C(21)	102.4(3)	C(22)-Si(2)-C(21)	110.2(3)
C(23)-Si(2)-C(2)	117.9(2)	C(22)-Si(2)-C(2)	111.8(2)
C(21)-Si(2)-C(2)	107.5(2)	N(1)-Si(3)-C(32)	114.1(2)
N(1)-Si(3)-C(31)	111.3(2)	C(32)-Si(3)-C(31)	107.0(3)
N(1)-Si(3)-C(33)	108.3(2)	C(32)-Si(3)-C(33)	106.8(3)
C(31)-Si(3)-C(33)	109.2(3)	C(41)-O(1)-C(44)	108.3(4)
C(41)-O(1)-Al(1)	123.0(3)	C(44)-O(1)-Al(1)	127.1(3)
O(1)-C(41)-C(42)	103.5(5)	C(43)-C(42)-C(41)	111.2(7)
C(42)-C(43)-C(44)	111.5(7)	C(43)-C(44)-O(1)	104.6(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Al(1)	42(1)	37(1)	31(1)	-2(1)	5(1)	-5(1)
Cl(1)	53(1)	77(1)	27(1)	2(1)	5(1)	-4(1)
Cl(2)	75(1)	36(1)	66(1)	-10(1)	2(1)	-9(1)
N(1)	40(2)	30(2)	25(2)	2(2)	9(2)	-5(2)
C(1)	36(3)	32(3)	26(2)	4(2)	-3(2)	-1(2)
C(2)	32(3)	41(3)	33(3)	1(2)	0(2)	3(2)
C(3)	38(3)	33(3)	38(3)	5(2)	10(2)	-3(2)
C(4)	46(3)	34(3)	47(3)	2(2)	1(2)	1(2)
C(5)	65(4)	42(3)	71(4)	-7(3)	3(3)	-8(3)
C(6)	73(4)	30(3)	83(4)	2(3)	9(3)	2(3)
C(7)	49(3)	44(3)	76(4)	11(3)	7(3)	13(3)
C(8)	39(3)	38(3)	58(3)	6(2)	6(2)	-6(2)
Si(1)	38(1)	68(1)	42(1)	6(1)	7(1)	-9(1)
C(11)	71(4)	88(5)	69(4)	39(3)	25(3)	-4(3)
C(12)	55(3)	95(5)	65(4)	-8(3)	11(3)	-33(3)
C(13)	53(3)	111(5)	50(3)	3(3)	20(3)	-12(3)
Si(2)	46(1)	51(1)	48(1)	-3(1)	1(1)	14(1)
C(21)	51(3)	87(5)	79(4)	-1(3)	0(3)	24(3)
C(22)	67(4)	68(4)	65(4)	-22(3)	5(3)	17(3)
C(23)	79(4)	47(3)	66(4)	9(3)	6(3)	19(3)
Si(3)	51(1)	41(1)	26(1)	2(1)	6(1)	-2(1)
C(31)	75(4)	88(4)	35(3)	3(3)	-7(3)	-2(3)
C(32)	107(5)	87(5)	47(3)	9(3)	29(3)	39(4)
C(33)	121(5)	78(4)	42(3)	5(3)	26(3)	-42(4)
O(1)	39(2)	43(2)	45(2)	3(2)	7(1)	-11(2)
C(41)	52(3)	61(4)	79(4)	28(3)	19(3)	8(3)
C(42)	51(4)	161(9)	280(12)	139(9)	60(6)	45(5)
C(43)	66(5)	125(8)	318(15)	-117(9)	84(7)	-34(5)
C(44)	62(4)	78(5)	127(6)	-20(4)	30(4)	-29(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(4A)	3513(3)	4962(4)	9740(2)	52
H(5A)	3258(4)	6982(5)	9887(3)	72
H(6A)	1946(4)	7901(5)	9228(3)	75
H(7A)	867(4)	6764(5)	8454(3)	68
H(8A)	1132(3)	4754(4)	8303(3)	54
H(11A)	2811(13)	4894(8)	7404(17)	112
H(11B)	3776(12)	5543(22)	7328(15)	112
H(11C)	3263(23)	5793(16)	8021(4)	112
H(12A)	5391(16)	3927(9)	9129(14)	107
H(12B)	4877(5)	5180(23)	9112(15)	107
H(12C)	5557(13)	4884(31)	8527(3)	107
H(13A)	4042(4)	2791(28)	7075(11)	105
H(13B)	4952(21)	2450(20)	7635(4)	105
H(13C)	4936(21)	3643(9)	7170(13)	105
H(21A)	5232(5)	452(7)	8971(20)	109
H(21B)	5165(4)	1558(32)	9498(8)	109
H(21C)	5299(4)	1766(27)	8666(13)	109
H(22A)	2673(6)	581(27)	7673(11)	101
H(22B)	3481(24)	-366(7)	7911(5)	101
H(22C)	3700(19)	791(22)	7469(6)	101
H(23A)	2584(5)	268(26)	9354(11)	97
H(23B)	3429(22)	747(16)	9934(4)	97
H(23C)	3563(19)	-417(12)	9471(13)	97
H(31A)	2933(13)	3651(6)	10716(16)	101
H(31B)	3259(6)	2384(27)	10467(11)	101
H(31C)	2716(8)	2495(30)	11158(6)	101
H(32A)	1071(16)	4603(7)	10126(20)	118
H(32B)	848(23)	3876(24)	10821(3)	118
H(32C)	205(7)	3707(19)	10050(18)	118
H(33A)	438(12)	1146(17)	10004(16)	118
H(33B)	1003(26)	1198(16)	10811(5)	118
H(33C)	1448(14)	545(5)	10177(20)	118
H(41A)	-529(3)	3837(5)	7945(3)	76
H(41B)	-323(3)	4050(5)	8813(3)	76
H(42A)	-1823(5)	3877(9)	8876(6)	192
H(42B)	-2028(5)	3674(9)	8013(6)	192
H(43A)	-2400(5)	2043(8)	8202(7)	197
H(43B)	-2086(5)	2207(8)	9060(7)	197
H(44A)	-1172(4)	999(6)	8100(4)	105
H(44B)	-967(4)	973(6)	8977(4)	105

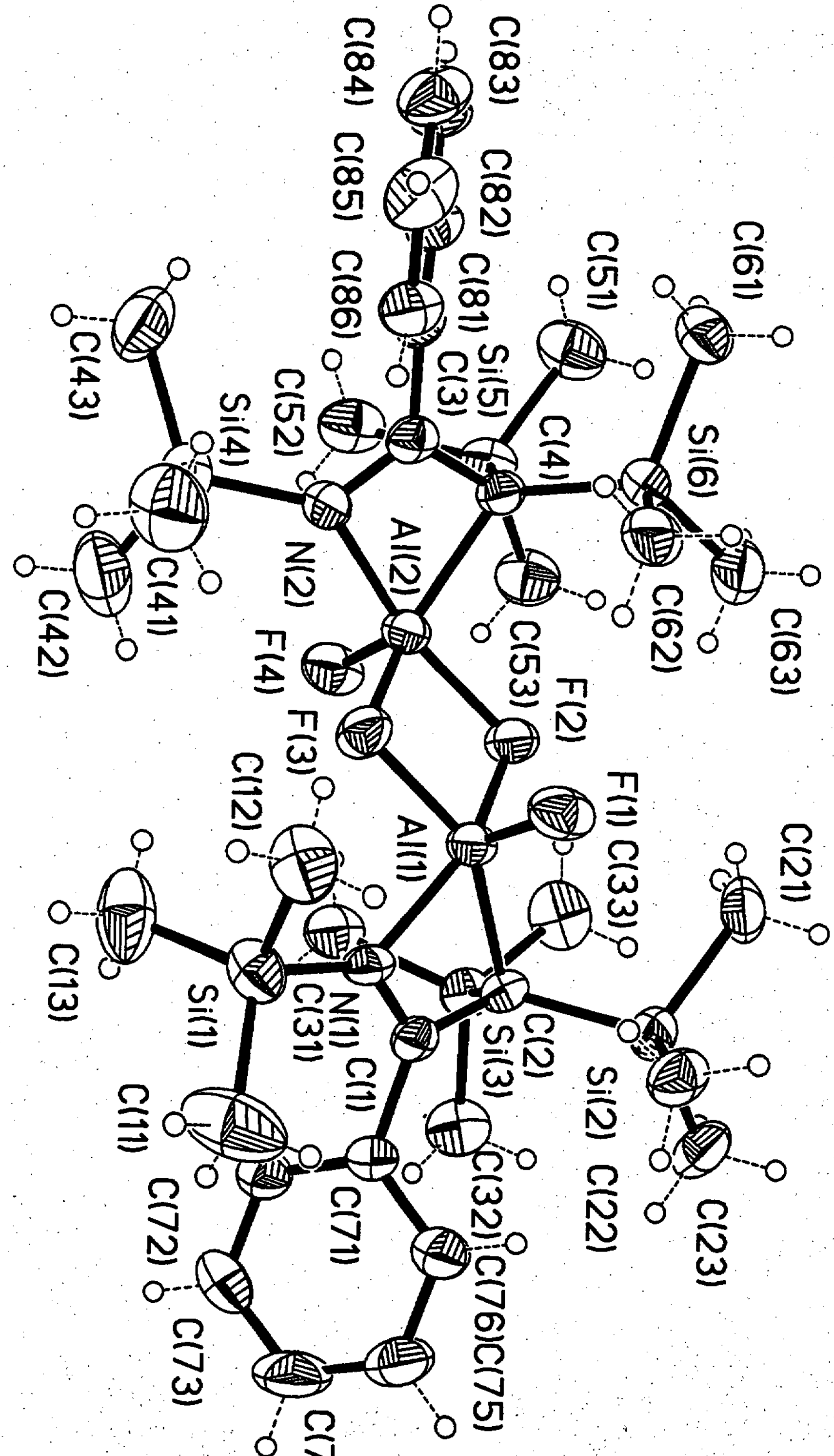
C(83)
C(84)
C(82)
C(85)
C(61)
C(51)
C(81)
C(86)
Si(5)
C(3)
C(43)
Si(4)
C(52)
C(4)
Si(6)
Al(2)
N(2)
C(41)
C(42)
C(62)
C(53)
C(63)
F(4)
F(2)
F(3)
F(1)
C(33)
C(12)
Al(1)
C(21)
C(13)
Si(1)
C(31)
N(1)
C(1)
Si(3)
C(2)
Si(2)
C(22)
C(11)
C(32)
C(71)
C(72)
C(23)
C(76)
C(75)
C(73)
C(74)

Table 1. Crystal data and structure refinement for 1.

Identification code	roe756
Empirical formula	$C_{37}H_{71}Al_2F_4N_2Si_6$ incl. $_{0.5}$hexa
Formula weight	842.46
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 10.916(3) Å alpha = 79.13(3)°
	b = 13.712(6) Å beta = 80.207(13)°
	c = 18.242(6) Å gamma = 69.784(15)°
Volume, Z	2499.9(15) $Å^3$, 2
Density (calculated)	1.119 Mg/m^3
Absorption coefficient	0.243 mm^{-1}
F(000)	906
Crystal size	0.50 x 0.50 x 0.50 mm
θ range for data collection	3.55 to 20.04°
Limiting indices	$-10 \le h \le 10$, $-13 \le k \le 13$, $-17 \le l \le 17$
Reflections collected	8628
Independent reflections	4653 (R_{int} = 0.0498)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4634 / 319 / 493
Goodness-of-fit on F^2	1.040
Final R indices [$I>2\sigma(I)$]	R1 = 0.0493, wR2 = 0.1130
R indices (all data)	R1 = 0.0744, wR2 = 0.1390
Largest diff. peak and hole	0.272 and -0.323 $eÅ^{-3}$

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

	x	y	z	U(eq)
Al(1)	1554(2)	5356(1)	2294(1)	34(1)
Al(2)	1903(2)	3152(1)	2331(1)	36(1)
F(1)	1537(3)	5860(2)	1389(1)	52(1)
F(2)	2837(2)	4074(2)	2245(1)	41(1)
F(3)	634(3)	4433(2)	2379(2)	46(1)
F(4)	2010(3)	2657(2)	3236(1)	54(1)
N(1)	81(4)	6367(3)	2833(2)	35(1)
N(2)	726(4)	2574(3)	1980(2)	38(1)
C(1)	901(5)	6635(3)	3135(2)	34(1)
C(2)	2308(5)	6059(3)	2923(2)	32(1)
C(3)	1646(5)	2175(3)	1453(3)	35(1)
C(4)	2948(5)	2246(4)	1511(2)	36(1)
Si(1)	-1653(2)	6796(1)	2843(1)	48(1)
C(11)	-2465(7)	8168(5)	3042(4)	93(2)
C(12)	-1919(5)	6716(5)	1886(3)	61(2)
C(13)	-2225(6)	5835(5)	3543(3)	77(2)
Si(2)	3305(1)	6794(1)	2252(1)	41(1)
C(21)	4502(5)	5874(4)	1621(3)	61(2)
C(22)	2232(5)	7910(4)	1640(3)	50(2)
C(23)	4274(5)	7344(4)	2718(3)	56(2)
Si(3)	3131(2)	5213(1)	3761(1)	42(1)
C(31)	2100(6)	4401(4)	4265(3)	53(2)
C(32)	3333(6)	5968(4)	4470(3)	55(2)
C(33)	4795(5)	4315(4)	3454(3)	63(2)
Si(4)	-875(2)	2471(1)	2268(1)	54(1)
C(41)	-2112(6)	3613(5)	1805(4)	83(2)
C(42)	-1108(6)	2495(5)	3294(3)	89(2)
C(43)	-971(6)	1205(5)	2084(4)	83(2)
Si(5)	4065(2)	1044(1)	2051(1)	44(1)
C(51)	5290(6)	82(4)	1455(3)	64(2)
C(52)	3044(6)	324(4)	2706(3)	55(2)
C(53)	5059(6)	1432(4)	2611(3)	59(2)
Si(6)	3754(2)	2810(1)	608(1)	44(1)
C(61)	4279(6)	1940(4)	-150(3)	55(2)
C(62)	2569(6)	4072(4)	208(3)	59(2)
C(63)	5243(6)	3063(5)	797(3)	70(2)
C(71)	439(5)	7401(4)	3697(3)	35(1)
C(72)	-311(5)	7188(4)	4362(3)	45(1)
C(73)	-721(6)	7864(5)	4895(3)	60(2)
C(74)	-393(7)	8772(5)	4751(3)	77(2)
C(75)	333(7)	9002(5)	4092(3)	73(2)
C(76)	774(6)	8311(4)	3570(3)	53(2)
C(81)	1342(5)	1751(4)	829(3)	37(1)
C(82)	1987(5)	727(4)	688(3)	44(1)
C(83)	1667(6)	357(4)	115(3)	53(2)
C(84)	728(7)	1031(5)	-335(3)	64(2)
C(85)	101(6)	2048(5)	-210(3)	63(2)
C(86)	403(5)	2409(4)	377(3)	49(1)
C(91)	6093(21)	1455(17)	5059(20)	207(13)
C(92)	4988(18)	1116(16)	5004(17)	206(11)
C(93)	5368(20)	[illegible]		

C(92A)	4405(25)	-1429(19)	5179(24)	259(17)
C(91A)	3200(26)	-1814(23)	5028(21)	354(21)

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

Al(1)-F(1)	1.665(3)	Al(1)-F(2)	1.837(3)
Al(1)-F(3)	1.841(3)	Al(1)-N(1)	1.977(4)
Al(1)-C(2)	2.051(5)	Al(1)-C(1)	2.392(5)
Al(1)-Al(2)	2.902(2)	Al(2)-F(4)	1.670(3)
Al(2)-F(3)	1.829(3)	Al(2)-F(2)	1.850(3)
Al(2)-N(2)	1.964(4)	Al(2)-C(4)	2.055(5)
Al(2)-C(3)	2.378(5)	N(1)-C(1)	1.308(6)
N(1)-Si(1)	1.776(4)	N(2)-C(3)	1.312(6)
N(2)-Si(4)	1.783(4)	C(1)-C(2)	1.486(6)
C(1)-C(71)	1.508(6)	C(2)-Si(2)	1.881(5)
C(2)-Si(3)	1.889(5)	C(3)-C(4)	1.480(7)
C(3)-C(81)	1.504(7)	C(4)-Si(5)	1.891(5)
C(4)-Si(6)	1.892(5)	Si(1)-C(12)	1.846(5)
Si(1)-C(13)	1.849(6)	Si(1)-C(11)	1.860(6)
Si(2)-C(23)	1.874(5)	Si(2)-C(21)	1.875(5)
Si(2)-C(22)	1.876(5)	Si(3)-C(31)	1.865(5)
Si(3)-C(33)	1.870(5)	Si(3)-C(32)	1.886(5)
Si(4)-C(41)	1.848(6)	Si(4)-C(42)	1.850(6)
Si(4)-C(43)	1.869(6)	Si(5)-C(53)	1.867(5)
Si(5)-C(52)	1.873(5)	Si(5)-C(51)	1.881(5)
Si(6)-C(62)	1.871(5)	Si(6)-C(63)	1.873(6)
Si(6)-C(61)	1.883(5)	C(71)-C(76)	1.385(7)
C(71)-C(72)	1.386(7)	C(72)-C(73)	1.382(7)
C(73)-C(74)	1.377(8)	C(74)-C(75)	1.371(8)
C(75)-C(76)	1.381(7)	C(81)-C(86)	1.383(7)
C(81)-C(82)	1.386(6)	C(82)-C(83)	1.385(7)
C(83)-C(84)	1.387(8)	C(84)-C(85)	1.369(8)
C(85)-C(86)	1.389(7)	C(91)-C(92A)#1	0.77(5)
C(91)-C(91A)#1	1.03(3)	C(91)-C(92)	1.46
C(91)-C(93A)#1	1.66(4)	C(92)-C(92A)#1	0.90(3)
C(92)-C(93A)#1	1.13(4)	C(92)-C(93)	1.55
C(92)-C(93)#1	1.64(4)	C(93)-C(93A)#1	0.91(3)
C(93)-C(93)#1	0.93(5)	C(93)-C(93A)	1.53
C(93)-C(92)#1	1.64(4)	C(93A)-C(93)#1	0.91(3)
C(93A)-C(92)#1	1.13(5)	C(93A)-C(92A)	1.39
C(93A)-C(91)#1	1.66(4)	C(92A)-C(91)#1	0.77(5)
C(92A)-C(92)#1	0.90(4)	C(92A)-C(91A)	1.66
C(91A)-C(91)#1	1.03(3)		
F(1)-Al(1)-F(2)	101.40(14)	F(1)-Al(1)-F(3)	102.23(15)
F(2)-Al(1)-F(3)	75.86(13)	F(1)-Al(1)-N(1)	105.6(2)
F(2)-Al(1)-N(1)	152.4(2)	F(3)-Al(1)-N(1)	92.7(2)
F(1)-Al(1)-C(2)	114.9(2)	F(2)-Al(1)-C(2)	102.5(2)
F(3)-Al(1)-C(2)	142.2(2)	N(1)-Al(1)-C(2)	71.3(2)
F(1)-Al(1)-C(1)	114.3(2)	F(2)-Al(1)-C(1)	134.9(2)
F(3)-Al(1)-C(1)	119.4(2)	N(1)-Al(1)-C(1)	33.2(2)
C(2)-Al(1)-C(1)	38.1(2)	F(1)-Al(1)-Al(2)	105.04(11)
F(2)-Al(1)-Al(2)	38.26(9)	F(3)-Al(1)-Al(2)	37.60(9)
N(1)-Al(1)-Al(2)	125.98(13)	C(2)-Al(1)-Al(2)	129.81(14)
C(1)-Al(1)-Al(2)	139.21(12)	F(4)-Al(2)-F(3)	102.56(15)
F(4)-Al(2)-F(2)	99.10(15)	F(3)-Al(2)-F(2)	75.81(12)
F(4)-Al(2)-N(2)	106.6(2)	F(3)-Al(2)-N(2)	92.6(2)
F(2)-Al(2)-N(2)	153.6(2)	F(4)-Al(2)-C(4)	120.0(2)
F(3)-Al(2)-C(4)	137.1(2)	F(2)-Al(2)-C(4)	100.9(2)
N(2)-Al(2)-C(4)	71.4(2)	F(4)-Al(2)-C(3)	121.6(2)
F(3)-Al(2)-C(3)	114.7(2)	F(2)-Al(2)-C(3)	131.8(2)
N(2)-Al(2)-C(3)	33.5(2)	C(4)-Al(2)-C(3)	38.1(2)
F(4)-Al(2)-Al(1)	[illegible]		

C(4)-Al(2)-Al(1)	125.77(15)	C(3)-Al(2)-Al(1)	133.35(12)
Al(1)-F(2)-Al(2)	103.81(14)	Al(2)-F(3)-Al(1)	104.52(15)
C(1)-N(1)-Si(1)	134.9(3)	C(1)-N(1)-Al(1)	91.1(3)
Si(1)-N(1)-Al(1)	133.9(2)	C(3)-N(2)-Si(4)	131.6(3)
C(3)-N(2)-Al(2)	90.8(3)	Si(4)-N(2)-Al(2)	137.3(2)
N(1)-C(1)-C(2)	114.2(4)	N(1)-C(1)-C(71)	122.2(4)
C(2)-C(1)-C(71)	123.5(4)	N(1)-C(1)-Al(1)	55.8(2)
C(2)-C(1)-Al(1)	58.4(2)	C(71)-C(1)-Al(1)	176.4(3)
C(1)-C(2)-Si(2)	117.8(3)	C(1)-C(2)-Si(3)	111.8(3)
Si(2)-C(2)-Si(3)	115.5(2)	C(1)-C(2)-Al(1)	83.4(3)
Si(2)-C(2)-Al(1)	107.3(2)	Si(3)-C(2)-Al(1)	117.0(2)
N(2)-C(3)-C(4)	114.2(4)	N(2)-C(3)-C(81)	121.3(4)
C(4)-C(3)-C(81)	124.4(4)	N(2)-C(3)-Al(2)	55.7(2)
C(4)-C(3)-Al(2)	59.1(2)	C(81)-C(3)-Al(2)	169.5(3)
C(3)-C(4)-Si(5)	114.4(3)	C(3)-C(4)-Si(6)	114.6(3)
Si(5)-C(4)-Si(6)	115.4(3)	C(3)-C(4)-Al(2)	82.8(3)
Si(5)-C(4)-Al(2)	103.5(2)	Si(6)-C(4)-Al(2)	121.9(2)
N(1)-Si(1)-C(12)	104.7(2)	N(1)-Si(1)-C(13)	105.7(2)
C(12)-Si(1)-C(13)	110.9(3)	N(1)-Si(1)-C(11)	113.3(3)
C(12)-Si(1)-C(11)	109.1(3)	C(13)-Si(1)-C(11)	112.8(3)
C(23)-Si(2)-C(21)	107.4(3)	C(23)-Si(2)-C(22)	107.6(2)
C(21)-Si(2)-C(22)	107.6(3)	C(23)-Si(2)-C(2)	114.2(2)
C(21)-Si(2)-C(2)	108.6(2)	C(22)-Si(2)-C(2)	111.1(2)
C(31)-Si(3)-C(33)	108.7(3)	C(31)-Si(3)-C(32)	106.6(2)
C(33)-Si(3)-C(32)	107.7(3)	C(31)-Si(3)-C(2)	108.5(2)
C(33)-Si(3)-C(2)	110.7(2)	C(32)-Si(3)-C(2)	114.5(2)
N(2)-Si(4)-C(41)	110.0(3)	N(2)-Si(4)-C(42)	103.8(3)
C(41)-Si(4)-C(42)	110.3(3)	N(2)-Si(4)-C(43)	111.7(2)
C(41)-Si(4)-C(43)	111.6(3)	C(42)-Si(4)-C(43)	109.2(3)
C(53)-Si(5)-C(52)	108.9(3)	C(53)-Si(5)-C(51)	105.6(3)
C(52)-Si(5)-C(51)	107.3(3)	C(53)-Si(5)-C(4)	110.5(2)
C(52)-Si(5)-C(4)	109.3(2)	C(51)-Si(5)-C(4)	115.1(2)
C(62)-Si(6)-C(63)	109.1(3)	C(62)-Si(6)-C(61)	106.1(2)
C(63)-Si(6)-C(61)	107.8(3)	C(62)-Si(6)-C(4)	109.7(2)
C(63)-Si(6)-C(4)	110.0(2)	C(61)-Si(6)-C(4)	114.0(2)
C(76)-C(71)-C(72)	118.9(4)	C(76)-C(71)-C(1)	121.2(4)
C(72)-C(71)-C(1)	119.9(4)	C(73)-C(72)-C(71)	121.1(5)
C(74)-C(73)-C(72)	118.9(5)	C(75)-C(74)-C(73)	120.8(5)
C(74)-C(75)-C(76)	120.1(5)	C(75)-C(76)-C(71)	120.1(5)
C(86)-C(81)-C(82)	119.3(5)	C(86)-C(81)-C(3)	118.7(5)
C(82)-C(81)-C(3)	122.0(4)	C(83)-C(82)-C(81)	120.4(5)
C(82)-C(83)-C(84)	119.4(5)	C(85)-C(84)-C(83)	120.7(5)
C(84)-C(85)-C(86)	119.7(6)	C(81)-C(86)-C(85)	120.5(5)
C(92A)#1-C(91)-C(91A)#1	135(8)	C(92A)#1-C(91)-C(92)	31(4)
C(91A)#1-C(91)-C(92)	165(5)	C(92A)#1-C(91)-C(93A)#1	56(2)
C(91A)#1-C(91)-C(93A)#1	143(5)	C(92)-C(91)-C(93A)#1	41.9(13)
C(92A)#1-C(92)-C(93A)#1	85(3)	C(92A)#1-C(92)-C(91)	26(4)
C(93A)#1-C(92)-C(91)	78.7(16)	C(92A)#1-C(92)-C(93)	121(3)
C(93A)#1-C(92)-C(93)	35.4(17)	C(91)-C(92)-C(93)	111.7
C(92A)#1-C(92)-C(93)#1	138(5)	C(93A)#1-C(92)-C(93)#1	63.6(19)
C(91)-C(92)-C(93)#1	142.2(15)	C(93)-C(92)-C(93)#1	33.7(17)
C(93A)#1-C(93)-C(93)#1	112(6)	C(93A)#1-C(93)-C(93A)	146(4)
C(93)#1-C(93)-C(93A)	33(3)	C(93A)#1-C(93)-C(92)	46(3)
C(93)#1-C(93)-C(92)	79(3)	C(93A)-C(93)-C(92)	106.9
C(93A)#1-C(93)-C(92)#1	150(7)	C(93)#1-C(93)-C(92)#1	68(2)
C(93A)-C(93)-C(92)#1	41.6(16)	C(92)-C(93)-C(92)#1	146(2)
C(93)#1-C(93A)-C(92)#1	98(3)	C(93)#1-C(93A)-C(92A)	138(3)
C(92)#1-C(93A)-C(92A)	40(2)	C(93)#1-C(93A)-C(93)	34(3)
C(92)#1-C(93A)-C(93)	74.7(19)	C(92A)-C(93A)-C(93)	109.9
C(93)#1-C(93A)-C(91)#1	150(5)	C(92)#1-C(93A)-C(91)#1	59.4(18)
C(92A)-C(93A)-C(91)#1	27.2(18)	C(93)-C(93A)-C(91)#1	134.0(13)
C(91)#1-C(92A)-C(92)#1	123(9)	C(91)#1-C(92A)-C(93A)	97(3)

C(92)#1-C(92A)-C(91A)	149(6)	C(93A)-C(92A)-C(91A)	114.3
C(91)#1-C(91A)-C(92A)	19(4)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Al(1)	40(1)	31(1)	33(1)	-7(1)	-4(1)	-11(1)
Al(2)	44(1)	33(1)	32(1)	-7(1)	-1(1)	-13(1)
F(1)	78(2)	40(2)	35(2)	-6(1)	-6(2)	-16(2)
F(2)	37(2)	36(2)	53(2)	-16(1)	-5(1)	-11(1)
F(3)	37(2)	34(2)	69(2)	-14(1)	-3(1)	-12(1)
F(4)	85(2)	40(2)	33(2)	-2(1)	-4(2)	-18(2)
N(1)	40(2)	33(2)	37(2)	-12(2)	-5(2)	-14(2)
N(2)	41(3)	35(2)	36(2)	-8(2)	-2(2)	-12(2)
C(1)	46(3)	25(3)	29(3)	2(2)	-2(2)	-15(2)
C(2)	36(3)	26(3)	35(3)	-2(2)	-7(2)	-11(2)
C(3)	47(3)	24(3)	34(3)	2(2)	-7(2)	-15(2)
C(4)	41(3)	34(3)	35(3)	-8(2)	-5(2)	-14(2)
Si(1)	37(1)	61(1)	43(1)	-13(1)	-6(1)	-10(1)
C(11)	72(5)	82(4)	111(6)	-46(4)	-38(4)	24(4)
C(12)	48(4)	83(4)	52(3)	-9(3)	-14(3)	-20(3)
C(13)	54(4)	126(5)	57(4)	1(4)	-7(3)	-45(4)
Si(2)	42(1)	35(1)	43(1)	-2(1)	1(1)	-15(1)
C(21)	55(4)	51(4)	65(4)	-7(3)	23(3)	-18(3)
C(22)	71(4)	41(3)	43(3)	2(2)	-8(3)	-26(3)
C(23)	47(4)	44(3)	84(4)	-4(3)	-9(3)	-25(3)
Si(3)	48(1)	39(1)	38(1)	-2(1)	-9(1)	-14(1)
C(31)	77(4)	49(3)	36(3)	0(3)	-7(3)	-24(3)
C(32)	62(4)	55(4)	53(4)	-5(3)	-21(3)	-17(3)
C(33)	54(4)	61(4)	63(4)	2(3)	-16(3)	-4(3)
Si(4)	41(1)	60(1)	62(1)	-12(1)	4(1)	-20(1)
C(41)	49(4)	85(4)	102(5)	-18(4)	-12(4)	-1(4)
C(42)	71(5)	121(6)	70(4)	-17(4)	21(3)	-39(4)
C(43)	68(5)	69(4)	120(6)	-17(4)	9(4)	-42(4)
Si(5)	48(1)	38(1)	43(1)	-10(1)	-10(1)	-7(1)
C(51)	54(4)	59(4)	71(4)	-22(3)	-13(3)	1(3)
C(52)	80(4)	32(3)	49(3)	2(3)	-17(3)	-14(3)
C(53)	60(4)	60(4)	58(4)	-13(3)	-20(3)	-13(3)
Si(6)	54(1)	49(1)	35(1)	-13(1)	5(1)	-25(1)
C(61)	72(4)	57(4)	39(3)	-12(3)	4(3)	-27(3)
C(62)	92(5)	48(3)	37(3)	-5(3)	7(3)	-30(3)
C(63)	72(4)	98(5)	57(4)	-20(3)	10(3)	-53(4)
C(71)	38(3)	33(3)	35(3)	-9(2)	-7(2)	-9(2)
C(72)	56(4)	49(3)	38(3)	-16(3)	-1(3)	-23(3)
C(73)	63(4)	68(4)	45(3)	-21(3)	15(3)	-22(3)
C(74)	118(6)	62(4)	61(4)	-35(4)	3(4)	-34(4)
C(75)	115(6)	52(4)	67(4)	-26(3)	8(4)	-46(4)
C(76)	71(4)	44(3)	47(3)	-15(3)	6(3)	-24(3)
C(81)	46(3)	40(3)	33(3)	-2(2)	-7(2)	-23(3)
C(82)	56(4)	40(3)	45(3)	-5(3)	-11(3)	-25(3)
C(83)	73(4)	44(3)	53(4)	-17(3)	-2(3)	-29(3)
C(84)	98(5)	71(4)	45(4)	-4(3)	-20(3)	-52(4)
C(85)	79(5)	67(4)	55(4)	8(3)	-29(3)	-37(4)
C(86)	55(4)	45(3)	48(3)	-1(3)	-13(3)	-19(3)
C(91)	219(29)	197(23)	209(27)	44(22)	-81(24)	-86(22)
C(92)	167(25)	232(23)	198(23)	-26(25)	-13(21)	-47(20)
C(93)	207(27)	229(24)	254(25)	23(22)	78(19)	-121(19)

C(92A)	295(39)	193(21)	287(37)	81(25)	-66(30)	-122(22)
C(91A)	352(47)	333(35)	423(44)	-20(36)	-115(40)	-154(29)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(11A)	-2376(40)	8207(9)	3561(9)	140
H(11B)	-3398(11)	8390(13)	2975(25)	140
H(11C)	-2048(30)	8632(7)	2697(17)	140
H(12A)	-1391(26)	6022(11)	1750(8)	91
H(12B)	-1655(32)	7257(18)	1528(4)	91
H(12C)	-2851(8)	6826(27)	1871(6)	91
H(13A)	-1788(29)	5129(7)	3403(12)	115
H(13B)	-3178(8)	6013(19)	3556(16)	115
H(13C)	-2012(35)	5853(23)	4039(5)	115
H(21A)	4030(7)	5730(21)	1265(13)	91
H(21B)	4951(25)	5215(11)	1925(3)	91
H(21C)	5150(20)	6196(12)	1345(15)	91
H(22A)	1461(16)	7740(11)	1573(14)	75
H(22B)	2728(11)	8026(16)	1150(6)	75
H(22C)	1947(25)	8548(7)	1879(8)	75
H(23A)	4931(22)	6767(4)	2987(15)	84
H(23B)	3681(7)	7797(21)	3075(14)	84
H(23C)	4717(26)	7754(22)	2337(4)	84
H(31A)	1972(26)	3990(19)	3917(5)	80
H(31B)	1244(12)	4862(4)	4459(15)	80
H(31C)	2540(15)	3927(18)	4684(11)	80
H(32A)	2481(8)	6475(18)	4620(14)	83
H(32B)	3957(24)	6342(20)	4247(6)	83
H(32C)	3666(30)	5480(5)	4913(8)	83
H(33A)	4717(7)	3902(20)	3091(15)	95
H(33B)	5174(15)	3842(19)	3892(4)	95
H(33C)	5366(11)	4731(5)	3219(18)	95
H(41A)	-1900(24)	4252(7)	1803(22)	125
H(41B)	-2984(8)	3679(20)	2079(14)	125
H(41C)	-2108(30)	3513(16)	1286(8)	125
H(42A)	-1040(43)	3152(16)	3393(3)	133
H(42B)	-430(27)	1899(20)	3531(4)	133
H(42C)	-1978(18)	2447(35)	3502(5)	133
H(43A)	-185(20)	630(6)	2231(22)	124
H(43B)	-1025(42)	1245(13)	1548(6)	124
H(43C)	-1754(23)	1076(17)	2378(19)	124
H(51A)	4828(6)	-124(21)	1126(14)	96
H(51B)	5769(25)	-541(13)	1781(3)	96
H(51C)	5912(21)	409(10)	1149(15)	96
H(52A)	2383(21)	808(7)	3019(13)	82
H(52B)	3611(7)	-252(16)	3027(12)	82
H(52C)	2605(25)	40(22)	2414(3)	82
H(53A)	4473(6)	1856(22)	2986(12)	88
H(53B)	5560(25)	1844(22)	2276(4)	88
H(53C)	5667(23)	801(4)	2865(15)	88
H(61A)	4846(26)	1243(9)	46(6)	82
H(61B)	4765(28)	2247(14)	-579(8)	82
H(61C)	3501(6)	1876(20)	-311(13)	82
H(62A)	2261(26)	4557(10)	582(7)	89
H(62B)	1818(17)	3936(5)	73(17)	89
H(62C)	3007(11)	4385(14)	-241(11)	89
H(63A)	[illegible]			

H(63C)	5576(22)	3453(26)	346(7)	104
H(72A)	-548(5)	6568(4)	4453(3)	54
H(73A)	-1220(6)	7706(5)	5354(3)	72
H(74A)	-675(7)	9243(5)	5113(3)	92
H(75A)	535(7)	9639(5)	3995(3)	88
H(76A)	1307(6)	8459(4)	3123(3)	64
H(82A)	2651(5)	277(4)	986(3)	53
H(83A)	2087(6)	-351(4)	31(3)	64
H(84A)	518(7)	784(5)	-734(3)	77
H(85A)	-537(6)	2506(5)	-523(3)	76
H(86A)	-39(5)	3112(4)	468(3)	59
H(91A)	5823(22)	2224(17)	4970(19)	310
H(91B)	6823(23)	1167(23)	4683(32)	310
H(91C)	6377(45)	1203(26)	5563(26)	310
H(92A)	4684(38)	1394(22)	4502(22)	247
H(92B)	4253(27)	1407(25)	5385(26)	247
H(93A)	6121(20)	-402(21)	4760(36)	285
H(93B)	5619(47)	-384(26)	5640(29)	285
H(93C)	3397(24)	10(25)	5355(26)	261
H(93D)	3962(40)	-108(26)	4493(19)	261
H(92C)	4562(51)	-1658(28)	5713(28)	311
H(92D)	5217(24)	-1786(21)	4869(38)	311
H(91D)	3458(31)	-2581(23)	5131(25)	531
H(91E)	3023(46)	-1580(30)	4503(22)	531
H(91F)	2406(29)	-1507(28)	5360(28)	531